# Numerical Simulation of acoustic and electromagnetic scattering problems

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## Chapter 1

# The acoustic scattering Problem in full space

#### 1.1 Introduction

We study the wave equation in full space  $\mathbb{R}^d$ ,  $d \in \{1, 2, 3\}$ .

$$\frac{\partial^2}{\partial t^2} p + \gamma \frac{\partial}{\partial t} p = c^2 \Delta p$$

Where

$$c = c(x)$$
 speed of sound  
 $\gamma = \gamma(x)$  damping coefficient

Assume time-periodic behaviour

$$p(x,t) = Re[u(x)e^{-i\omega t}]$$

with frequency  $\omega$  and a real-valued function u. Since

$$\frac{\partial^2 p(x,t)}{\partial t^2} = \text{Re}[-\omega^2 u(x)e^{-i\omega t}]$$
$$\frac{\partial p(x,t)}{\partial t} = Re[-i\omega u(x)e^{-i\omega t}]$$
$$\Delta p(x,t) = \text{Re}[\Delta u(x)]e^{-i\omega t}$$

for all times t > 0, we infer

$$-\omega^2 u - \gamma i \omega u = c^2 \Delta u, \quad \text{in } \mathbb{R}^d.$$

This is equivalent to

$$\Delta u + \frac{\omega^2}{c^2} \left( 1 + \frac{i\gamma}{\omega} \right) u = 0.$$

We assume, that  $c = c_0$  is constant in free space (reference value). We can now define a wave number

$$\kappa = \underbrace{\frac{0}{c_0}}_{>0} > 0$$

and the index of refraction

$$n(x) = \frac{c_0^2}{c(x)^2} \left( 1 + i \frac{\gamma}{\omega} \right).$$

This results in the Helmholtz-Equation

$$\Delta u + \kappa^2 n u = 0, \quad \text{in } \mathbb{R}^d.$$

We assume that there exists  $\alpha > 0$  such that

$$c(x) = c_0$$
 and  $\gamma(x) = 0$ ,  $\forall |x| > \alpha$ ,

that means inhomogeneities of the medium lie inside some bounded region (inside a ball). Furthermore we assume, that outside this ball of radius  $\alpha$ ,  $\overline{B_{\alpha}(0)}$ , there are sources that generate plane waves, that is functions of the type

$$u^{in}(x) = e^{ikx \cdot \hat{\theta}},$$

where  $|\hat{\theta}| = 1$  for  $\hat{\theta} \in \mathbb{R}^d$  and  $\cdot$  denotes the inner product in  $\mathbb{R}^d$ . Then,  $u^{in}$  satisfies

$$\Delta u^{in} + k^2 u^{in} = 0.$$

(just calculation). This  $u^{in}$  generates a scattered field  $u^s$ . The total field

$$u = u^{in} + u^s$$

satisfies

$$\Delta u + \kappa^2 n u = 0.$$

Furthermore we assume Sommerfeld's radiation condition (r = |x|):

$$\frac{\partial u^s}{\partial r} - i\kappa u^s(x) = o\left(r^{\frac{1-d}{2}}\right), \text{ as } r = |x| \to \infty$$

uniformly in  $\frac{x}{|x|}$ .

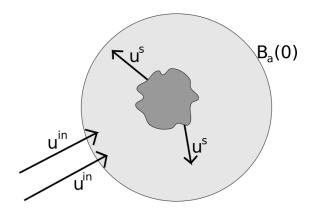


Figure 1.1: Visualization of the problem

### 1.2 Theory for the direct Scattering Problem in $\mathbb{R}^3$

Throughout this section d = 3 holds! Furthermore

1.  $\hat{\theta} \in \mathbb{R}^3$  with  $|\hat{\theta}| = 1$  defines the indicent field

$$u^{in}(x) = e^{-i\kappa\hat{\theta}\cdot x}, \quad x \in \mathbb{R}^d$$

- $2. \ \kappa \in \mathbb{R}, \kappa > 0$
- 3.  $n \in L^{\infty}(\mathbb{R}^3)$ , Re  $n \geq 0$ , Im  $n \geq 0$  and n(x) = 1 for all  $x \in \mathbb{R}^3 \setminus B_{\alpha}(0)$  and some  $\alpha > 0$

We recall

$$H^1_{loc}(\mathbb{R}^3) := \{ u : \mathbb{R}^3 \to \mathbb{C} : u|_K \in H^1(K), \text{ for every } K = B_R(0) \text{ and any } R > 0 \}$$

The Scattering Problem reads as follows

**Problem 1.1 (Scattering Problem (S)).** Given  $\hat{\theta}$ ,  $\kappa$ , n as above. Seek  $u \in H^1_{loc}(\mathbb{R}^3)$  such that

$$\Delta u + \kappa^2 n u = 0$$

in  $\mathbb{R}^3$  in the weak sense, that is

$$\int_{\mathbb{R}^3} \left( \nabla u \cdot \nabla \bar{\Psi} - \kappa n u \bar{\Psi} \right) \, dx = 0$$

for any  $\Psi \in H^1(\mathbb{R}^3)$  with compact support, and s.t.

$$u^s = u - u^{in}$$

satisfies Sommerfeld's radiation condition (d = 3, sharper version)

$$\frac{\partial u^s}{\partial r} - i\kappa u^s = O\left(\frac{1}{r^2}\right), \quad \text{uniformly in } \hat{x} = \frac{x}{|x|} \text{ as } r = |x| \to \infty$$

Remark 1.1. Regularity-theory tells us, that the radiation condition is well-defined, given the assumptions from Problem 1.1.

