Derivation, Analysis and Numerical Analysis of the Helmholtz–Korteweg equation

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Oxford Mathematics

University of Oxford Mathematical Institute

L. S. Hirst, G. Charras, *Liquid crystals in living tissue*, Nature, 2017.

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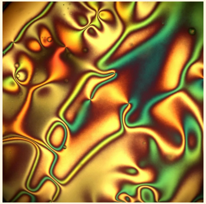
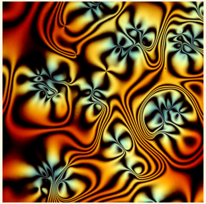
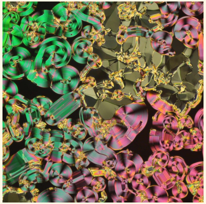

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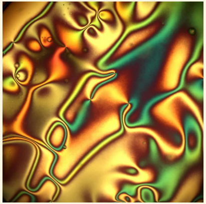
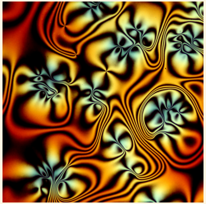
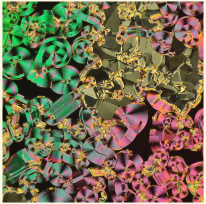
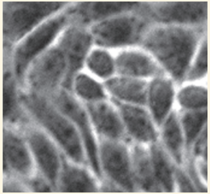
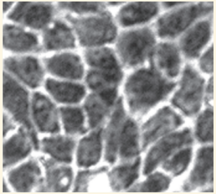

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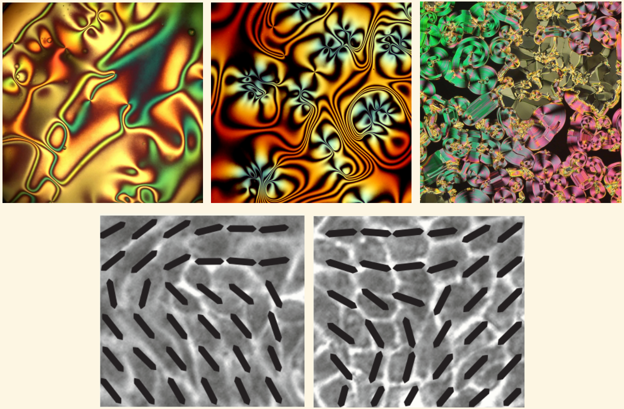

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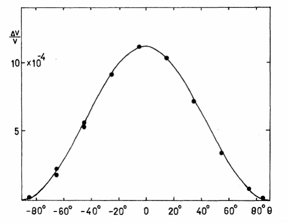

Figure: Angular dependence of sound velocity. $T = 21$ C, $v = 10$ MHz, and $H = 5$ kOe. θ is the angle between the field direction and propagation direction. Solid line is $12.5 \cdot 10^{-4}\cos(\theta)^2$.

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- Historically the interaction of acoustic waves with the nematic director field was first explained by means of the minimal entropy production principle, i.e. the acoustic anisotropy is assumed to be the result of calamitic molecules reorienting in order to minimize the propagation losses.

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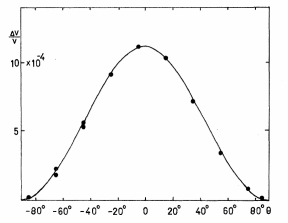

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- Historically the interaction of acoustic waves with the nematic director field was first explained by means of the minimal entropy production principle, i.e. the acoustic anisotropy is assumed to be the result of calamitic molecules reorienting in order to minimize the propagation losses.
- We here assume the aligning torque acting on the nematic director field is of elastic nature, rather than of a dissipative viscous one. This idea was already proposed, and validated experimentally, by Mullen, Lüthi, and Stephen.

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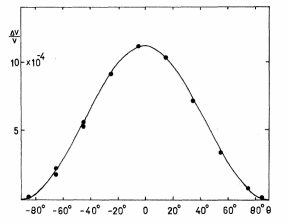

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THE HELMHOLTZ–KORTEWEG EQUATION

1

TIME-HARMONIC CONDENSATION WAVES

Let us consider the continuity equation and the balance law of linear momentum in the absence of external body forces, i.e.

$$\partial_t \rho + \nabla \cdot (\rho \boldsymbol{v}) = 0, \qquad \rho \left[\partial_t \boldsymbol{v} + (\underline{\underline{\nabla \boldsymbol{v}}})\boldsymbol{v}\right] = -(\nabla \cdot \underline{\underline{\sigma}}), \tag{1}$$

where $\boldsymbol{v}(\boldsymbol{x}, t)$ is the fluid velocity and $\underline{\underline{\sigma}}$ is the Cauchy stress tensor.

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where $\boldsymbol{v}(\boldsymbol{x}, t)$ is the fluid velocity and $\underline{\underline{\sigma}}$ is the Cauchy stress tensor.
We are interested in disturbances in the density field of the form $\rho(\boldsymbol{x}, t) = \rho_0 \left(1 + s(\boldsymbol{x}, t)\right)$, where $s(\boldsymbol{x}, t)$ is a time-harmonic condensation, i.e.

$$s(\boldsymbol{x}, t) = \Re \left[S(\boldsymbol{x}) e^{-i\omega t} \right] ,$$

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$$s(\boldsymbol{x}, t) = \Re\left[S(\boldsymbol{x}) e^{-i\omega t}\right],$$

with ω being the frequency of the disturbances. Furthermore, we will assume that the condensation is a small perturbation of the density field, i.e. $|s(\boldsymbol{x}, t)| = \mathcal{O}(\varepsilon)$, with $\varepsilon \ll 1$. Lastly, we will assume that the velocity field is a small perturbation around the stationary regime, i.e. $\|\boldsymbol{v}(\boldsymbol{x}, t)\| = \mathcal{O}(\varepsilon)$.

