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Anisotropic Acoustic Waves In Rarefied Ne- matic Liquid Crystals

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22nd GAMM Seminar on Microstructures, 27th of January
2023, Vienna

Oxford
Mathematics

Why Rarefied Nematic Liquid Crystal ?

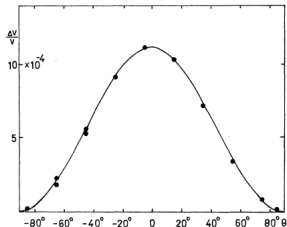


FIG. 2. Angular dependence of sound velocity. $T = 21^\circ\text{C}$, $\nu = 10$ MHz, and $H = 5$ kOe. θ is the angle between the field direction and propagation direction. Solid line is $12.5 \times 10^{-4} \cos^2 \theta$.

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

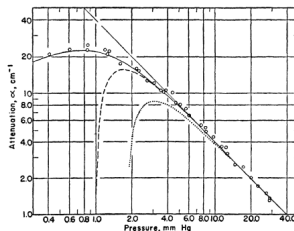
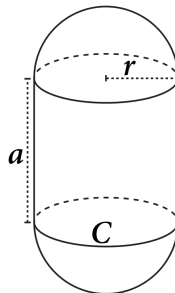


FIG. 1. Attenuation of sound at 1 Mc/sec. in helium. Circles—experimental results. Heavy full line—exact hydrodynamic. Light full line—first approximation, hydrodynamic and Burnett. Dashed line—second approximation, hydrodynamic. Dotted line—second approximation, Burnett.

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

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

- ▶ He considered a larger configuration space made by **position**, **velocity**, **Euler's angles** for describing the orientation of each molecule 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,

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

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

$$C[f, f] = - \int \int \int \int (f'_1 f' - f_1 f)(\mathbf{k} \cdot \mathbf{g}) S(\mathbf{k}) d\mathbf{k} d\mathbf{v}_1 d\alpha_1 d\omega_1$$

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

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

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

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

¹The inertia tensor for the spherocylinder we are considering.

The Hydrodynamic Equations – Notation

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

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

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

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

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

$$\mathbf{v}_0 := \langle\langle \mathbf{v} \rangle\rangle, \quad \omega_0 := \langle\langle \omega \rangle\rangle.$$

The Hydrodynamic Equations – Curtis Balance Laws

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

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

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

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

The Hydrodynamic Equations – Surprise Balance Laws

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

$$\rho \left[\partial_t \boldsymbol{\eta} + (\nabla_{\mathbf{r}} \boldsymbol{\eta}) \mathbf{v}_0 \right] + \nabla_{\mathbf{r}} \cdot (\rho \mathbb{N}) = \boldsymbol{\xi},$$

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

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

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** $\theta = \langle \langle \frac{m}{2} \mathbf{V} \cdot \mathbf{V} + \frac{1}{2} \boldsymbol{\Omega} \cdot \mathbb{I} \cdot \boldsymbol{\Omega} \rangle \rangle$ are fixed.

Momentum Closure Around The Equilibrium

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

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

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




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

which is the well known **Euler equation** that if linearised yield the **wave equation**.

Unfortunately same procedure result in a **vanishing** $\mathbb{N}^{(0)}$.

²This shows that the pressure is a monotonically increasing function of the

References

-  C. F. Curtiss, *Kinetic theory of nonspherical molecules*, The Journal of Chemical Physics **24** (1956), no. 2, 225–241.
-  Martin Greenspan, *Attenuation of sound in rarefied helium*, Phys. Rev. **75** (1949), 197–198.
-  M. E. Mullen, B. Lüthi, and M. J. Stephen, *Sound velocity in a nematic liquid crystal*, Phys. Rev. Lett. **28** (1972), 799–801.