

Forward and inverse problems in nonlinear acoustics

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Abstract. The importance of ultrasound is well established in the imaging of human tissue. In order to enhance image quality by exploiting nonlinear effects, recently techniques such as harmonic imaging and nonlinearity parameter tomography have been put forward. As soon as the pressure amplitude exceeds a certain bound, the classical linear wave equation loses its validity, and more general nonlinear versions have to be used. Another characteristic property of ultrasound propagation in human tissue is frequency power law attenuation, leading to fractional derivative damping models in the time domain. In this contribution, we will first of all dwell on modeling nonlinearity on the one hand and fractional damping on the other hand. Moreover, we will give an idea of the challenges in the analysis of the resulting PDEs and discuss some parameter asymptotics. Finally, we address a relevant inverse problem in this context, the above-mentioned task of nonlinearity parameter imaging, which leads to a coefficient identification problem for a quasilinear wave equation.

1. Introduction

The difference between linear and nonlinear acoustic wave propagation becomes apparent through the steepening of waves; see Figure 1. This is due to a pressure-dependent wave speed, which is higher in compressed areas and lower in low-density regions. This fact is visible in the wave profiles from both a space and from a time perspective and can also be read off from the PDEs; cf. (2.7) below. Another way of characterizing nonlinearity is by looking at contributions in the frequency domain in the case of a sinusoidal excitation, which in the linear case results in a response at the excitation frequency only, whereas in the nonlinear case, so-called higher harmonics are generated; see Figure 2. Also this effect is very well visible in the governing mathematical models; cf. (5.4).

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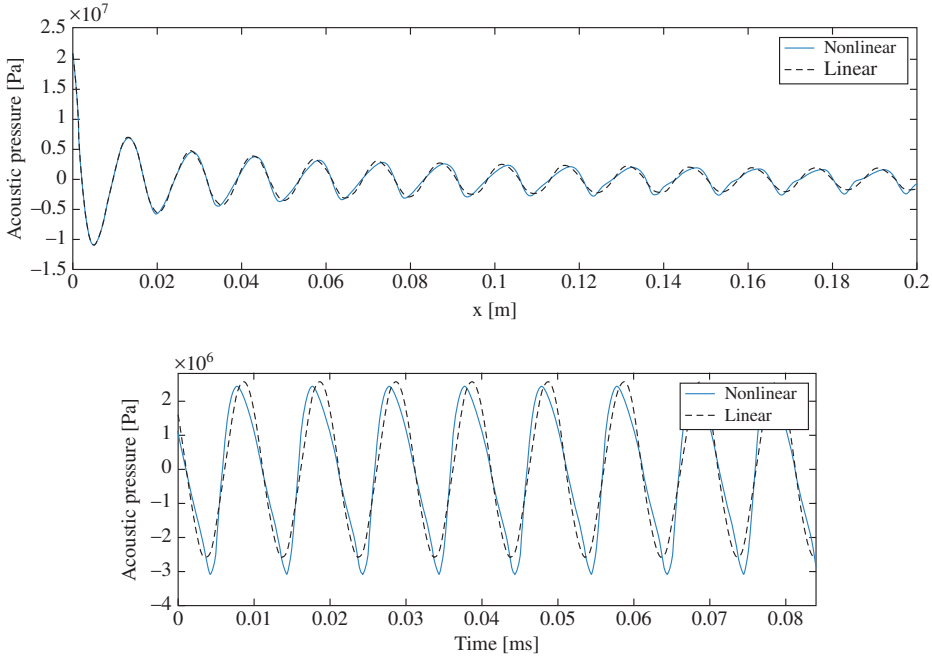


Figure 1. Linear versus nonlinear wave propagation in space (top) and time (bottom) domains.

2. Models of nonlinear acoustics

2.1. Physical principles

The main physical quantities in acoustics are

- acoustic particle velocity $\mathbf{v}$;
- absolute temperature ϑ ;
- acoustic pressure p ;
- heat flux $\mathbf{q}$;
- mass density ϱ ;
- entropy η .

These are usually decomposed into mean (zero-order) and fluctuating (first-order) parts

$$\mathbf{v} = \mathbf{v}_0 + \mathbf{v}_\sim = \mathbf{v}, \quad p = p_0 + p_\sim, \quad \varrho = \varrho_0 + \varrho_\sim, \quad \text{etc.}$$

and subject to the following physical laws:

- momentum conservation = Navier–Stokes equation (with $\nabla \times \mathbf{v} = 0$):

$$\varrho(\mathbf{v}_t + \nabla(\mathbf{v} \cdot \mathbf{v})) + \nabla p = \left(\frac{4\mu_V}{3} + \zeta_V \right) \Delta \mathbf{v};$$

- mass conservation = equation of continuity: $\varrho_t + \nabla \cdot (\varrho \mathbf{v}) = 0$;
- entropy equation: $\varrho \vartheta (\eta_t + \mathbf{v} \cdot \nabla \eta) = -\nabla \cdot \mathbf{q}$;

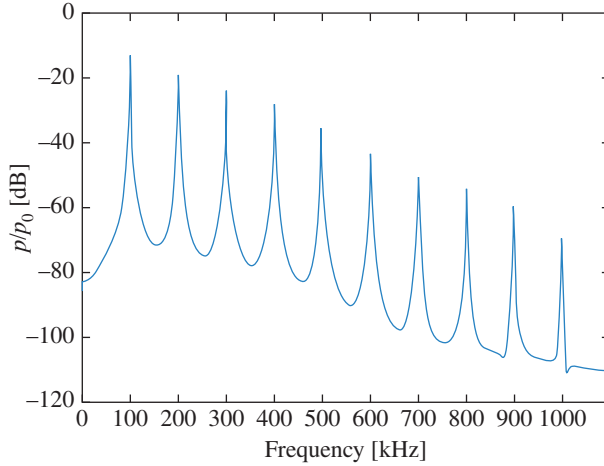


Figure 2. Higher harmonics in frequency domain.

- equation of state: $\varrho \sim = \frac{1}{c^2} p \sim - \frac{1}{\varrho_0 c^4} \frac{B}{2A} p \sim^2 - \frac{a}{\varrho_0 c^4} \left(\frac{1}{c_V} - \frac{1}{c_p} \right) p \sim_t$;
- Gibbs equation: $\vartheta d\eta = c_V d\vartheta - p \frac{1}{\varrho^2} d\varrho$,

where c_p / c_V is the specific heat at constant pressure / volume and ζ_V / μ_V the bulk / shear viscosity. The missing sixth equation in this system governing the six unknown functions $\mathbf{v}$, p , ϱ , ϑ , $\mathbf{q}$, η is the relation between temperature and heat flux, which (like the pressure-density relation) is subject to constitutive modeling. Classically, Fourier's law

$$\mathbf{q} = -K \nabla \vartheta \quad (2.1)$$

(with K denoting the thermal conductivity) has been employed for this purpose. However, this is known to lead to the infinite speed of propagation paradox. For this reason, a relaxation term has been introduced that leads to the Maxwell–Cattaneo law

$$\tau \mathbf{q}_t + \mathbf{q} = -K \nabla \vartheta, \quad (2.2)$$

which contains the relaxation time τ as an additional parameter and allows for so-called “thermal waves” (also called the second sound phenomenon).

