Anisotropic Acoustic Waves In Rarefied Nematic Liquid Crystals

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Why Rarefied Nematic Liquid Crystal ?

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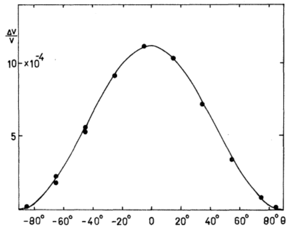


FIG. 2. Angular dependence of sound velocity. $T=21°C$, $\nu=10$ MHz, and $H=5$ kOe. θ is the angle between the field direction and propagation direction. Solid line is $12.5\times10^{-4}\cos^2\theta$.

Figure: It was observed in [MLS72] that acoustic waves travel in NLC faster in the direction parallel to the nematic director.

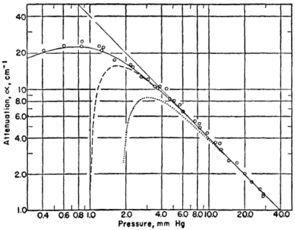


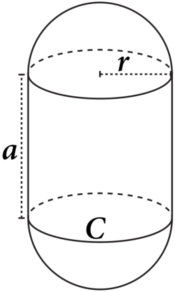
FIG. 1. Attenuation of sound at 1 Mc/sec. in helium. Circles—experimental results. Heavy full line—exact hydrodynamic. Light full line—first approximation, hydrodynamic and Burnett. Dashed line—second approximation, hydrodynamic. Dotted line—second approximation, Burnett.

Figure: It was observed in [Gre49] that first order theory better fit experimental data on acoustic attenuation at low pressure.

Curtiss Collision Operator

Curtis in his seminal paper [Cur56] proposed a kinetic theory for spherocylindrical molecules as an idealisation of polyatomic gas.

- His considered a larger configuration space made by **position**, **velocity**, **Euler's angles** for describing the orientation of each molecules and the **angular velocity** with respect to a fixed coordinate system.
- Molecules would interact by **excluded volume**, which give rise to **short range interactions** hence the **nematic ordering**.



This led Curtiss to formulate the following **Boltzmann** type equation,

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

where $f(\boldsymbol{r}, \boldsymbol{v}, \boldsymbol{\alpha}, \boldsymbol{\omega})$ is the usual first reduced distribution function and $C[f, f]$ is the collision operator defined as

$$C[f, f] = -\int\int\int\int (f_1' f' - f_1 f)(\boldsymbol{k} \cdot \boldsymbol{g}) S(\boldsymbol{k}) d\boldsymbol{k} d\boldsymbol{v}_1 d\boldsymbol{\alpha}_1 d\boldsymbol{\omega}_1$$

with $\S(\boldsymbol{k}) d\boldsymbol{k}$ being the surface element of the excluded volume and $\boldsymbol{g} = \boldsymbol{v} - \boldsymbol{v}_1$. Here with out loss of generality the equation is stated in **absence of external force** and **torque**.

Collision Invariants

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

$$\int\int\int \psi^{(i)} d\boldsymbol{v}_1 d\boldsymbol{\omega}_1 d\boldsymbol{\alpha}_1 = 0.$$

- $\psi^{(1)} = 1$, the **number of particle** in the system;
- $\psi^{(2)} = m\boldsymbol{v}$, the **linear momentum**;
- $\psi^{(3)} = \mathbb{I}^1 \cdot \omega + \boldsymbol{r} \times m\boldsymbol{v}$, the **angular momentum**;
- $\psi^{(4)} = \frac{1}{2} m\boldsymbol{v} \cdot \boldsymbol{v} + \frac{1}{2}\boldsymbol{\omega} \cdot \mathbb{I} \cdot \boldsymbol{\omega}$, the **kinetic energy of the system**.

[1] The inertia tensor for the spherocylinder we are considering.

The Hydrodynamic Equations – Notation

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

$$n(\boldsymbol{r}) = \int\int\int f(\boldsymbol{r}, \boldsymbol{v}, \alpha, \boldsymbol{\omega}) d\boldsymbol{v} d\alpha d\boldsymbol{\omega}.$$

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

$$\langle\langle\cdot\rangle\rangle(\boldsymbol{r}) = \frac{1}{n(\boldsymbol{r})}\int\int\int \cdot\, f(\boldsymbol{r}, \boldsymbol{v}, \alpha, \boldsymbol{\omega}) d\boldsymbol{v} d\alpha d\boldsymbol{\omega}.$$

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

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

The Hydrodynamic Equations – Curtis Balance Laws

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

$$\partial_t \rho + \nabla_{\boldsymbol{r}} \cdot (\rho \boldsymbol{v}_0) = 0,$$

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

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

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For the third collision invariant we took a different rout then Curtis, which led to the following balance law

$$\rho\Big[\partial_t \boldsymbol{\eta} + (\nabla_{\boldsymbol{r}}\boldsymbol{\eta})\boldsymbol{v}_0\Big] + \nabla_{\boldsymbol{r}} \cdot (\rho \mathbb{N}) = \boldsymbol{\xi}, \tag{2}$$

where $\boldsymbol{\eta}$ is the **macroscopic intrinsic angular momentum** defined as $\boldsymbol{\eta}(\boldsymbol{r}) = \langle\langle \mathbb{I} \cdot \omega \rangle\rangle$ and $\mathbb{P}$ is the **couple tensor** defined as $\mathbb{N} = \langle\langle \boldsymbol{V} \otimes (\mathbb{I}\boldsymbol{\omega} \rangle\rangle$. Here $\boldsymbol{\xi}$ is defined in tensor notation as $\langle\langle mn(\varepsilon_{lki} v_i v_k)\boldsymbol{e}_l \rangle\rangle$ and we proved that $\boldsymbol{\xi}$ vanish (as stated by Curtis in [Cur56]) in this particular setting.

