Towards a description of twist waves in liquid crystals using mesoscopic continuum physics

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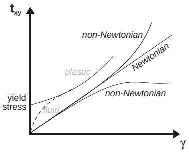
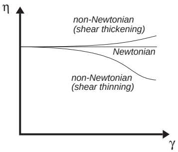
Introduction: Complex Materials

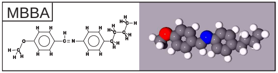
Examples:

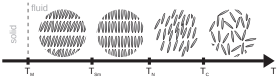
- Steel etc.
- Memory alloys
- Polymer solutions



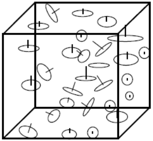


- **Liquid crystals**





- Micro-cracks in brittle materia



distribution of crack orientations $\underline{n}$ and diameters 2l: f($\underline{x}$,t,$\underline{n}$,l)

Internal Variables, Order Parameters

One approach is to define additional fields on the configuration space:

- macrocopic director (unit vector),
- scalar order parameter,
- alignment tensors,
- ...

Mesoscopic Space I

A different approach is to include additional variables in the configuration space.

$$(\boldsymbol{x}, t) \quad \rightarrow \quad (\boldsymbol{x}, \boldsymbol{m}, t)$$

These variables can be

- **orientation (of liquid crystals)** $(\boldsymbol{x}, t) \rightarrow ((\boldsymbol{x}, \boldsymbol{m}), t), \boldsymbol{m} \in S^2$
- length and orientation of end-to-end vector (of polymer chain) $(\boldsymbol{x}, t) \rightarrow ((\boldsymbol{x}, \boldsymbol{m}, l), t), \boldsymbol{m} \in S^2, l \in [0, l_{\max}]$
- diameter and orientation (of micro-crack) $(\boldsymbol{x}, t) \rightarrow ((\boldsymbol{x}, \boldsymbol{m}, d), t), \boldsymbol{m} \in S^2, d \in \mathbb{R}^+$, orientations of micro-cracks do not change

Mesoscopic Space II

phys. object	generalization	
Space	$\boldsymbol{x} \to (\boldsymbol{x}, \boldsymbol{n}) = \tilde{\mathbf{x}}$	$\boldsymbol{x} \in \mathbb{R}^3,\ \boldsymbol{n} \in S^2,\ \tilde{\mathbf{x}} \in \mathbb{R}^3 \times S^2$
velocity	$\boldsymbol{v} \to (\boldsymbol{v}, \boldsymbol{u}) = \tilde{\mathbf{v}}$	
mass density	$\varrho(\boldsymbol{x}) \to \tilde{\varrho}(\tilde{\mathbf{x}})$	
internal energy density	$\varepsilon(\boldsymbol{x}) \to \tilde{\varepsilon}(\tilde{\mathbf{x}})$	
gradient	$\nabla \to (\nabla_{\boldsymbol{x}}, \nabla_{\boldsymbol{n}}) = \nabla_{\tilde{\mathbf{x}}}$	
stress tensor	$\mathbf{t}(\boldsymbol{x}) \to \tilde{\mathbf{t}}(\tilde{\mathbf{x}})$	
force density	$\boldsymbol{f}(\boldsymbol{x}) \to (f, k)(\tilde{\mathbf{x}}) = \tilde{\mathbf{f}}(\tilde{\mathbf{x}})$	
heat flux density		
heat supply		

LC: Mesoscopic Balances I

mesoscopic mass

$$\frac{\partial}{\partial t}\tilde{\varrho}(\tilde{\mathbf{x}}, t) + \nabla_{\tilde{\mathbf{x}}} \cdot (\tilde{\mathbf{v}}(\tilde{\mathbf{x}}, t)\tilde{\varrho}(\tilde{\mathbf{x}}, t)) = 0 \quad (1)$$

mesoscopic momentum

$$\frac{\partial}{\partial t}(\tilde{\varrho}(\tilde{\mathbf{x}}, t)\tilde{\mathbf{v}}(\tilde{\mathbf{x}}, t)) + \\ + \nabla_{\tilde{\mathbf{x}}} \cdot \left(\tilde{\mathbf{v}}(\tilde{\mathbf{x}}, t)\tilde{\varrho}(\tilde{\mathbf{x}}, t)\tilde{\mathbf{v}}(\tilde{\mathbf{x}}, t)) - \tilde{\mathbf{t}}^{\top}_{\tilde{\mathbf{x}},\tilde{\mathbf{x}}}(\tilde{\mathbf{x}}, t)\right) = \tilde{\varrho}(\tilde{\mathbf{x}}, t)\tilde{\mathbf{f}}(\tilde{\mathbf{x}}, t) \quad (2)$$

Note that these are equations for 5 components (3 for the linear momentum and 2 for the angular momentum). Thus the balance of spin is naturally introduced and does not need to be postulated.