2.2. Classical models of nonlinear acoustics

In the linear case, where quadratic and higher-order terms (e.g., products of first-order terms) are skipped, it suffices to consider momentum and mass conservation along with the equation of state, and the velocity can be eliminated by taking the divergence in momentum conservation and subtracting the time derivative of mass conservation. Upon substitution of the (linearized) pressure-density relation, this

leads to the well-known second-order wave equation $p_{tt} - c^2 \Delta p = 0$. In the nonlinear case, the same procedure, but retaining quadratic terms (that is, application of the so-called Blackstock's scheme in nonlinear acoustics), leads to the classical models of nonlinear acoustics.

- *Kuznetsov's equation* [46, 47]:

$$p_{\sim tt} - c^2 \Delta p_{\sim} - \delta \Delta p_{\sim t} = \left(\frac{B}{2A \varrho_0 c^2} p_{\sim}^2 + \varrho_0 |\mathbf{v}|^2 \right)_{tt},$$

where $\varrho_0 \mathbf{v}_t = -\nabla p$ for the particle velocity $\mathbf{v}$ and the pressure p , that is,

$$\psi_{tt} - c^2 \Delta \psi - \delta \Delta \psi_t = \left(\frac{B}{2A c^2} (\psi_t)^2 + |\nabla \psi|^2 \right)_t, \quad (2.3)$$

since $\nabla \times \mathbf{v} = 0$, hence $\mathbf{v} = -\nabla \psi$ for some velocity potential ψ .

- The *Westervelt equation* [55], which is obtained from Kuznetsov's equation via the approximation $\varrho_0 |\mathbf{v}|^2 \approx \frac{1}{\varrho_0 c^2} (p_{\sim})^2$ that corresponds to neglecting non-cumulative nonlinear effects:

$$p_{\sim tt} - c^2 \Delta p_{\sim} - \delta \Delta p_{\sim t} = \frac{1}{\varrho_0 c^2} \left(1 + \frac{B}{2A} \right) p_{\sim tt}^2. \quad (2.4)$$

Here, $\delta = h \left(\text{Pr} \left(\frac{4}{3} + \frac{\xi_V}{\mu_V} \right) + \gamma - 1 \right)$ is the diffusivity of sound (containing the thermal diffusivity h and the Prandtl number Pr) and $\frac{B}{A}$ is the nonlinearity parameter.

2.3. Advanced models of nonlinear acoustics

Taking into account further physical effects requires considering temperature, heat flux and entropy as variables as well. Modeling in nonlinear acoustics is a highly active field, and only a small portion of the resulting PDE models has been subject to rigorous mathematical investigation so far. We mention here a few examples of these.

- The *Jordan–Moore–Gibson–Thompson* (JMGT) equation [14, 28, 51]

$$\tau \psi_{ttt} + \psi_{tt} - c^2 \Delta \psi - (\delta + \tau c^2) \Delta \psi_t = \left(\frac{B}{2A c^2} (\psi_t)^2 + |\nabla \psi|^2 \right)_t, \quad (2.5)$$

where τ is the relaxation time, results from replacing Fourier's law (2.1) of heat conduction by (2.2); later on, we will also encounter fractional versions thereof. The mentioned second sound phenomenon can be seen by considering the auxiliary quantity $z := \psi_t + \frac{c^2}{\delta + \tau c^2} \psi$, which solves a weakly damped wave equation

$$z_{tt} - \tilde{c} \Delta z + \gamma z_t = r(z, \psi)$$

with $\tilde{c} = c^2 + \frac{\delta}{\tau}$, $\gamma = \frac{1}{\tau} - \frac{c^2}{\delta + \tau c^2} > 0$ and a lower-order term $r(z, \psi)$.

- The *Blackstock–Crighton* (BCBJ) equation [5, 8, 16]

$$(\partial_t - a\Delta)(\psi_{tt} - c^2\Delta\psi - \delta\Delta\psi_t) - ra\Delta\psi_t = \left(\frac{B}{2Ac^2}(\psi_t^2) + |\nabla\psi|^2 \right)_{tt}, \quad (2.6)$$

where $a = \frac{\nu}{\rho r}$ is the thermal diffusivity and r another constant.

Both models can be related to the classical Kuznetsov equation (2.3) by – first of all just formally – setting the parameters τ and a to zero. We will take a look at the mathematical justification of these parameter limits in Section 3.

The amount of literature on the analysis of these and some other advanced models of nonlinear acoustics is vast, and we do not attempt to provide an overview that could claim completeness in any sense. Some selected references are [9, 17, 18, 22, 32, 33, 44, 48, 49].

Just to get an idea of the mathematical challenges arising in the analysis (referring to the above quoted literature for details), let us take a look at the question of well-posedness of a prototypical initial-boundary value problem for the Westervelt equation as the most simple of the abovementioned models:

$$\begin{aligned} u_{tt} - c^2\Delta u - b\Delta u_t &= \frac{\kappa}{2}(u^2)_{tt} && \text{in } \Omega, \\ \frac{\partial u}{\partial n} &= g && \text{on } \partial\Omega, \\ u(t=0) &= u_0, \quad u_t(t=0) = u_1 && \text{in } \Omega, \end{aligned}$$

where we use the mathematically common notation u for the PDE solution, which plays the physical role of the acoustic pressure. Differentiating out the quadratic term and a slight rearrangement leads to

$$(1 - \kappa u)u_{tt} - c^2\Delta u - b\Delta u_t = \kappa(u_t)^2$$

which reveals the fact that the coefficient of the second time derivative depends on u itself. This leads to potential degeneracy for $u \geq \frac{1}{\kappa}$ and similarly affects the other models (Kuznetsov, Jordan–Moore–Gibson–Thompson, Blackstock–Crighton). The typical approach of proving well-posedness therefore relies on smallness of the state and proceeds as follows:

- employ energy estimates to obtain a bound on u in $C(0, T; H^2(\Omega))$;
- use smallness of u in $C(0, T; H^2(\Omega))$ and the embedding $H^2(\Omega) \rightarrow L^\infty(\Omega)$ to guarantee $1 - \kappa u \geq \underline{\alpha} > 0$;
- apply a combination of these arguments in a fixed-point scheme.

This also illustrates the state dependence of the effective wave speed, since a further rearrangement allows rewriting the equation as

$$u_{tt} - \tilde{c}^2\Delta u - \tilde{b}(u)\Delta u_t = f(u)$$

with

$$\tilde{c}(u) = \frac{c}{\sqrt{1 - \kappa u}}, \quad \tilde{b}(u) = \frac{b}{1 - \kappa u}, \quad f(u) = \frac{\kappa(u_t)^2}{1 - \kappa u}, \quad (2.7)$$

as long as $1 - \kappa u > 0$ (otherwise the equation loses its validity as a wave propagation model).

3. Parameter asymptotics

In this section, we point to a few analytical results on limits that interrelate the models in Section 2. We will be explicit about function space settings and mathematical tools only in part for the first example (the limit as $\tau \searrow$ in the JMGT equation; cf. Section 3.1). The other limits will be discussed briefly and collectively in Section 3.2; details can be found in the cited papers.