A GENERALIZED HELMHOLTZ EQUATION

Under these assumptions, we can rewrite (1) as

$$\rho_0 \left[\partial_t s + \nabla \cdot \boldsymbol{v} + \mathcal{O}(\varepsilon^2)\right] = 0, \qquad \partial_t \boldsymbol{v} + \mathcal{O}(\varepsilon^2) = -\rho^{-1}(\nabla \cdot \underline{\underline{\sigma}}) \,.$$

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Neglecting terms of order $\mathcal{O}(\varepsilon^2)$, since $|s(\boldsymbol{x},t)| \ll 1$ we have $\rho^{-1} \approx \rho_0^{-1}$, thus

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Substituting the time-harmonic ansatz (2) in the general wave equation (1) yields

$$\Re\left[-\rho_0\omega^2 S(\boldsymbol{x})e^{-i\omega t}\right] = -\Re\left[\nabla\cdot\left(\nabla\cdot\underline{\underline{\sigma}}\right)\right].$$

STRESS TENSOR: SPHERICAL RESPONSE

The Cauchy stress tensor $\underline{\underline{\sigma}}$ encodes the elastic response of the liquid crystal to any defromation.

Spherical response

The isotropic response of a compressible fluid is usually modeled as a spherical stress tensor, i.e. the stress tensor is given by

$$\underline{\underline{\sigma}}^{(I)} = -p\underline{\underline{\mathrm{Id}}}$$

where p is the fluid pressure, which we assume is of the form $p = \rho c_0^2$, with c_0 being the speed of sound in the isotropic phase and ρ the density of the liquid crystal.

STRESS TENSOR: TRANSVERSALLY ISOTROPIC RESPONSE

P. Biscari, A. DiCarlo, S. S. Turzi *Anisotropic wave propagation in nematic liquid crystals*, Soft Matter, 2014.

Transversally isotropic response

Originally Ericksen modeled the elastic response of the liquid crystal as a transversally isotropic material, i.e. the stress tensor is given by

$$\underline{\underline{\sigma}}^{(T)} = -p\underline{\underline{\mathsf{Id}}} + \mu\,(\boldsymbol{n}\otimes\boldsymbol{n})$$

where $\boldsymbol{n}$ is the nematic director field and μ is a fixed constant.

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- The transversally isotropic stress tensor, is incompatible with an hyperelastic formulation.

STRESS TENSOR: NEMATIC–KORTEWEG RESPONSE

E. Virga *Variational theory for nematoacoustics*, Physics Review E (2009).

Nematic–Korteweg response

Virga proposed a different model for the elastic response of the liquid crystal, which is compatible with an hyperelastic formulation. The stress tensor is given by

$$\underline{\underline{\sigma}}^{(V)} = p\underline{\underline{I}} - \alpha\rho\left(\nabla\rho \otimes \nabla\rho\right) - \beta\left(\nabla\rho \cdot \boldsymbol{n}\right)\nabla\rho \otimes \boldsymbol{n},$$

where the coefficients α and β are positive constants and the pressure is given by

$$p = \rho c_0^2 - \rho\nabla \cdot \left[\rho\left(\alpha\nabla\rho + \beta(\nabla\rho \cdot \boldsymbol{n})\boldsymbol{n}\right)\right].$$

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- It can be proven that this stress tensor is compatible with an hyperelastic formulation, i.e. it can be derived from the free energy functional

$$W(\rho,\nabla\rho,\boldsymbol{n}) = c_0^2\rho + \frac{1}{2}\alpha\|\nabla\rho\|^2 + \frac{1}{2}\beta(\nabla\rho\cdot\boldsymbol{n})^2.$$

THE NEMATIC HELMHOLTZ–KORTEWEG EQUATION

Consider the nematic Korteweg stress tensor and the time-harmonic ansatz we can rewrite the right-hand side of the generalised wave equation (1) as

$$\nabla \cdot \underline{\underline{\sigma}} \approx \Re\Big[-\rho_0 c_0^2 \nabla S(\boldsymbol{x}) + \alpha \rho_0^3 \nabla(\Delta S(\boldsymbol{x})) + \rho_0^3 u_2 \nabla\left((\nabla S \cdot \boldsymbol{n})\boldsymbol{n}\right)\Big].$$

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Dividing by $\rho_0 e^{-\omega t}$ the generalised wave equation (1) yields

$$-\omega^2 S(\boldsymbol{x}) - c_0^2 \Delta S(\boldsymbol{x}) + \rho_0^2 \alpha \Delta^2 S(\boldsymbol{x}) + \rho_0^2 u_2 \nabla \cdot \nabla \Big[\underline{\underline{\mathcal{H}S}}\boldsymbol{n} \cdot \boldsymbol{n} + \underline{\underline{\nabla \boldsymbol{n}}} \nabla S \cdot \boldsymbol{n} + (\nabla S \cdot \boldsymbol{n})(\nabla \cdot \boldsymbol{n})\Big] = 0.$$

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A reasonable assumption is that the nematic director field $\boldsymbol{n}$ is regarded as undistorted at the acoustic length scale, so that we can assume $\underline{\underline{\nabla \boldsymbol{n}}} = 0$.