LC: Mesoscopic Balances II

mesoscopic internal energy

$$
\begin{aligned}
\frac{\partial}{\partial t}(\tilde{\varrho}(\tilde{\mathbf{x}},t)\tilde{\varepsilon}(\tilde{\mathbf{x}},t)) + \\
+\nabla_{\tilde{\mathbf{x}}}\cdot(\tilde{\mathbf{v}}(\tilde{\mathbf{x}},t)\tilde{\varrho}(\tilde{\mathbf{x}},t)\tilde{\varepsilon}(\tilde{\mathbf{x}},t)+\tilde{\mathbf{q}}(\tilde{\mathbf{x}},t)) - \\
-\tilde{\mathbf{t}}(\tilde{\mathbf{x}},t) : \nabla_{\tilde{\mathbf{x}}}\tilde{\mathbf{v}}(\tilde{\mathbf{x}},t) &= \tilde{\varrho}(\tilde{\mathbf{x}},t)\tilde{r}(\tilde{\mathbf{x}},t) - \\
&\quad \tilde{\varrho}(\tilde{\mathbf{x}},t)\tilde{\mathbf{v}}(\tilde{\mathbf{x}},t)\cdot\tilde{\mathbf{f}}(\tilde{\mathbf{x}},t)
\end{aligned}
\tag{3}
$$

with $\tilde{\mathbf{t}} : \nabla_{\tilde{\mathbf{x}}}\tilde{\mathbf{v}}$ defined as $t_{\mu\nu}\nabla^{\nu}v^{\mu}$, using Einstein's sum convention.

Orientation Waves

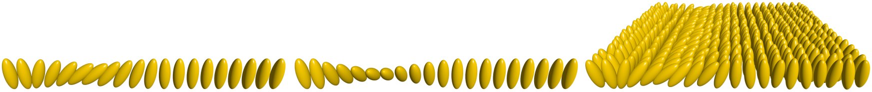
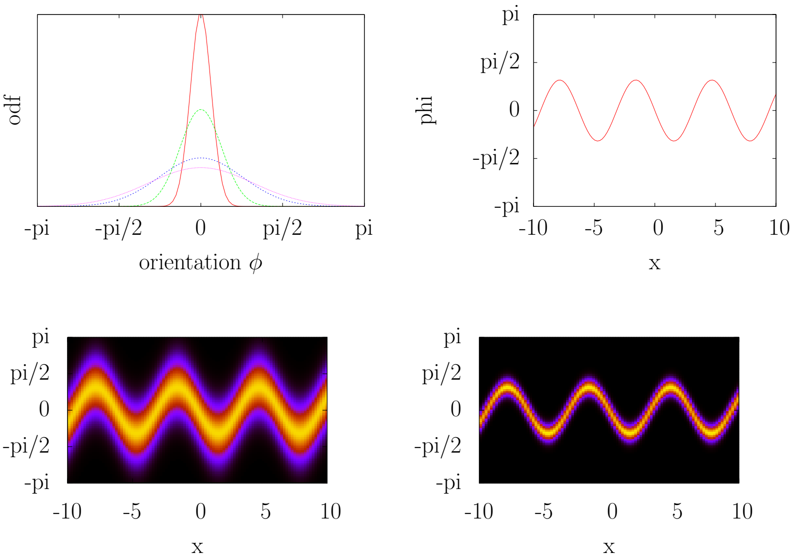


Figure: Schematic representation of orientation waves in liquid crystals. (propagation from left to right)

First descriptions by Ericksen in 1968.

Why use mesoscopic description?