3.1. Vanishing relaxation time in the Jordan–Moore–Gibson–Thompson equation

Considering a family of solutions $(\psi^\tau)_{\tau \in (0, \bar{\tau}]}$ to

$$\tau \psi_{ttt}^\tau + \psi_{tt}^\tau - c^2 \Delta \psi^\tau - b \Delta \psi_t^\tau = \left(\frac{B}{2Ac^2} (\psi_t^\tau)^2 + |\nabla \psi^\tau|^2 \right)_t$$

with $b = \delta + \tau c^2$, the typical question to be answered is whether and in which function spaces a limit ψ^0 of ψ^τ as $\tau \searrow 0$ exists and under which conditions it can be shown to solve Kuznetsov’s equation (2.3).

Some comments are in order.

- We will consider the “Westervelt-type” and the “Kuznetsov-type” equations, without and with the gradient nonlinearity $|\nabla \psi|_t^2$.
- For $\tau = 0$ (classical Westervelt and Kuznetsov equations), the reformulation of the linearization as a first-order system leads to an analytic semigroup and maximal parabolic regularity. These properties do not hold anymore with $\tau > 0$, that is, the equation loses its “parabolic nature”. This is consistent with physics, corresponding to a transition from infinite to finite propagation speed. As $\tau \rightarrow 0$, the PDE changes from hyperbolic to parabolic.
- As in the classical models (2.3) and (2.4), potential degeneracy can be an issue, since we have

$$\begin{aligned} \tau \psi_{ttt}^\tau + \psi_{tt}^\tau - c^2 \Delta \psi^\tau - b \Delta \psi_t^\tau &= \left(\frac{\kappa}{2} (\psi_t^\tau)^2 + |\nabla \psi^\tau|^2 \right)_t \\ &= \kappa \psi_t^\tau \psi_{tt}^\tau + |\nabla \psi^\tau|_t^2 \\ \iff \tau \psi_{ttt}^\tau + (1 - \kappa \psi_t^\tau) \psi_{tt}^\tau - c^2 \Delta \psi^\tau - b \Delta \psi_t^\tau &= |\nabla \psi^\tau|_t^2. \end{aligned}$$

The plan of the analysis is to first establish well-posedness of the linearized equation along with energy estimates and use these results to prove well-posedness of the Westervelt- or Kuznetsov-type JMGT equation for $\tau > 0$ by a fixed-point argument. Relying on uniform in τ bounds obtained in the energy analysis and (weak) compactness of bounded sets in the underlying solution spaces, we then take limits as $\tau \rightarrow 0$. We refer to [6, 34, 35] for details and only sketch the above steps in a concrete function space setting for the Westervelt-type case while mentioning in passing that an extension to the Kuznetsov-type JMGT equation requires higher-order energy estimates.

We start by considering the linearized problem with variable coefficient α :

$$\begin{cases} \tau \psi_{ttt} + \alpha(x, t) \psi_{tt} - c^2 \Delta \psi - b \Delta \psi_t = f & \text{in } \Omega \times (0, T), \\ \psi = 0 & \text{on } \partial\Omega \times (0, T), \\ (\psi, \psi_t, \psi_{tt}) = (\psi_0, \psi_1, \psi_2) & \text{in } \Omega \times \{0\}. \end{cases} \quad (3.1)$$

Under the assumptions

$$\alpha(x, t) \geq \underline{\alpha} > 0 \quad \text{on } \Omega \quad \text{a.e. in } \Omega \times (0, T), \quad (3.2)$$

$$\begin{aligned} \alpha &\in L^\infty(0, T; L^\infty(\Omega)) \cap L^\infty(0, T; W^{1,3}(\Omega)), \\ f &\in H^1(0, T; L^2(\Omega)), \end{aligned} \quad (3.3)$$

$$(\psi_0, \psi_1, \psi_2) \in H_0^1(\Omega) \cap H^2(\Omega) \times H_0^1(\Omega) \cap H^2(\Omega) \times H_0^1(\Omega), \quad (3.4)$$

we obtain the following result.

Theorem 3.1. *Let c^2 , b , $\tau > 0$, and let $T > 0$. Let assumptions (3.2), (3.3), (3.4) hold. Then there exists a unique solution*

$$\begin{aligned} \psi &\in X^W := W^{1,\infty}(0, T; H_0^1(\Omega) \cap H^2(\Omega)) \\ &\quad \cap W^{2,\infty}(0, T; H_0^1(\Omega)) \cap H^3(0, T; L^2(\Omega)). \end{aligned}$$

The solution fulfills the estimate

$$\begin{aligned} \|\psi\|_{W,\tau}^2 &:= \tau^2 \|\psi_{ttt}\|_{L^2 L^2}^2 + \tau \|\psi_{tt}\|_{L^\infty H^1}^2 + \|\psi_{tt}\|_{L^2 H^1}^2 + \|\psi\|_{W^{1,\infty} H^2}^2 \\ &\leq C(\alpha, T, \tau) (\|\psi_0\|_{H^2}^2 + \|\psi_1\|_{H^2}^2 + \tau \|\psi_2\|_{H^1}^2 + \|f\|_{L^\infty L^2}^2 + \|f_t\|_{L^2 L^2}^2). \end{aligned}$$

If additionally $\|\nabla \alpha\|_{L^\infty L^3} < \frac{\alpha}{C_{H^1, L^6}^\Omega}$ holds, then $C(\alpha, T, \tau)$ is independent of τ .

Idea of proof. As a standard for proving well-posedness of evolutionary PDEs, we combine a Galerkin discretization with energy estimates and weak limits; however, due to the need for higher regularity, we derive energy estimates by nonstandard testing; in this case, we test by $-\Delta \psi_{tt}$ and with $\tau \psi_{ttt}$. ■

This allows us to prove well-posedness of the Westervelt-type JMGT equation

$$\begin{cases} \tau \psi_{ttt} + (1 - \kappa \psi_t) \psi_{tt} - c^2 \Delta \psi - b \Delta \psi_t = 0 & \text{in } \Omega \times (0, T), \\ \psi = 0 & \text{on } \partial\Omega \times (0, T), \\ (\psi, \psi_t, \psi_{tt}) = (\psi_0, \psi_1, \psi_2) & \text{in } \Omega \times \{0\}. \end{cases}$$

Theorem 3.2. *Let $c^2, b > 0, \kappa \in \mathbb{R}$ and $T > 0$. There exist $\rho, \rho_0 > 0$ such that for all $(\psi_0, \psi_1, \psi_2) \in H_0^1(\Omega) \cap H^2(\Omega) \times H_0^1(\Omega) \cap H^2(\Omega) \times H_0^1(\Omega)$ satisfying*

$$\|\psi_0\|_{H^2(\Omega)}^2 + \|\psi_1\|_{H^2(\Omega)}^2 + \tau \|\psi_2\|_{H^1(\Omega)}^2 \leq \rho_0^2,$$

there exists a unique solution $\psi \in X^W$ and $\|\psi\|_{W, \tau}^2 \leq \rho^2$.