Under this hypothesis we obtain the **nematic Helmholtz–Korteweg equation**, i.e.

$$-\omega^2 S(\boldsymbol{x}) - c_0^2 \Delta S(\boldsymbol{x}) + \rho_0^2 \alpha \Delta^2 S(\boldsymbol{x}) + \rho_0^2 u_2 \nabla \cdot \nabla \left[\boldsymbol{n} \cdot \underline{\underline{\mathcal{H}S}}\boldsymbol{n}\right] = 0.$$

BOUNDARY CONDITIONS

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Sound-soft boundary conditions

Sound-soft boundary conditions impose that the excess-pressure defined as

$$c_0^2\rho_0 S(\boldsymbol{x}) - \rho_0^3\alpha\Delta S(\boldsymbol{x}) - u_2\rho_0^3\left(\boldsymbol{n}\cdot\underline{\underline{\mathcal{H}S}}\boldsymbol{n}\right) = 0.$$

vanish along the boundary. Sound-soft boundary conditions thus correspond to imposing homogeneous Dirichlet boundary conditions on $S(\boldsymbol{x})$ and

$$\Delta S(\boldsymbol{x}) = -\frac{u_2}{\alpha}\left(\boldsymbol{n}\cdot\underline{\underline{\mathcal{H}S}}\boldsymbol{n}\right).$$

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Sound-hard boundary conditions

Sound-hard boundary conditions also change since the normal derivative of the fluid velocity $\partial_{\boldsymbol{\nu}} \boldsymbol{v}$ now satisfies the equation

$$i\omega\rho_0(\boldsymbol{n}\cdot\boldsymbol{\nu}) = c_0^2\partial_{\boldsymbol{\nu}}S(\boldsymbol{x}) - \rho_0^2\alpha\partial_{\boldsymbol{\nu}}\Delta S(\boldsymbol{x}) - \rho_0^2 u_2\partial_{\boldsymbol{\nu}}\left(\boldsymbol{n}\cdot\underline{\underline{\mathcal{H}S}}\boldsymbol{n}\right).$$

Sound-hard boundary conditions thus correspond to imposing homogeneous Neumann boundary conditions on $S(\boldsymbol{x})$ and

$$\partial_{\boldsymbol{\nu}}\Delta S(\boldsymbol{x}) = -\frac{u_2}{\alpha}\partial_{\boldsymbol{\nu}}\left(\boldsymbol{n}\cdot\underline{\underline{\mathcal{H}S}}\boldsymbol{n}\right).$$

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Impedance boundary conditions

Some computation shows that the impedance boundary conditions for the nematic Helmholtz–Korteweg equation are equivalent to imposing Robin boundary conditions on $S(\boldsymbol{x})$ and

$$\partial_{\boldsymbol{\nu}} \Delta S(\boldsymbol{x}) = i\zeta \Delta S(\boldsymbol{x}) + i\zeta \frac{u_2}{\alpha} \left(\boldsymbol{n} \cdot \underline{\underline{\mathcal{H}S}}\boldsymbol{n}\right) - \frac{u_2}{\alpha} \partial_{\boldsymbol{\nu}} \left(\boldsymbol{n} \cdot \underline{\underline{\mathcal{H}S}}\boldsymbol{n}\right),$$

where ζ is the impedance of the boundary.

FEATURES

2

DISPERSION RELATION

We consider plane wave solutions, given by $S(\boldsymbol{x}) = s_0 e^{ik(\boldsymbol{x}\cdot\boldsymbol{d})}$, where $s_0 = \mathcal{O}(\varepsilon)$, $\boldsymbol{d}$ is the unit vector that prescribes the direction in which the wave propagates, k is the wave-number and the wave-vector $\boldsymbol{k}$ is given by $\boldsymbol{k} := k\boldsymbol{d}$.

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Substituting the plane-wave ansatz in the nematic Helmholtz–Korteweg equation yields the following dispersion relation

$$-\omega^2 + c_0^2 k^2 + \rho_0^2 \alpha k^4 + \rho_0^2 u_2 k^4 (\boldsymbol{d}\cdot\boldsymbol{n})^2 = 0,$$

CHARACTERISTIC TIME SCALE

Collecting the fourth order terms and defining ξ as the angle between $\boldsymbol{d}$ and $\boldsymbol{n}$ we find

$$-\omega^2 + c_0^2 k^2 + \left[\rho_0^2\alpha + \rho_0^2 u_2 \cos^2(\xi)\right] k^4 = 0.$$

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If we introduce the nematic Korteweg characteristic time scale τ_2, defined as

$$\tau_2 := 4\frac{\rho_0\sqrt{\alpha + u_2\cos^2(\xi)}}{c_0^2}.$$

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We can rewrite the previous equation as $-1 + \kappa^2 + \frac{1}{4}\tau_2^2\omega^2\kappa^4 = 0$, which has roots

$$\kappa = \pm\frac{1}{\tau_2\omega}\left[-2 \pm 2\sqrt{1+\tau_2^2\omega^2}\right]^{\frac{1}{2}}.$$

ANISOTROPIC SPEED OF SOUND

By analogy to the Helmholtz equation we assume that the wave-number k can be decomposed as

$$k = k^{(R)} + ik^{(I)}, \qquad k^{(R)} = \frac{\omega}{c}, \qquad \kappa^{(I)} := \frac{c_0}{\omega} k^{(I)}.$$

where $k^{(R)}, k^{(I)} \in \mathbb{R}$ and where $c > 0$ is the effective speed of sound, i.e. the actual (and possibly anisotropic) speed of sound with which the wave propagates, as opposed to the isotropic speed of sound c_0.

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Considering first the imaginary part, we find two non-trivial solutions for $\kappa_0^{(I)}$, i.e.

$$\kappa^{(I)} = \pm\sqrt{\frac{2}{\tau_2^2\omega^2} - \left(\frac{c_0}{c}\right)^2}.$$

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$$k = k^{(R)} + ik^{(I)}, \qquad k^{(R)} = \frac{\omega}{c}, \qquad \kappa^{(I)} := \frac{c_0}{\omega} k^{(I)}.$$

where $k^{(R)}, k^{(I)} \in \mathbb{R}$ and where $c > 0$ is the effective speed of sound, i.e. the actual (and possibly anisotropic) speed of sound with which the wave propagates, as opposed to the isotropic speed of sound c_0.