Maxwell-Boltzmann Distribution

In [Cur56] Curtis gives an expression for the Maxwell-Boltzmann distribution, i.e. such distribution $f^{(0)}$ such that $C[f^{(0)}, f^{(0)}]$ vanish.

$$f^{(0)}(\boldsymbol{v},\boldsymbol{\omega}) = n\frac{\sin(\alpha_2)Q}{\int Q\sin(\alpha_2)d\boldsymbol{\alpha}}\frac{m^{\frac{3}{2}}}{2\pi\theta}^{3}(\Gamma_1\Gamma_2\Gamma_3)^{\frac{1}{2}}\exp\left[-m\frac{|\boldsymbol{V}|}{2\theta}-\frac{\boldsymbol{\Omega}\cdot\mathbb{I}\cdot\boldsymbol{\Omega}}{2\theta}\right]$$

where the **peculiar angular velocity** defined as $\boldsymbol{\Omega} = \boldsymbol{\omega} - \boldsymbol{\omega}_0$, Γ_i are the moments of inertia of the spherocylinder we are considering and Q is defined as $Q = \exp\left[\frac{\boldsymbol{\omega}_0\cdot\mathbb{I}\cdot\boldsymbol{\omega}_0}{2\theta}\right]$.

Notice in particular that we assumed $\boldsymbol{\omega}_0$ and the **kinetic temperature** $\theta = \langle\langle \frac{m}{2}\boldsymbol{V}\cdot\boldsymbol{V} + \frac{1}{2}\boldsymbol{\Omega}\cdot\mathbb{I}\cdot\boldsymbol{\Omega}\rangle\rangle$ are fixed.

Momentum Closure Around The Equilibrium

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Now we can use the previous distribution to compute an approximation of the **pressure tensor** near the equilibrium, i.e.

$$\mathbb{P}^{(0)} = \theta \boldsymbol{Id}$$

We can define the **pressure** as $p = \rho\theta^2$ and rewrite,

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

which is the well known **Euler equation** that if linearised yield the **wave equation**.
Unfortunately same procedure result in a **vanishing** $\mathbb{N}^{(0)}$.

[2]This shows that the pressure is a monotonically increasing function of the density which is needed in order to have a positive speed of sound.

Balance Laws For Kinetic Temperature

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We need an other way to formulate **constitutive relation** for the **couple tensor**, we begin observing that testing $\psi^{(4)}$ we get the following balance law:

$$\dot{\psi} + \nabla_{\boldsymbol{r}} \boldsymbol{v}_0 : \mathbb{P} + \nabla_{\boldsymbol{r}} \boldsymbol{\omega}_0 : \mathbb{N} - \nabla \cdot \left[\mathbb{P}^T \boldsymbol{v}_0 + \mathbb{N}^T \boldsymbol{\omega}_0 \right] \geq 0$$

where $\psi = \langle\langle \theta \rangle\rangle$. We add $\boldsymbol{\xi}$ and observe that if we integrate with appropriate boundary condition the expression is the **rate of work** theorem that was the starting point of Leslie-Ericksen theory

$$\dot{\psi} + \nabla_{\boldsymbol{r}} \boldsymbol{v}_0 : \mathbb{P} + \nabla_{\boldsymbol{r}} \boldsymbol{\omega}_0 : \mathbb{N} - \nabla \cdot \left[\mathbb{P}^T \boldsymbol{v}_0 + \mathbb{N}^T \boldsymbol{\omega}_0 \right] + \boldsymbol{\xi} \geq 0 \qquad (3)$$

Noll–Coleman Procedure

Since we are happy with our **pressure tensor** so far we make the following **ansatz**

$$\psi = \psi(\nu, \nabla\nu)$$

where ν is the **nematic director**. Expanding the total derivative and using Ericksen identity we get the following expression in tensor notation

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

Noll–Coleman Procedure

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Substituting this expression inside of (3) and considering thermodynamic process for which the exact divergences disappear we get:

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

Once again since the above expression must hold for all thermodynamic process for which the exact divergences disappear we get the following **constitutive relations**:

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

Anisotropic Waves

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It can be showed that steady spherical solution of (2) are of the form $\boldsymbol{\nu} = \frac{\boldsymbol{r}}{|\boldsymbol{r}|}$ and that $\nabla\boldsymbol{\nu}^T\nabla\boldsymbol{\nu} = \boldsymbol{Id} - \boldsymbol{\nu}\otimes\boldsymbol{\nu}$. Therefore for this particular case we have the following choice of **pressure tensor**:

$$\mathbb{P} = \mathbb{P}^{(0)} + \boldsymbol{Id} + \boldsymbol{\nu}\otimes\boldsymbol{\nu}.$$

If we linearise the **Euler equation** with this choice of **pressure tensor** we get the eave equation:

$$\partial_t^2 p - \nabla\cdot\Big[(\boldsymbol{Id} + \boldsymbol{\nu}\otimes\boldsymbol{\nu})\nabla p\Big] = 0.$$

Anisotropic Waves

And it is well known that when we have a planer wave

$$p(\boldsymbol{r}, t) = A\cos(\boldsymbol{k} \cdot \boldsymbol{r} - \omega t)$$

travelling in a transversely isotropic medium has speed of sound

$$\boxed{c_s = (1 + cos(\theta))^2}$$

where θ is the angle between $\boldsymbol{k}$ and $\boldsymbol{\nu}$.

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