Idea of proof. We apply Banach's contraction principle to the fixed-point operator $\mathcal{T} : \phi \mapsto \psi$ solving (3.1) with $\alpha = 1 - \kappa \phi_t$, $f = 0$. Invariance of $\mathcal{T}$ on $B_\rho^{X^W}$ can be obtained from the energy estimate in Theorem 3.1. Also contractivity $\|\mathcal{T}(\phi_1) - \mathcal{T}(\phi_2)\|_{W, \tau} \leq q \|\phi_1 - \phi_2\|_{W, \tau}$ can be established by means of the estimate in Theorem 3.1, since $\hat{\psi} = \psi_1 - \psi_2 = \mathcal{T}(\phi_1) - \mathcal{T}(\phi_2)$ solves (3.1) with $\alpha = 1 - \kappa \phi_{1t}$ and $f = \kappa \hat{\phi}_t \psi_{2tt}$, where $\hat{\phi} = \phi_1 - \phi_2$. ■

To take limits for vanishing relaxation time, we consider the τ -independent part of the norms

$$\|\psi\|_{W, \tau}^2 := \tau^2 \|\psi_{ttt}\|_{L^2 L^2}^2 + \tau \|\psi_{tt}\|_{L^\infty H^1}^2 + \|\psi_{tt}\|_{L^2 H^1}^2 + \|\psi\|_{W^{1, \infty} H^2}^2,$$

that is,

$$\|\psi\|_{\bar{X}^W}^2 := \|\psi_{tt}\|_{L^2 H^1}^2 + \|\psi\|_{W^{1, \infty} H^2}^2,$$

since these norms are uniformly bounded, independently of τ , and impose smallness of initial data in the space

$$X_0^W := H_0^1(\Omega) \cap H^2(\Omega) \times H_0^1(\Omega) \cap H^2(\Omega) \times H_0^1(\Omega).$$

This allows us to prove the following; cf [34].

Theorem 3.3. *Let $c^2, b, \kappa \in \mathbb{R}$ and $T > 0$. Then there exist $\bar{\tau}, \rho_0 > 0$ such that for all $(\psi_0, \psi_1, \psi_2) \in B_{\rho_0}^{X_0^W}$, the family $(\psi^\tau)_{\tau \in (0, \bar{\tau})}$ of solutions to the Westervelt-type JMGT equation converges weakly* in $\bar{X}^W$ to a solution $\bar{\psi} \in \bar{X}^W$ of the Westervelt equation with initial conditions $\bar{\psi}(0) = \psi_0$, $\bar{\psi}_t(0) = \psi_1$ as $\tau \searrow 0$.*

Figures 3–5 illustrate these convergence results by showing some numerical simulations comparing Westervelt-type JMGT and Westervelt solutions in the following setting:

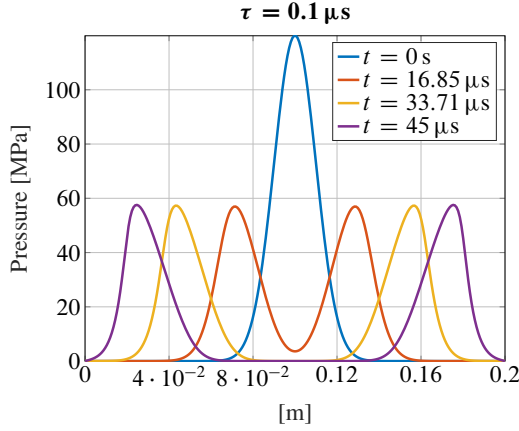


Figure 3. Snapshots of pressure $p = \varrho \psi_t$ for fixed relaxation time $\tau = 0.1 \mu\text{s}$.

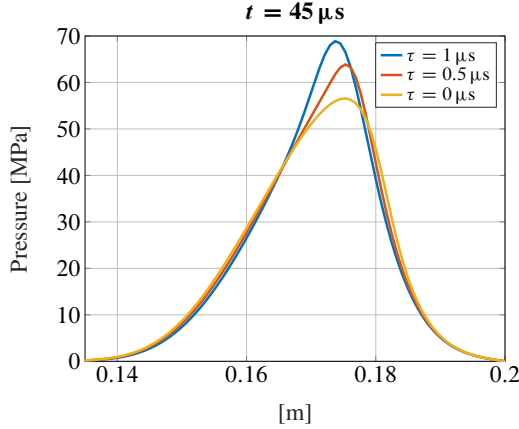


Figure 4. Pressure wave for different relaxation parameters τ at final time $t = 45 \mu\text{s}$.

- water in a 1D channel geometry

$$c = 1500 \text{ m/s}, \quad \delta = 6 \cdot 10^{-9} \text{ m}^2/\text{s}, \quad \varrho = 1000 \text{ kg/m}^3, \quad \frac{B}{A} = 5;$$

- space discretization with B-splines (isogeometric analysis): quadratic basis functions, globally C^2 ; 251 DOFs on $\Omega = [0, 0.2 \text{ m}]$;
- time discretization by Newmark scheme, adapted to third-order equation; 800 time steps on $[0, T] = [0, 45 \mu\text{s}]$;
- initial conditions $(\psi_0, \psi_1, \psi_2) = (0, \mathcal{A} \exp(-\frac{(x-0.1)^2}{2\sigma^2}), 0)$ with amplitude $\mathcal{A} = 8 \cdot 10^4 \text{ m}^2/\text{s}^2$.

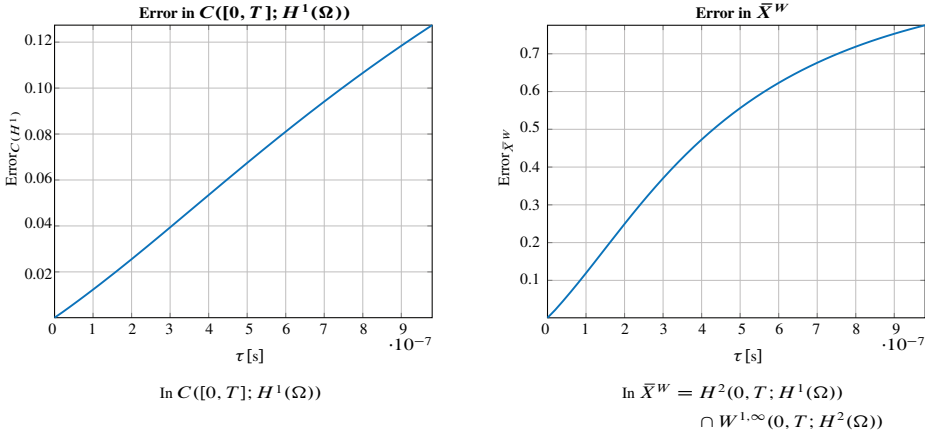


Figure 5. Relative errors as $\tau \rightarrow 0$.