Considering first the imaginary part, we find two non-trivial solutions for $\kappa_0^{(I)}$, i.e.

$$\kappa^{(I)} = \pm\sqrt{\frac{2}{\tau_2^2\omega^2} - \left(\frac{c_0}{c}\right)^2}.$$

Focusing on the vanishing imaginary part we can rewrite the dispersion relation as,

$$-1 + \left(\frac{c_0}{c}\right)^2 + \frac{1}{4}\tau_2^2\omega^2\left(\frac{c_0}{c}\right)^4 = 0.$$

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Solving for c_0/c we find only one real positive root, $\frac{c_0}{c} = \omega\tau_2\left[2\left(\sqrt{1+\omega^2\tau_2^2} - 1\right)\right]^{-\frac{1}{2}}$.

ANISOTROPIC PENETRATION DEPTH

We next consider the other case where k is purely imaginary, i.e. $k = ik^{(I)}$. We will assume

$$k^{(I)} = -\frac{\omega}{c}\sqrt{\alpha}, \qquad \alpha \geq 0. \tag{1}$$

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Substituting (2) in (1) and discarding the imaginary part of $\sqrt{\alpha}$ to get

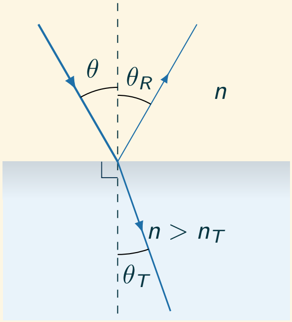
$$\delta = \frac{c_0}{2\omega}\left[\frac{-1+\sqrt{1+\tau_2^2\omega^2}}{\tau_2^2\omega^2}\right]^{-\frac{1}{2}}, \qquad \delta \approx \frac{c_0}{2\omega}\sqrt{\tau_2\omega}, \omega\tau_2 >> 1$$

TOTAL INTERNAL REFLECTION

We now turn our attention to the total internal reflection case, described by imaginary wave-numbers. The transmitted wave will have wave number $k^T = \frac{n_T}{n} k$, where n_T is the refractive index of the lower half-plane and n is the refractive index of the upper half-plane. Using Snell's law we can compute the direction $\boldsymbol{d}^T$ of the transmitted wave, i.e.

$$d_1^T = \sin(\theta)\frac{n}{n_T}, \qquad d_2^T = \sqrt{1 - \sin^2(\theta)\frac{n^2}{n_T^2}},$$

where θ is the angle of incidence of S^+. When the angle of incidence is greater than the critical angle, i.e. $\theta > \theta_c$, with $\theta_c = \sin^{-1}\left(\frac{n_T}{n}\right)$, the transmitted wave will undergo total internal reflection.



SCATTERING BY A CIRCULAR OBSTACLE: A SINGULARLY PERTURBED PROBLEM

Mathematical Institute

We next consider the scattering of a plane wave by a circular sound soft obstacle, immersed in a nematic Korteweg fluid. We assume $u_2 \ll \alpha$, $\rho_0^2\alpha \approx \ell^2$, $\rho_0^2 u_2 \approx \gamma^{-1}\ell^2$, with $\gamma \gg 1 \gg \ell$.

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Scattering problem

$$\begin{aligned}
-\omega^2 S^+(\boldsymbol{x}) - c_0^2\Delta S^+(\boldsymbol{x}) + \ell^2\Delta^2 S^+(\boldsymbol{x})& \\
+\gamma^{-1}\ell^2\nabla\cdot\nabla\left[\boldsymbol{n}\cdot\underline{\underline{\mathcal{H}S^+}}\boldsymbol{n}\right] = 0 &\quad |\boldsymbol{x}| > 1,\\
S^+(\boldsymbol{x}) = S^-(\boldsymbol{x}) &\quad |\boldsymbol{x}| = 1,\\
\Delta(S^+ - S^-) + \gamma^{-1}\boldsymbol{n}\cdot\underline{\underline{\mathcal{H}}}(S^+ - S^-)\boldsymbol{n} = 0 &\quad |\boldsymbol{x}| = 1,\\
|\partial_{|\boldsymbol{x}|}S^+(\boldsymbol{x}) - ikS^+(\boldsymbol{x})| = \mathcal{O}(|\boldsymbol{x}|^{-\frac{1}{2}}) &\quad |\boldsymbol{x}| \to \infty,
\end{aligned}$$

where S^+ is the scattered wave and S^- is the incoming plane wave.

SCATTERING BY A CIRCULAR OBSTACLE: BOUNDARY LAYERS

To study the boundary layer we introduce the change of variables $\boldsymbol{\xi} = \ell\,\boldsymbol{x}$, and rewrite the first equation of the scattering problem as

$$-\omega^2 S^+(\boldsymbol{\xi}) - \frac{c_0^2}{\ell^2}\Delta S^+(\boldsymbol{\xi}) + \frac{1}{\ell^2}\Delta^2 S^+(\boldsymbol{\xi}) + \frac{\gamma^{-1}}{\ell^2}\nabla\cdot\nabla\left[\underline{\underline{\mathcal{H}S^+}}\boldsymbol{n}\cdot\boldsymbol{n}\right] = 0.$$

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As $\ell \to 0$ we can consider only the dominant terms, to derive a partial differential equation for the boundary layer S_ℓ, i.e.

$$-c_0^2\Delta S_\ell^+(\boldsymbol{\xi}) + \Delta^2 S_\ell^+(\boldsymbol{\xi}) + \gamma^{-1}\nabla\cdot\nabla\left[\boldsymbol{n}\cdot\underline{\underline{\mathcal{H}S_\ell^+}}\boldsymbol{n}\right] = 0.$$