Twist Waves in Mesoscopic Theory I

$$\frac{\partial}{\partial t}\tilde{\varrho}(\tilde{\mathbf{x}},t) + \nabla_x \cdot (\tilde{\mathbf{v}}_{\mathbf{x}}(\tilde{\mathbf{x}},t)\tilde{\varrho}(\tilde{\mathbf{x}},t)) + \nabla_n \cdot (\tilde{\mathbf{v}}_{\mathbf{n}}(\tilde{\mathbf{x}},t)\tilde{\varrho}(\tilde{\mathbf{x}},t)) = 0 \tag{4}$$

$$\rightarrow \quad \frac{\partial}{\partial t}\tilde{\varrho}(x_3,\varphi,t) + \frac{\partial}{\partial \varphi}(\tilde{v}_{\varphi}(x_3,\varphi,t)\tilde{\varrho}(x_3,\varphi,t)) = 0 \tag{5}$$

$$\begin{aligned} &\frac{\partial}{\partial t}(\tilde{\varrho}(\tilde{\mathbf{x}},t)\tilde{\mathbf{v}}(\tilde{\mathbf{x}},t)) + \\ &+\nabla_x \cdot \left(\tilde{\mathbf{v}}_{\mathbf{x}}(\tilde{\mathbf{x}},t)\tilde{\varrho}(\tilde{\mathbf{x}},t)\tilde{\mathbf{v}}(\tilde{\mathbf{x}},t) - \tilde{\mathbf{t}}^{\top}_{\tilde{\mathbf{x}},\mathbf{x}}(\tilde{\mathbf{x}},t)\right) + \\ &+\nabla_n \cdot \left(\tilde{\mathbf{v}}_{\mathbf{n}}(\tilde{\mathbf{x}},t)\tilde{\varrho}(\tilde{\mathbf{x}},t)\tilde{\mathbf{v}}(\tilde{\mathbf{x}},t) - \tilde{\mathbf{t}}^{\top}_{\tilde{\mathbf{x}},\mathbf{n}}(\tilde{\mathbf{x}},t)\right) = \tilde{\varrho}(\tilde{\mathbf{x}},t)\tilde{\mathbf{f}}(\tilde{\mathbf{x}},t) \end{aligned} \tag{6}$$

Twist Waves in Mesoscopic Theory II

This balance can be split into two balances:

$$
\begin{aligned}
&\frac{\partial}{\partial t}(\tilde{\varrho}(\tilde{\mathbf{x}},t)\mathbf{v}(\tilde{\mathbf{x}},t)) + \\
&+\nabla_x \cdot \left(\tilde{\mathbf{v}}_{\mathbf{x}}(\tilde{\mathbf{x}},t)\tilde{\varrho}(\tilde{\mathbf{x}},t)\tilde{\mathbf{v}}_{\mathbf{x}}(\tilde{\mathbf{x}},t) - \tilde{\mathbf{t}}^{\top}_{\mathbf{x},\mathbf{x}}(\tilde{\mathbf{x}},t)\right) + \\
&+\nabla_n \cdot \left(\tilde{\mathbf{v}}_{\mathbf{n}}(\tilde{\mathbf{x}},t)\tilde{\varrho}(\tilde{\mathbf{x}},t)\tilde{\mathbf{v}}_{\mathbf{x}}(\tilde{\mathbf{x}},t) - \tilde{\mathbf{t}}^{\top}_{\mathbf{x},\mathbf{n}}(\tilde{\mathbf{x}},t)\right) = \tilde{\varrho}(\tilde{\mathbf{x}},t)\tilde{\mathbf{f}}_{\mathbf{x}}(\tilde{\mathbf{x}},t)
\end{aligned}
\tag{7}
$$

$$
\rightarrow \quad -\frac{\partial}{\partial x_3}\tilde{\mathbf{t}}^{\top}_{x_3x_3}(x_3,\varphi,t) - \frac{\partial}{\partial \varphi}\tilde{\mathbf{t}}^{\top}_{x_3\varphi}(x_3,\varphi,t) = 0 \tag{8}
$$

$$
\begin{aligned}
&\frac{\partial}{\partial t}(\tilde{\varrho}(\tilde{\mathbf{x}},t)\tilde{\mathbf{v}}_{\mathbf{n}}(\tilde{\mathbf{x}},t)) + \\
&+\nabla_x \cdot \left(\tilde{\mathbf{v}}_{\mathbf{x}}(\tilde{\mathbf{x}},t)\tilde{\varrho}(\tilde{\mathbf{x}},t)\tilde{\mathbf{v}}_{\mathbf{n}}(\tilde{\mathbf{x}},t) - \tilde{\mathbf{t}}^{\top}_{\mathbf{n},\mathbf{x}}(\tilde{\mathbf{x}},t)\right) + \\
&+\nabla_n \cdot \left(\tilde{\mathbf{v}}_{\mathbf{n}}(\tilde{\mathbf{x}},t)\tilde{\varrho}(\tilde{\mathbf{x}},t)\tilde{\mathbf{v}}_{\mathbf{n}}(\tilde{\mathbf{x}},t) - \tilde{\mathbf{t}}^{\top}_{\mathbf{n},\mathbf{n}}(\tilde{\mathbf{x}},t)\right) = \tilde{\varrho}(\tilde{\mathbf{x}},t)\tilde{\mathbf{f}}_{\mathbf{n}}(\tilde{\mathbf{x}},t)
\end{aligned}
\tag{9}
$$