3.2. Some further parameter limits

- Vanishing diffusivity of sound $\delta \searrow 0$ in Kuznetsov's equation (2.3):

$$\psi_{tt}^\delta - c^2 \Delta \psi^\delta - \delta \Delta \psi_t^\delta = \left(\frac{B}{2Ac^2} (\psi_t^\delta)^2 + |\nabla \psi^\delta|^2 \right)_t$$

with an undamped quasilinear wave equation

$$\psi_{tt} - c^2 \Delta \psi = \left(\frac{B}{2Ac^2} (\psi_t)^2 + |\nabla \psi|^2 \right)_t \quad (3.5)$$

as a limiting problem; cf. [37]. The challenge here lies in the fact that $\delta > 0$ is crucial for global-in-time well-posedness and exponential decay in $d \in \{2, 3\}$ space dimensions. As a byproduct, for $\delta = 0$ we recover results (in particular on required regularity of initial data) from [19] on the undamped Westervelt equation and obtain a new result on local-in-time well-posedness of the undamped Kuznetsov equation (3.5). A similar limiting analysis for $\delta \searrow 0$ has been carried out for the JMGT equation (2.5) in [36].

- Vanishing thermal diffusivity in the Blackstock–Crighton equation (2.6):
Here, the aim is to recover solutions to Kuznetsov's equation (2.3) as a limit for $a \searrow 0$ of solutions ψ^a to

$$(\partial_t - a\Delta)(\psi_{tt}^a - c^2 \Delta \psi^a - \delta \Delta \psi_t^a) - ra \Delta \psi_t^a = \left(\frac{B}{2Ac^2} (\psi_t^a)^2 + |\nabla \psi^a|^2 \right)_{tt};$$

cf. [44]. Note that this process also requires one integration with respect to time. To obtain sufficiently regular solutions (as needed for the underlying arguments

for nondegeneracy), consistency of the initial data is thus needed:

$$\psi_2 - c^2 \Delta \psi_0 - \delta \Delta \psi_1 = \frac{B}{Ac^2} \psi_1 \psi_2 + 2 \nabla \psi_0 \cdot \nabla \psi_1.$$

- Limit $\alpha \nearrow 1$ of the differentiation order in fractional JMGT equations:
Finally, we also consider families of time-fractional versions of the Jordan–Moore–Gibson–Thompson equation (2.5), such as

$$\tau^\alpha \partial_t^{2+\alpha} \psi^\alpha + \psi_{tt}^\alpha - c^2 \Delta \psi^\alpha - (\delta + \tau^\alpha c^2) \Delta \partial_t^\alpha \psi^\alpha = \left(\frac{B}{2Ac^2} (\psi_t^\alpha)^2 + |\nabla \psi^\alpha|^2 \right)_t$$

and convergence of their solutions to one of (2.5) (with fixed positive τ); cf. [38] and see also (4.1) below. Like in the $\tau \searrow 0$ limit, the leading order time derivative changes; however, here, this happens in a continuous manner. One of the key tasks in this work was the derivation of proper models from physical balance and constitutive laws. This brings us to the topic of the next section.

4. Fractional attenuation models in ultrasonics

As well known [13], attenuation of ultrasound depends both on the tissue type (which by the way also provides a way of imaging as mentioned in Section 6) and on the frequency. In view of the semilogarithmic scaling in the graph (the attenuation is given in decibels per centimeter), the slopes of the lines correspond to exponents of the frequency in the resulting attenuation law. Since physical balance equations by their nature only contain integer derivatives, fractional (or more generally, nonlocal) modeling happens on the level of constitutive laws. In acoustics, this can be done in terms of

- pressure-density relation and/or
- temperature-heat flux relation.

Below, we will partly describe the derivation of such models in the simpler linear setting; nonlinear versions can be obtained by inserting the constitutive equations into the balance laws and applying the procedure mentioned at the beginning of Section 2.2, leading to second (or higher) order in time wave equations.

As pressure-density relations often rely on analogies to viscoelasticity (which was one of the historical origins of fractional modeling [12]), we start with a brief recap on fractional modeling there.

4.1. Fractional models of (linear) viscoelasticity

In continuum mechanics, the deformation of a body is described by

- the equation of motion (resulting from balance of forces)

$$\varrho \mathbf{u}_{tt} = \operatorname{div} \sigma + \mathbf{f};$$

- the characterization of strain as the symmetric gradient of displacements (in a geometrically linearized setting)

$$\varepsilon = \frac{1}{2}(\nabla \mathbf{u} + (\nabla \mathbf{u})^T);$$

- a constitutive model, that is, a stress-strain relation.

Here, $\mathbf{u}$ is the vector of displacements, σ and ε are the stress and strain tensors and ϱ is the mass density.

Classical examples of constitutive models are

$$\text{Hooke's law (linear elasticity): } \sigma = b_0 \varepsilon,$$

$$\text{Newton model: } \sigma = b_1 \varepsilon_t,$$

$$\text{Kelvin–Voigt model: } \sigma = b_0 \varepsilon + b_1 \varepsilon_t,$$

$$\text{Maxwell model: } \sigma + a_1 \sigma_t = b_0 \varepsilon,$$

$$\text{Zener model: } \sigma + a_1 \sigma_t = b_0 \varepsilon + b_1 \varepsilon_t$$

with coefficients a_i, b_i . Replacing the first time derivatives in the equations by fractional ones ∂_t^β (cf. Section 4.4) with $\beta \in [0, 1)$, one arrives at (time-)fractional versions:

$$\text{fractional Newton model: } \sigma = b_1 \partial_t^\beta \varepsilon,$$

$$\text{fractional Kelvin–Voigt model: } \sigma = b_0 \varepsilon + b_1 \partial_t^\beta \varepsilon,$$

$$\text{fractional Maxwell model: } \sigma + a_1 \partial_t^\alpha \sigma = b_0 \varepsilon,$$

$$\text{fractional Zener model: } \sigma + a_1 \partial_t^\alpha \sigma = b_0 \varepsilon + b_1 \partial_t^\beta \varepsilon$$

$$\text{which are comprised in the general model class: } \sum_{n=0}^N a_n \partial_t^{\alpha_n} \sigma = \sum_{m=0}^M b_m \partial_t^{\beta_m} \varepsilon;$$

cf. [3, 12].

4.2. Fractional models of (linear) acoustics via pressure-density relation

As we have already seen in Section 2, the fundamental laws of acoustics are first of all

- balance of momentum

$$\varrho_0 \mathbf{v}_t = -\nabla p + \mathbf{f};$$

- balance of mass

$$\varrho \nabla \cdot \mathbf{v} = -\varrho_t;$$

- combined with an equation of state, the most simple linear one is

$$\frac{\varrho_{\sim}}{\varrho_0} = \frac{p_{\sim}}{p_0}$$

and, analogously to the general viscoelastic law above, can be generalized to

$$\sum_{m=0}^M b_m \partial_t^{\beta_m} \frac{\varrho_{\sim}}{\varrho_0} = \sum_{n=0}^N a_n \partial_t^{\alpha_n} \frac{p_{\sim}}{p_0}.$$

Inserting the equation of state into a combination of the balance laws that eliminates the velocity leads to fractional acoustic wave equations. Some of the most commonly used instances are as follows [25, 52]:

- Caputo–Wismer–Kelvin wave equation (fractional Kelvin–Voigt):

$$p_{tt} - b_0 \Delta p - b_1 \partial_t^{\beta} \Delta p = \tilde{f};$$

- modified Szabo wave equation (fractional Maxwell):

$$p_{tt} - a_1 \partial_t^{2+\alpha} p - b_0 \Delta p = \tilde{f};$$

- fractional Zener wave equation:

$$p_{tt} - a_1 \partial_t^{2+\alpha} p - b_0 \Delta p + b_1 \partial_t^{\beta} \Delta p = \tilde{f};$$

- general fractional model:

$$\sum_{n=0}^N a_n \partial_t^{2+\alpha_n} p - \sum_{m=0}^M b_m \partial_t^{\beta_m} \Delta p = \tilde{f}.$$

We refer to [41, Chapter 7] for their well-posedness analysis.