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Some solutions of this equation are given by solutions of

$$-c_0 S_\ell^+(\boldsymbol{\xi}) + \Delta S_\ell^+(\boldsymbol{\xi}) + \gamma^{-1}\boldsymbol{n}\cdot\underline{\underline{\mathcal{H}S_\ell^+}}\boldsymbol{n} = 0,$$

and using the assumption that $\underline{\underline{\nabla\boldsymbol{n}}} \equiv 0$ we obtain $-c_0 S_\ell^+(\boldsymbol{\xi}) + \nabla\cdot\left[(I + \gamma^{-1}\boldsymbol{n}\otimes\boldsymbol{n})\nabla S_\ell^+\right] = 0.$ From this we see that the boundary layer S_ℓ^+ is governed by a reaction-diffusion equation with a transversally isotropic diffusion tensor $(I + \gamma^{-1}\boldsymbol{n}\otimes\boldsymbol{n})$.

SCATTERING BY A CIRCULAR OBSTACLE: VISHIK–LYUSTERNIK METHOD

Using the Vishik–Lyusternik method, we assume $S^+(\boldsymbol{x}) = S_0^+(\boldsymbol{x}) + S_\ell^+(\boldsymbol{\xi})$, where $S_0^+(\boldsymbol{x})$ is the solution of the Helmholtz equation for $|\boldsymbol{x}| > 1$.
We know the value of the boundary layer S_ℓ^+ on the perimeter of the circular obstacle we can rewrite the S^+ as being an $\mathcal{O}(\ell^2)$ perturbation of the solution of the following Helmholtz scattering problem

$$\begin{aligned} -\omega^2 S^+(\boldsymbol{x}) - c_0^2 \Delta S^+(\boldsymbol{x}) &= 0, && |\boldsymbol{x}| > 1,\\ S^+(\boldsymbol{x}) &= S^-(\boldsymbol{x}) + \mathcal{O}(\ell^2), && |\boldsymbol{x}| = 1,\\ |\partial_{|\boldsymbol{x}|} S^+(\boldsymbol{x}) - ikS^+(\boldsymbol{x})| &= \mathcal{O}(|\boldsymbol{x}|^{-\frac{1}{2}}), && |\boldsymbol{x}| \to \infty. \end{aligned}$$

The solution of the previous equation can be expressed as a Mie series and using the Jacobi-Anger formula we obtain the following asymptotic expansion

$$S^+(r,\theta) = -\sqrt{\frac{2}{\pi k r}} \sum_{j\in\mathbb{Z}} a_j \frac{e^{i(kr - j\frac{\pi}{2}) - \frac{\pi}{4} + j\theta}}{H_j^{(1)}(kR)}, \qquad r \to \infty.$$

ANALYSIS

3

INDEFINITENESS OF HELMHOLTZ-LIKE PROBLEMS

Mathematical Institute

Let X be a separable Hilbert space. For given $k \gg 0$, $f \in L^2(\Omega)$, find $u \in X$ s.t.

$$a(u,v) := e(u,v) - k^2(u,v)_{L^2(\Omega)} = (f,v)_{L^2(\Omega)} \quad \forall v \in X, \tag{P}$$

where $e(\cdot,\cdot)$ is the bilinear form associated to the eigenvalue problem: find $u \in X$, $\lambda \in \mathbb{C}$ such that

$$e(u,v) = \lambda(u,v)_{L^2(\Omega)}.$$

We will assume this eigenvalue problem is well-posed and the associated solution operator is compact and self-adjoint.

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- the eigenfunctions $\{e^{(i)}\}_{i\in\mathbb{N}}$ form an orthonormal basis of X
- suppose $\exists i_*$ s.t. $\lambda^{(i_*)} < k^2 < \lambda^{(i_*+1)}$, then (P) is indefinite:

$$a(e^{(i_*)}, e^{(i_*)}) = \lambda^{(i_*)} - k^2 < 0 < \lambda^{(i_*+1)} - k^2 = a(e^{(i_*+1)}, e^{(i_*+1)})$$

WELL-POSEDNESS

F. Brezzi, *On the existence, uniqueness and approximation of saddle-point problems arising from Lagrangian multipliers.*, R.A.I.R.O., 1974.

Let X be a Hilbert space, $a : X \times X \to \mathbb{C}$ be a **bounded** sesquilinear form and $A \in L(X, X')$ be the associated operator: $\langle Au, v\rangle_{X',X} = a(u, v)\ \forall u, v \in X$. We search for $u \in X$ such that $Au = f$ in X' is **well-posed**

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Lax-Milgram

A is coercive, i.e. $\exists \alpha > 0$ s.t. $\Re\{\langle Au, u\rangle_{X',X}\} \geq \|u\|_X^2 \Rightarrow A$ is a bounded isomorphism

T-COERCIVITY

P. Ciarlet Jr., *T-coercivity: Application to the discretization of Helmholtz-like problems*. CAMWA, 2012.

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- recover coercivity with $T = \mathrm{Id}$
- not directly inherited to the discrete level

CONSTRUCTION OF T – EXAMPLE

For given $k \gg 0$, $f \in L^2(\Omega)$, find $u \in X$ s.t.

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- construct $T \in L(X)$ bijective, s.t.

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- can show coercivity of $a(T\cdot,\cdot)$ since

$$a(Te^{(i)}, e^{(i)}) = \begin{cases} k^2 - \lambda^{(i)} & \text{if } i \leq i_* \\ \lambda^{(i)} - k^2 & \text{if } i > i_* \end{cases} > 0.$$

THE DISCRETE LEVEL

Mathematical Institute

T-coercivity not inherited to the discrete level.