$$
\begin{aligned}
\rightarrow \quad &\frac{\partial}{\partial t}(\tilde{\varrho}(x_3,\varphi,t)\tilde{v}_{\varphi}(x_3,\varphi,t)) - \frac{\partial}{\partial x_3}\tilde{\mathbf{t}}^{\top}_{\varphi x_3}(x_3,\varphi,t) + \\
&+\frac{\partial}{\partial \varphi}\left(\tilde{v}_{\varphi}(x_3,\varphi,t)\tilde{\varrho}(x_3,\varphi,t)\tilde{v}_{\varphi}(x_3,\varphi,t) - \tilde{\mathbf{t}}^{\top}_{\varphi\varphi}(x_3,\varphi,t)\right) = 0
\end{aligned}
\tag{10}
$$

Transformation into a wave-like equation I

1. differentiation of the continuity equation with respect to time
2. taking the divergence of the balances of linear and angular momentum
3. subtraction of these equations

Transformation into a wave-like equation II

Taking the time derivative

$$\frac{\partial^2}{\partial t^2}\tilde{\varrho}(x_3,\varphi,t)+\frac{\partial}{\partial t}\frac{\partial}{\partial\varphi}\left(\tilde{v}_\varphi(x_3,\varphi,t)\tilde{\varrho}(x_3,\varphi,t)\right) \quad = \quad 0 \quad , \tag{11}$$

the divergence

$$-\frac{\partial^2}{\partial x_3^2}\tilde{\mathbf{t}}^\top_{x_3x_3}(x_3,\varphi,t)-\frac{\partial}{\partial x_3}\frac{\partial}{\partial\varphi}\tilde{\mathbf{t}}^\top_{x_3\varphi}(x_3,\varphi,t) \quad = \quad 0 \tag{12}$$

and the divergence

$$\begin{aligned}\frac{\partial}{\partial\varphi}\frac{\partial}{\partial t}\left(\tilde{\varrho}(x_3,\varphi,t)\tilde{v}_\varphi(x_3,\varphi,t)\right)-\frac{\partial}{\partial\varphi}\frac{\partial}{\partial x_3}\tilde{\mathbf{t}}^\top_{\varphi x_3}(x_3,\varphi,t)+&\\ +\frac{\partial^2}{\partial\varphi^2}\left(\tilde{v}_\varphi(x_3,\varphi,t)\tilde{\varrho}(x_3,\varphi,t)\tilde{v}_\varphi(x_3,\varphi,t)-\tilde{\mathbf{t}}^\top_{\varphi\varphi}(x_3,\varphi,t)\right) \quad &= \quad 0 \quad .\end{aligned} \tag{13}$$

Transformation into a wave-like equation III

if $\frac{\partial}{\partial x_3}\frac{\partial}{\partial \varphi}\tilde{\mathbf{t}}^{\top}_{x_3\varphi}(x_3,\varphi,t)+\frac{\partial}{\partial \varphi}\frac{\partial}{\partial x_3}\tilde{\mathbf{t}}^{\top}_{\varphi x_3}(x_3,\varphi,t) \;=\; 0$, i.e. the "mixed" part of the mesoscopic stress tensor is skew-symmetric:

$$\begin{aligned}\frac{\partial^2}{\partial t^2}\tilde{\varrho}(x_3,\varphi,t)+\frac{\partial^2}{\partial x_3^2}\tilde{\mathbf{t}}^{\top}_{x_3x_3}(x_3,\varphi,t)-\\ -\frac{\partial^2}{\partial \varphi^2}\left(\tilde{v}_{\varphi}(x_3,\varphi,t)\tilde{\varrho}(x_3,\varphi,t)\tilde{v}_{\varphi}(x_3,\varphi,t)-\tilde{\mathbf{t}}^{\top}_{\varphi\varphi}(x_3,\varphi,t)\right) &= 0 \quad . \qquad (14)\end{aligned}$$

Conclusion

- Mesoscopic continuum theory was introduced
- Orientation waves have been explained
- Wave equation in the mesoscopic theory has been presented

And . . . I think I will stop here . . .

Thank You!