4.3. Fractional models of nonlinear acoustics via temperature-heat flux relation

Recall that the classical Fourier law (2.1) leads to an infinite speed of propagation paradox, which can be amended by substituting it with the Maxwell–Cattaneo law (2.2), allowing for “thermal waves” (aka the second sound phenomenon). However, this can lead to a violation of the second law of thermodynamics and moreover is unable to reproduce the fractional power law frequency dependence of attenuation as relevant in ultrasonics. Some research in physics has therefore been devoted to

an appropriate and physically consistent modeling of the temperature-heat flux relation. This can be achieved by “interpolating” between (2.1) and (2.2), using fractional derivatives [15, 24, 50]:

$$\begin{aligned}
 (\text{GFE}) \quad & (1 + \tau^\alpha \partial_t^\alpha) \mathbf{q}(t) = -K \nabla \vartheta, \\
 (\text{GFE I}) \quad & (1 + \tau^\alpha \partial_t^\alpha) \mathbf{q}(t) = -K \tau_\vartheta^{1-\alpha} \partial_t^{1-\alpha} \nabla \vartheta, \\
 (\text{GFE II}) \quad & (1 + \tau^\alpha \partial_t^\alpha) \mathbf{q}(t) = -K \tau_\vartheta^{\alpha-1} \partial_t^{\alpha-1} \nabla \vartheta, \\
 (\text{GFE III}) \quad & (1 + \tau \partial_t) \mathbf{q}(t) = -K \tau_\vartheta^{1-\alpha} \partial_t^{1-\alpha} \nabla \vartheta.
 \end{aligned}$$

Using these in place of (2.2) leads to the models

$$\begin{aligned}
 \tau^\alpha \partial_t^\alpha \psi_{tt} + (1 - \kappa \psi_t) \psi_{tt} - c^2 \Delta \psi - \tau^\alpha c^2 \partial_t^\alpha \Delta \psi - \delta \Delta \psi_t + \partial_t |\nabla \psi|^2 &= 0, \\
 \tau^\alpha \partial_t^\alpha \psi_{tt} + (1 - \kappa \psi_t) \psi_{tt} - c^2 \Delta \psi - \tau^\alpha c^2 \partial_t^\alpha \Delta \psi - \delta \partial_t^{2-\alpha} \Delta \psi + \partial_t |\nabla \psi|^2 &= 0, \\
 \tau^\alpha \partial_t^\alpha \psi_{tt} + (1 - \kappa \psi_t) \psi_{tt} - c^2 \Delta \psi - \tau^\alpha c^2 \partial_t^\alpha \Delta \psi - \delta \partial_t^\alpha \Delta \psi + \partial_t |\nabla \psi|^2 &= 0, \\
 \tau \psi_{ttt} + (1 - \kappa \psi_t) \psi_{tt} - c^2 \Delta \psi - \tau c^2 \Delta \psi_t - \delta \partial_t^{2-\alpha} \Delta \psi + \partial_t |\nabla \psi|^2 &= 0
 \end{aligned} \tag{4.1}$$

that have been analyzed in [38].

4.4. Fractional derivatives

To clarify what we mean by ∂_t^α in the models above, we provide a brief intermission on some of the most commonly used fractional derivative concepts.

With the Abel fractional integral operator

$$I_{t_0}^\gamma f(x) = \frac{1}{\Gamma(\gamma)} \int_{t_0}^t \frac{f(s)}{(t-s)^{1-\gamma}} ds,$$

a fractional (time) derivative can be defined by either

$${}^{RL}D_t^\alpha f = \frac{d}{dt} I_{t_0}^{1-\alpha} f \quad \text{Riemann–Liouville derivative}$$

or

$${}^{DC}D_t^\alpha f = I_{t_0}^{1-\alpha} \frac{df}{ds} \quad \text{Djrbashian–Caputo derivative.}$$

These are nonlocal operators and have a definite starting point t_0 . The R-L derivative is defined on a larger function space than the D-C one. However, the R-L derivative of a constant is nonzero; it even exhibits a singularity at initial time t_0 . This is why the D-C derivative, which maps constants to zero, is often preferred in physical applications. Some recent books on fractional PDEs (also containing many classical references on fractional differentiation) are [27, 41, 45].

The nonlocal and causal character of these derivatives provides the models in which they are used with a “memory”. In the context of inverse problems, it is important to note that initial values are therefore tied to later values and hence can be better reconstructed backward in time than in integer derivative models.

Some of the challenges in the analysis of fractional PDEs, in particular in deriving energy estimates, are as follows:

- The chain rule identity $u u_t = \frac{1}{2} \frac{d}{dt} u^2$ is lost.

- Likewise, there is no product rule of differentiation.

“Substitutes” for these devices in the fractional derivative case are

- the chain rule inequality

$$w(t) D_t^\alpha w(t) \geq \frac{1}{2} (D_t^\alpha w^2)(t)$$

for $w \in W^{1,1}(0, T)$ [2];

- coercivity of the Abel integral operator

$$\int_0^T \langle I^{1-\alpha} w(s), w(s) \rangle ds \geq \cos\left(\frac{\pi(1-\alpha)}{2}\right) \|w\|_{H^{-(1-\alpha)/2}(0,T)}^2$$

for $w \in H^{-(1-\alpha)/2}(0, T)$ [20, 54];

- the Kato–Ponce inequality

$$\|f g\|_{W^{\rho,r}(0,T)} \lesssim \|f\|_{W^{\rho,p_1}(0,T)} \|g\|_{L^{q_1}(0,T)} + \|f\|_{L^{p_2}(0,T)} \|g\|_{W^{\rho,q_2}(0,T)}$$

for f, g such that the right-hand side is finite, $0 \leq \rho \leq \bar{\rho} < 1$, $1 < r < \infty$, $p_1, p_2, q_1, q_2 \in (1, \infty]$, with $\frac{1}{r} = \frac{1}{p_i} + \frac{1}{q_i}$, $i = 1, 2$; see, e.g., [23].

5. Describing nonlinear wave propagation in the frequency domain by multiharmonic expansions

Motivated by the characteristic appearance of higher harmonics in nonlinear acoustics, cf. Figure 2, we now provide a mathematical formulation of this physical fact.