Uniform T_h-coercivity

Let $\{X_h\}_h \subset X$ be a seq. of discrete spaces. We call A uniformly T_h-coercive on $\{X_h\}_h$ if there exists a family of bijective operators $\{T_h\}_h$, $T_h \in L(X_h)$ and α_* independent of h s.t.

$$\Re\{(AT_h u_h, u_h)_{X_h}\} \geq \alpha_* \|u_h\|_X^2,$$

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Let $A \in L(X)$ be **injective** and $A = B + K$, where $B \in L(X)$ is **bijective** and $K \in L(X)$ **compact**. If B **is uniformly T$_h$-coercive** on $\{X_h\}_h \subset X$, then there exists $h_0 > 0$ s.t. A is uniformly T$_h$-coercive on $\{X_h\}_h$ for $h \leq h_0$.

WEAK FORMULATION

We want to find $u \in X$ such that

$$a(u, v) = (f, v)_{L^2(\Omega)} \qquad \forall v \in X,$$

where

$$a(u, v) := \underbrace{\alpha(\Delta u, \Delta v)_{L^2(\Omega)} + \beta(\boldsymbol{n}^T(\mathcal{H}u)\boldsymbol{n}, \Delta v)_{L^2(\Omega)} + (\nabla u, \nabla v)_{L^2(\Omega)}}_{=:e(u,v)} - k^2(u, v)_{L^2(\Omega)}$$

We will only consider sound-soft boundary conditions for which $X = H_0^2(\Omega) := H^2(\Omega) \cap H_0^1(\Omega)$

CONTINUOUS ANALYSIS: THE EIGENVALUE PROBLEM

Find $u \in H^2_0(\Omega)$, $\lambda \in \mathbb{C}$ s.t. $e(u,v) = \lambda(u,v)_{L^2(\Omega)}$ for all $v \in H^2_0(\Omega)$,

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CONTINUOUS ANALYSIS: THE EIGENVALUE PROBLEM

Oxford Mathematical Institute

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$$e(u, v) := \alpha(\Delta u, \Delta v)_{L^2(\Omega)} + \beta(\boldsymbol{n}^T(\mathcal{H}u)\boldsymbol{n}, \Delta v)_{L^2(\Omega)} + (\nabla u, \nabla v)_{L^2(\Omega)}.$$

If β is sufficiently small, the EVP is well-posed and the solution operator is compact and self-adjoint.

CONTINUOUS ANALYSIS: THE EIGENVALUE PROBLEM

Find $u \in H^2_0(\Omega)$, $\lambda \in \mathbb{C}$ s.t. $e(u,v) = \lambda(u,v)_{L^2(\Omega)}$ for all $v \in H^2_0(\Omega)$,

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CONTINUOUS ANALYSIS: THE EIGENVALUE PROBLEM

Find $u \in H_0^2(\Omega)$, $\lambda \in \mathbb{C}$ s.t. $e(u,v) = \lambda(u,v)_{L^2(\Omega)}$ for all $v \in H_0^2(\Omega)$,

$$e(u,v) := \alpha(\Delta u, \Delta v)_{L^2(\Omega)} + \beta(\boldsymbol{n}^T(\mathcal{H}u)\boldsymbol{n}, \Delta v)_{L^2(\Omega)} + (\nabla u, \nabla v)_{L^2(\Omega)}.$$

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If β is sufficiently small, the EVP is **well-posed** and the solution operator is **compact** and **self-adjoint**.

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- coercivity of $e(\cdot,\cdot)$ on $H^2_0(\Omega)$ can be proven using Poincaré inequality.
- compactness follows from the compact embedding $H^2_0(\Omega) \hookrightarrow L^2(\Omega)$.

CONTINUOUS ANALYSIS: T-COERCIVITY

- $\exists$ eigenpairs $(\lambda^{(i)}, e^{(i)})_{i\in\mathbb{N}}$ of $e(\cdot,\cdot)$ s.t. $(e^{(i)})_{i\in\mathbb{N}}$ forms an orthonormal basis of X

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- set $i_* := \min\{i \in \mathbb{N} : \lambda^{(i)} < k^2\}$ and define

$$W := \mathrm{span}_{0\leq i\leq i_*}\{e^{(i)}\}, \qquad T := \mathrm{Id}_X - 2P_W$$

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- We have that

$$\begin{aligned} & e(Tu, u) - k^2(Tu, u)_{L^2} \\ & \quad = \sum_{i\leq i_*} C_\lambda(k^2 - \lambda^{(i)})(u^{(i)})^2 + \sum_{i>i_*} C_\lambda(\lambda^{(i)} - k^2)(u^{(i)})^2 \geq \gamma\|u\|_X^2 \end{aligned}$$

NUMERICAL ANALYSIS

4

DISCRETIZATION

R.C. Kirby, L. Mitchell, *Code generation for generally mapped finite elements*. ACM TOMS, 2019.

Let $\{\mathcal{T}_h\}_h$ be a family of shape regular, quasi-uniform, simplicial triangulations. We choose an H^2-conforming finite element space, $p > 4$:

$$X_h := \{v \in H^2(\Omega) : v|_T \in \mathcal{P}^p(T) \quad \forall T \in \mathcal{T}_h\}$$

- imposing essential boundary conditions for $\mathcal{C}^1$-conforming FEM challenging.
- use Nitsche's method to impose BCs for *sound soft* boundary conditions.

DISCRETE PROBLEM

Find $u_h \in X_h$ s.t. $a_h(u_h, v_h) = (f, v_h)_{L^2(\Omega)}$ for all $v_h \in X_h$, where

$$a_h(u_h, v_h) := a(u_h, v_h) + \mathcal{N}_h(u_h, v_h)$$

- The discrete analysis follows similar steps as the continuous case:
  - analyse the discrete EVP (with potential Nitsche terms);
  - construct T_h and show uniform T_h-coercivity;

NITSCHE TERMS

$$
\begin{aligned}
\mathcal{N}_h(u_h, v_h) :=& \alpha(\nabla(\Delta u_h)\cdot\boldsymbol{\nu}, v_h)_{L^2(\partial\Omega)} - (\nabla u_h\cdot\boldsymbol{\nu}, v_h)_{L^2(\partial\Omega)} \\
&+\beta(\nabla(\boldsymbol{n}^T(\mathcal{H}u_h)\boldsymbol{n})\cdot\boldsymbol{\nu}, v_h)_{L^2(\partial\Omega)} \\
&+\alpha(u_h, \nabla(\Delta v_h)\cdot\boldsymbol{\nu})_{L^2(\partial\Omega)} - (u_h, \nabla v_h\cdot\boldsymbol{\nu})_{L^2(\partial\Omega)} \\
&+\beta(u_h, \nabla(\boldsymbol{n}^T(\mathcal{H}v_h)\boldsymbol{n})\cdot\boldsymbol{\nu})_{L^2(\partial\Omega)} \\
&+\alpha\frac{\eta_1}{h^3}(u_h, v_h)_{L^2(\partial\Omega)} + \frac{\eta_2}{h}(u_h, v_h)_{L^2(\partial\Omega)} \\
&+\beta\frac{\eta_3}{h^3}(u_h, v_h)_{L^2(\partial\Omega)}
\end{aligned}
$$

DISCRETE EIGENVALUE PROBLEM

Mathematical Institute

Find $u_h \in X_h$, $\lambda \in \mathbb{C}$, such that for all $v_h \in X_h$

$$e_h(u_h, v_h) := e(u_h, v_h) + \mathcal{N}_h(u_h, v_h) = \lambda(u_h, v_h)_{L^2(\Omega)}$$

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Lemma

For η_i, $i = 1, 2, 3$, large enough, the bilinear form $e_h(\cdot, \cdot)$ is uniformly coercive on $\tilde{X}_h$ with respect to $\|\cdot\|_2$.

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Lemma

For η_i, $i = 1, 2, 3$, large enough, the bilinear form $e_h(\cdot, \cdot)$ is uniformly coercive on $\tilde{X}_h$ with respect to $\|\cdot\|_2$.

$$|\mathcal{N}_h(u_h, u_h)| \gtrsim -\frac{\alpha\zeta_1}{h^3}\|\Delta u_h\|^2_{L^2(\Omega)} - \frac{\zeta_2}{h}\|\nabla u_h\|^2_{L^2(\Omega)} - \frac{\beta\zeta_3}{h^3}|u|^2_{H^2(\Omega)}$$
$$+\left(\frac{\alpha\eta_1}{h^3} - \frac{\alpha}{\zeta_1} + \frac{\eta_2}{h} - \frac{1}{\zeta_2} + \frac{\beta\eta_3}{h^3} - \frac{\beta}{\zeta_3}\right)\|u\|^2_{L^2(\partial\Omega)}$$

Pick ζ_i small enough, η_i large enough, $i = 1, 2, 3$.

DISCRETE T$_h$-COERCIVITY

- We define $T_h \in L(X_h)$ s.t $Te_h^{(i)} = \begin{cases} -e_h^{(i)} & \text{if } i \leq i_*; \\ +e_h^{(i)} & \text{if } i > i_*. \end{cases}$

DISCRETE T_h-COERCIVITY

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- As in the continuous case, we have that

$$e_h(T_h u_h, u_h) - k^2(T_h u_h, u_h) = \sum_{0 \leq i \leq i_*} C_{\lambda_h}(k^2 - \lambda_h^{(i)})(u_h^{(i)})^2 + \sum_{i > i_*} C_{\lambda_h}(\lambda_h^{(i)} - k^2)(u_h^{(i)})^2 \geq \gamma \|u_h\|_2^2,$$

provided that we pick h is **small enough** s.t. $\lambda_h^{(i_*)} < k^2$.

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- We define $T_h \in L(X_h)$ s.t $Te_h^{(i)} = \begin{cases} -e_h^{(i)} & \text{if } i \leq i_*; \\ +e_h^{(i)} & \text{if } i > i_*. \end{cases}$
- As in the continuous case, we have that

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provided that we pick h is **small enough** s.t. $\lambda_h^{(i_*)} < k^2$.

> There $\exists h_0$ s.t. $\forall h \leq h_0)$ $a_h(\cdot,\cdot)$ is uniformly T_h-coercive, thus the discrete problem has a unique solution for h small enough.

BEST APPROXIMATION

- $a_h(\cdot,\cdot)$ is **continuous** with respect to the **stronger** $\|\cdot\|_h$-norm:

$$\|u_h\|_h^2 := \|u_h\|_2^2 + \left(h^3\|\nabla(\Delta u_h)\|^2_{L^2(\partial\Omega)} + h^3\|\nabla(\boldsymbol{n}^T\mathcal{H}u_h\boldsymbol{n})\|^2_{L^2(\Omega)} + h\|\nabla u_h\|_{L^2(\partial\Omega)}\right)$$

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- a_h is **consistent**, i.e. $a_h(u-u_h, v_h) = 0$ for all $v_h \in X_h$