To this end, we recall the linear wave equation

$$u_{tt} - c^2 \Delta u = r, \tag{5.1}$$

where using a harmonic excitation $r(x, t) = \text{Re}(\hat{r}(x)e^{i\omega t})$ and a harmonic ansatz for u

$$u(x, t) = \text{Re}(\hat{u}(x)e^{i\omega t})$$

leads to the Helmholtz equation

$$-\omega^2 \hat{u} - c^2 \Delta \hat{u} = \hat{r}.$$

Replacing (5.1) by the Westervelt equation

$$u_{tt} - c^2 \Delta u - b \Delta u_t = \kappa(u^2)_{tt} + r \quad (5.2)$$

and still using a harmonic excitation $r(x, t) = \operatorname{Re}(\hat{r}(x)e^{i\omega t})$, we expect a response at multiples of the fundamental frequency ω . We therefore use a multiharmonic expansion of u

$$u(x, t) = \operatorname{Re}\left(\sum_{k=1}^{\infty} \hat{u}_k(x)e^{ik\omega t}\right), \quad (5.3)$$

which is mathematically justified by completeness of the system $(e^{ik\omega \cdot})_{k \in \mathbb{N}}$ in $L^2(0, T)$ as well as the fact that indeed a periodic solution to the Westervelt equation exists [29].

Theorem 5.1. *For $b, c^2, \beta, \gamma, T > 0$, $\kappa \in L^\infty(\Omega)$, there exists $\rho > 0$ such that for all $r \in L^2(0, T; L^2(\Omega))$ with $\|r\|_{L^2(0, T; L^2(\Omega))} \leq \rho$, there exists a unique solution*

$$u \in X := H^2(0, T; L^2(\Omega)) \cap H^1(0, T; H^{3/2}(\Omega)) \cap L^2(0, T; H^2(\Omega))$$

of

$$\begin{cases} u_{tt} - c^2 \Delta u - b \Delta u_t = \kappa(x)(u^2)_{tt} + r & \text{in } \Omega \times (0, T), \\ \beta u_t + \gamma u + \partial_\nu u = 0 & \text{on } \partial\Omega \times (0, T), \\ u(0) = u(T), \quad u_t(0) = u_t(T) & \text{in } \Omega, \end{cases}$$

and the solution fulfills the estimate

$$\|u\|_X \leq \tilde{C} \|r\|_{L^2(0, T; L^2(\Omega))}.$$

Inserting the ansatz (5.3) into (5.2) leads to the coupled system:

$$\begin{aligned} m = 1 : \quad & -\omega^2 \hat{u}_1 - (c^2 + i\omega b) \Delta \hat{u}_1 = \hat{r} - \frac{\kappa}{2} \omega^2 \sum_{k=3:2}^{\infty} \overline{\hat{u}_{\frac{k-1}{2}}} \hat{u}_{\frac{k+1}{2}}, \\ m = 2, 3, \dots : \quad & -\omega^2 m^2 \hat{u}_m - (c^2 + i\omega m b) \Delta \hat{u}_m = -\frac{\kappa}{4} \omega^2 m^2 \sum_{\ell=1}^{m-1} \hat{u}_\ell \hat{u}_{m-\ell} \\ & - \frac{\kappa}{2} \omega^2 m^2 \sum_{k=m+2:2}^{\infty} \overline{\hat{u}_{\frac{k-m}{2}}} \hat{u}_{\frac{k+m}{2}}. \end{aligned} \quad (5.4)$$

Note that the quadratic nonlinearity corresponds to a discrete autoconvolution in time. Skipping the last terms on the right-hand side corresponds to the simplification of dropping Re in (5.3) and leads to a triangular system that can be solved by forward substitution in a sequence of Helmholtz problems.

6. Inverse problems

In this section, we mainly focus on an innovative quantitative imaging methodology, based on some of the models in the previous sections, namely acoustic nonlinearity parameter tomography ANT. The key motivation for this comes from the experimentally proven qualification of the $\frac{B}{A}$ parameter in (2.3), (2.4), (2.5) or (2.6) as a characterizing and distinguishing material property of biological tissues. Thus, viewing $\kappa = \frac{1}{\rho c^2} \left(\frac{B}{2A} + 1 \right)$ as a spatially varying coefficient in the Westervelt equation, it can be used for medical imaging. While the physical and engineering literature on ANT has already been developing over many years, with initializing work going back to the 1980s and 1990s [4, 10, 11, 26, 57], mathematical results, as they are crucial for enabling any kind of advanced medical imaging technology, have only recently been started here. In particular, we point to [1, 53] for results on uniqueness from the Neumann–Dirichlet map in the Westervelt equation and to [21], which investigates and highlights the usefulness of geometric optics solutions to Westervelt equation for this imaging problem. In our own work [30, 39, 40, 42, 43], we mainly focused on uniqueness from a single boundary observation and on convergence of Newton’s method in the Westervelt equation as well as in [56] on linearized uniqueness and conditional stability of the inverse problem for the BCBJ model (2.6).

With the Westervelt equation as a forward model, the inverse problem of nonlinearity parameter imaging reads as follows.

Reconstruct $\kappa(x)$ in

$$\begin{aligned} (u - \kappa(x)u^2)_{tt} - c_0^2 \Delta u + Du &= r \quad \text{in } \Omega \times (0, T), \\ \partial_\nu u + \gamma u &= 0 \quad \text{on } \partial\Omega \times (0, T), \quad u(0) = 0, \quad u_t(0) = 0 \quad \text{in } \Omega \end{aligned}$$

(with excitation r) from observations

$$g = u \quad \text{on } \Sigma \times (0, T)$$

on a transducer array $\Sigma \subset \overline{\Omega}$, which we assume to be a surface or collection of discrete points.

The attenuation term D can be defined by one of the following common fractional models:

$$\begin{aligned} \text{Caputo–Wisner–Kelvin: } D &= -b\Delta\partial_t^\beta && \text{with } \beta \in [0, 1], b \geq 0, \\ \text{fractional Zener: } D &= a\partial_t^{2+\alpha} - b\Delta\partial_t^\beta && \text{with } a > 0, b \geq ac^2, \\ &&& 1 \geq \beta \geq \alpha > 0, \\ \text{space fractional Chen–Holm: } D &= b(-\Delta)^{\tilde{\beta}}\partial_t && \text{with } \tilde{\beta} \in [0, 1], b \geq 0. \end{aligned}$$

Since the speed of sound and the attenuation coefficient also depend on the underlying tissue type, they can be considered as additional unknowns in a multicoefficient inverse problem; see, e.g., [30, 42].

Chances and challenges of this inverse problem result from

- the difficulties in the analysis of the forward model (as well as its numerics) that have already been pointed to in Section 2;
- the fact that the unknown coefficient $\kappa(x)$ appears in the nonlinear term;
- $\kappa(x)$ being spatially varying, whereas the data $g(t)$ is in the “orthogonal” time direction; this is well known to lead to severe ill-conditioning of the inverse problem.

On the other hand, nonlinearity helps by adding information. In particular, the generation of higher harmonics and the fact that κ appears in each of the equations in (5.4) shows that information multiplies due to nonlinearity. As a consequence, it is in fact possible to achieve enhanced uniqueness results for the inverse problem formulated above, which we here illustrate by a uniqueness result for a general spatially variable coefficient from a single observation, while in the linear setting, this type of data would at most provide identifiability of piecewise constant coefficients.

6.1. Linearized and local nonlinear uniqueness

To this end, recalling (5.4), we reformulate the inverse problem in frequency domain, using the abbreviations

$$\vec{u} = (\hat{u}_j)_{j \in \mathbb{N}} \quad B_m(\vec{u}) = \frac{1}{4} \sum_{\ell=1}^{m-1} \hat{u}_\ell \hat{u}_{m-\ell} + \frac{1}{2} \sum_{k=m+2:2}^{\infty} \overline{\hat{u}_{\frac{k-m}{2}}} \hat{u}_{\frac{k+m}{2}},$$

defining the forward operator by

$$F_m(\kappa, \vec{u}) := \begin{pmatrix} -(\omega^2 m^2 + (c^2 + i\omega m b)\Delta)\hat{u}_m + \omega^2 m^2 \kappa B_m(\vec{u}) \\ \text{tr}_\Sigma \hat{u}_m \end{pmatrix}$$

and the data by

$$y_m := \begin{pmatrix} \hat{r} & \text{if } m = 1 \\ 0 & \text{if } m \geq 2 \end{pmatrix} \cdot \hat{g}_m.$$

This allows us to write the inverse problem as a nonlinear operator equation

$$\vec{F}(\kappa, \vec{u}) = y.$$

The linearized inverse problem is defined by considering the linearization of the forward operator

$$\vec{F}'(\kappa, \vec{u})(\underline{d\kappa}, \underline{d\vec{u}}) \approx F(\kappa, \vec{u}) - y,$$

where

$$\begin{aligned} F'_m(\kappa, \vec{u})(\underline{d\kappa}, \underline{d\vec{u}}) \\ = \begin{pmatrix} -(\omega^2 m^2 + (c^2 + \iota \omega m b) \Delta) \underline{d\hat{u}}_m + \omega^2 m^2 \kappa B'_m(\vec{u}) \underline{d\vec{u}} + \omega^2 m^2 \underline{d\kappa} B_m(\vec{u}) \\ \text{tr}_\Sigma \underline{d\hat{u}}_m \end{pmatrix} \end{aligned}$$

and in particular

$$F'_m(0, \vec{u})(\underline{d\kappa}, \underline{d\vec{u}}) = \begin{pmatrix} -(\omega^2 m^2 + (c^2 + \iota \omega m b) \Delta) \underline{d\hat{u}}_m + \omega^2 m^2 \underline{d\kappa} B_m(\vec{u}) \\ \text{tr}_\Sigma \underline{d\hat{u}}_m \end{pmatrix}.$$

This allows us to formulate the following linearized uniqueness result that has been obtained for the Westervelt equation in [43] and for the JMGT equation in [31].

Theorem 6.1. *The homogeneous linearized (at $\kappa = 0$, $\vec{u} = \phi(x)\vec{\psi}$ with $B_m(\vec{\psi}) \neq 0$, $m \in \mathbb{N}$) inverse problem of nonlinearity coefficient imaging in frequency domain only has the trivial solution, that is, $\vec{F}'(0, \vec{u})$ is injective.*

In the JMGT model, this even enables a (local) nonlinear uniqueness result [31].

Theorem 6.2. *For $(\kappa, \vec{u})$, $(\tilde{\kappa}, \tilde{\vec{u}})$ in a sufficiently small $H^s(\Omega) \times h^1(L^2(\Omega))$ neighborhood of $(0, \phi(x)\vec{\psi})$ with $s \in (\frac{1}{2}, 1]$, the uniqueness result*

$$\vec{F}(\kappa, \vec{u}) = \vec{F}(\tilde{\kappa}, \tilde{\vec{u}}) \quad \Rightarrow \quad \kappa = \tilde{\kappa} \text{ and } \vec{u} = \tilde{\vec{u}}$$

holds.

6.2. Some reconstruction results from two harmonics

Finally, we provide some images under the (practically often relevant) assumption of a piecewise constant nonlinearity coefficient, using only the information provided by the first two lines $m \in \{1, 2\}$ of the multiharmonic system (5.4). The reconstruction

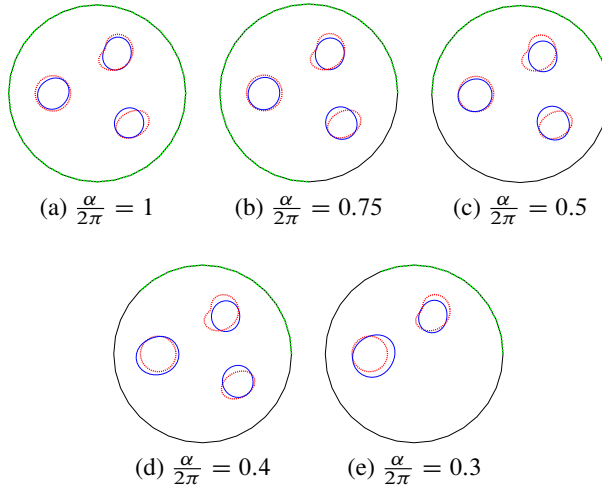


Figure 6. Reconstructions from limited data: measurements are taken on the green part of the boundary; α corresponds to the observation angle.

was carried out by parametrizing the boundary of the interface curves and applying Newton's method to the nonlinear system that arises from matching measurements to simulations. Starting curves for Newton's method were found by applying a sparsity-enhancing point source insertion algorithm [7] and extending the discovered point sources to disks whose radii are determined by a mean value property of solutions to the Helmholtz equation. While the geometry in Figures 6–8 is clearly idealized, we mimic a realistic measurement scenario by adding 1% random noise to the simulated data. For details, we refer to [43], from which the pictures shown here are also taken.

In Figure 6, we consider three objects and study the impact of limited data on the reconstruction quality, which clearly decreases under loss of information. Remarkably, all three objects are still found with less than half of the full view, and only upon reduction to less than a third of the data does one of the three objects become invisible.

Figure 7 illustrates a study of the influence of the distance between two objects on their reconstructability. Obviously, imaging both of them becomes harder as they move closer to each other. Still, up to the point where the two inclusions touch, they can be identified as two objects.

Finally, in Figure 8, we visualize how attenuation compromises the reconstruction as the object moves further away from the boundary on which observations are taken.

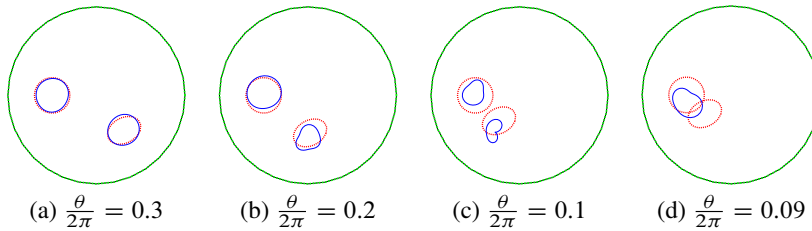


Figure 7. Reconstruction of two inclusions at different distances from each other; θ corresponds to the distance in polar coordinates.

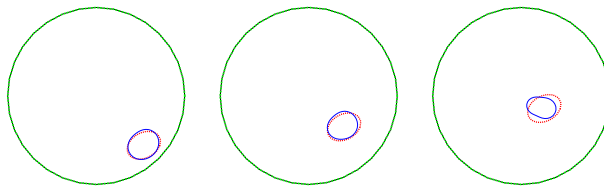


Figure 8. Reconstruction of one inclusion at different distances from the boundary.

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