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- a_h is **consistent**, i.e. $a_h(u-u_h, v_h) = 0$ for all $v_h \in X_h$
- With classical arguments, we can show that

$$\|u-u_h\|_h \leq C \inf_{v_h\in X_h} \|u-v_h\|_h.$$

BEST APPROXIMATION

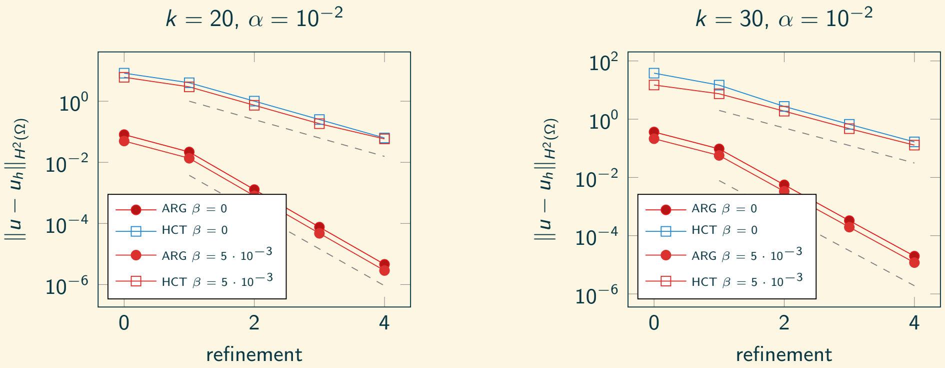
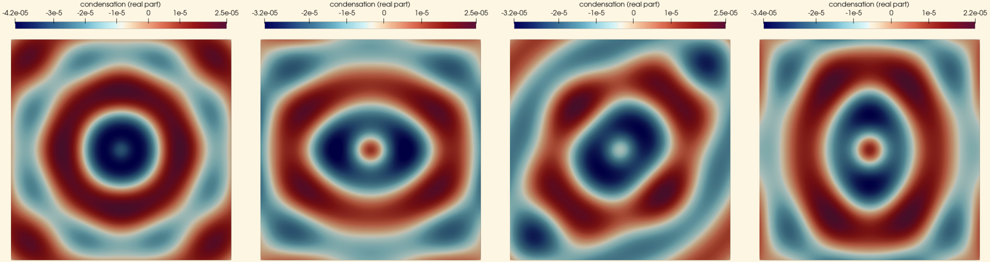


Figure: The convergence of the H^2-norm of the error for the Helmholtz–Korteweg equation for different values of k (top row) and the corresponding manufactured solution (bottom row).

Oxford Mathematical Institute

ANISOTROPIC SPEED OF SOUND

We demonstrate the anisotropic speed of sound considering as right-hand side asymmetric Gaussian pulse in $(0,0)$, *impedance* BCs, $k = 40$, $\alpha = 10^{-2}$



$\beta = 0$ | $\beta = 5 \cdot 10^{-3}$ | $\beta = 5 \cdot 10^{-3}$ | $\beta = 5 \cdot 10^{-3}$

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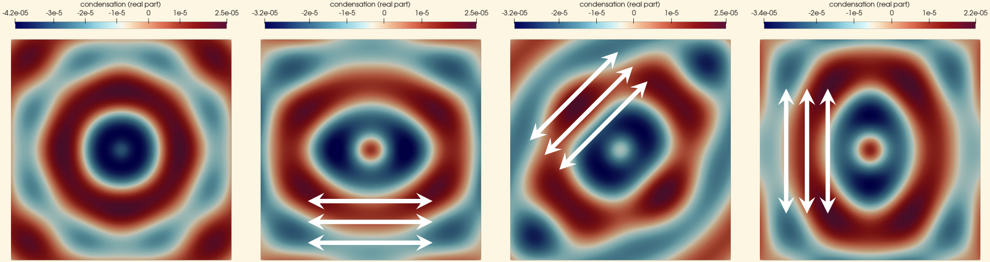

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TOTAL INTERNAL REFLECTION

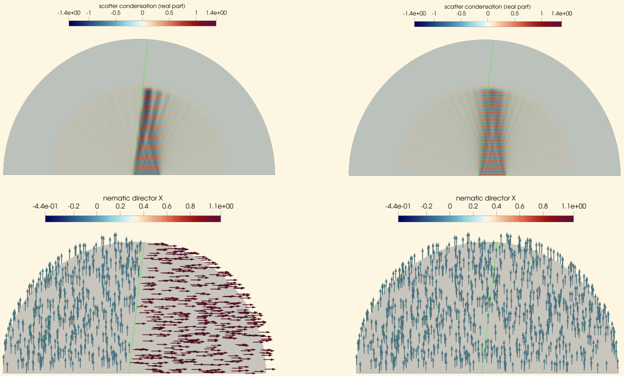

Figure: An acoustic reflection phenomenon in a nematic Korteweg fluid can be caused by a discontinuity in the nematic director field. We consider a Gaussian beam travelling upwards in a semicircular domain, with two different nematic director fields.

SCATTERING BY A CIRCULAR OBSTACLE

Mathematical Institute

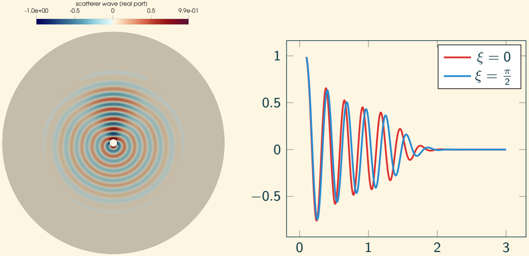

Figure: The scattered wave produced by a circular obstacle in a nematic Korteweg fluid with $\alpha = 10^{-3}$ and $u_2 = 5 \cdot 10^{-4}$, has a greater amplitude when the incoming plane wave is orthogonal to the nematic director field. Recall that ξ is the angle between $\boldsymbol{d}$ and $\boldsymbol{n}$. We simulated a plane wave propagating parallel to the y-axis and impinging on a circular obstacle, centered at the origin (left). The amplitude of the scattered wave, for different values of ξ, is measured along the y-axis (right). An adiabatic layer has been used to implement the Sommerfeld radiation condition on the outer bounday.

THANK YOU!

Derivation, Analysis and Numerical Analysis of the Helmholtz–Korteweg equation

Umberto Zerbinati*