#### Theorem 1.2 (Rellich's Lemma)

Let u satisfy  $\Delta u + \kappa^2 u$  for every  $|x| > \alpha$ . The following property

$$\lim_{R \to \infty} \int_{|x|=R} |u(x)|^2 dS = 0$$

implies, that u(x) = 0 for all  $|x| > \alpha$ .

Remark 1.3. Vice versa, if the property in Theorem 1.2 does not hold, then u cannot vanish for all  $|x| > \alpha$ .

Proof. Employs spherical Bessel functions, see e.g.

For the proof of uniqueness, we require results on periodic differential equations. We recall *Fourier representations of periodic functions*:

Define

$$Q \coloneqq (-\pi, \pi)^3 \subseteq \mathbb{R}^3.$$

The functions

$$\{\varphi_j: j \in \mathbb{Z}^3\}$$

with

$$\varphi_j(x) = \frac{1}{(2\pi)^3} e^{ij \cdot x}, \quad \forall x \in Q, j \in \mathbb{Z}^3$$

define a complete orthonormal system (ONS) of  $L^2(Q)$  and every  $g \in L^2(Q)$  has the expansion

$$g = \sum_{j \in \mathbb{Z}^3} g_j \varphi_j$$
, with  $g_j = \int_Q g \varphi_j \, dx$ , for  $j \in \mathbb{Z}^3$ .

Panceval's inequality shows

$$||g||_{L^2(Q)} = \sum_{j \in \mathbb{Z}^3} |g_j|^2.$$

Furthermore, if  $g \in L^2(Q)$  and  $\sum_{j \in \mathbb{Z}^3} |j|^2 |g_j|^2 < \infty$ , where  $|j| = |j_1| + |j_2| + |j_3|$ , then  $g \in H^1(Q)$ .

Define

$$H_{per}^1(Q) := \left\{ g \in L^2(Q) : \sum_{j \in \mathbb{Z}^3} (1 + |j|)^2 |g_j|^2 < \infty \right\}$$

and identify  $L^2(Q)$  and  $H^1_{per}(Q)$  with the corresponding periodic functions in  $\mathbb{R}^3$  by

$$g(2\pi j + x) = g(x)$$
, for  $x \in Q, j \in \mathbb{Z}^3$ .

# **Lemma 1.4** Let $p \in \mathbb{R}^3$ , $\alpha \in \mathbb{R}$ and $\hat{e} = \begin{bmatrix} 1 \\ i \\ 0 \end{bmatrix}$ . Then, for every t > 0 and every $g \in L^2(Q)$ there

exists a unique solution  $w = w_t(g) \in H^1_{per}(Q)$  to the differential equation

$$\Delta w + \lambda_t \cdot \nabla w + \mu_t w = g \tag{*}$$

understood weakly, that is

$$\forall \Psi \in C_c^{\infty}(Q): \quad \int \left( -\nabla w \cdot \nabla \bar{\Psi} + (\lambda_t \cdot \nabla w + \mu_t w) \,\bar{\Psi} \right) \, dx = \int_Q g \bar{\Psi} \, dx$$

for  $\lambda_t := 2t\hat{e} - ip$ ,  $\mu_t = -(it + \alpha)$ . It holds that

$$||w||_{L^2(Q)} \le \frac{1}{t} ||g||_{L^2(Q)},$$

this means that

$$L_t: L^2(Q) \to L^2(Q)$$
 defined by  $g \mapsto w_t(g)$ 

defines a bounded operator

$$||L_t|| \le \frac{1}{t}, \quad \forall t > 0.$$

PROOF. With the Fourier expansions

$$g = \sum_{j \in \mathbb{Z}^3} g_j \varphi_j$$
 and  $w = \sum_{j \in \mathbb{Z}^3} w_j \varphi_j$ ,

Eq. (\*) transforms to

$$\forall j \in \mathbb{Z}^3 : \quad c_j w_j = g_j, \quad \text{with } c_j = -|j|^2 + ij \cdot \lambda_t + \mu_t.$$

We have

$$|c_j| \ge |\operatorname{Im} c_j| \stackrel{insert}{=} |2tj \cdot \hat{e} - t| = t \underbrace{|2\hat{e} \cdot j - 1|}_{>1} \ge t.$$

Thus, the operator

$$(L_t g) \coloneqq \sum_{j \in \mathbb{Z}^3} \frac{g_j}{c_j} \varphi_j, \quad \text{with } g \in L^2(Q),$$

is well-defined and satisfies

$$||L_t|| \le \frac{1}{t}, \quad \forall t > 0.$$

It remains to show, that w is really a solution to the differential equation. In order to do so, let  $\Psi \in C_c^{\infty}(Q)$ . As  $\Psi$  has compact support, function-value and all derivatives are zero on the boundary of Q, and therefore we have also that  $\Psi$  is periodic. We can represent

$$\Psi = \sum_{j \in \mathbb{Z}^3} \Psi_j \varphi_j.$$

Then

$$\int_{Q} \left( -\nabla w \cdot \nabla \bar{\Psi} + (\lambda_t \nabla w + \mu_t w) \, \bar{\Psi} \right) dx = \sum_{j \in \mathbb{Z}^3} c_j w_j \cdot \bar{\Psi}_j$$

$$= \sum_{j \in \mathbb{Z}^3} g_j \cdot \bar{\Psi}_j$$

$$= \int_{Q} g \bar{\Psi} \, dx.$$

#### Theorem 1.5 (Unique continuation principle)

Let  $u \in H^1_{loc}(\mathbb{R}^3)$  solve  $\Delta u + \kappa^2 nu = 0$ , where  $n \in L^{\infty}(\mathbb{R}^3)$  with n(x) = 1 for  $|x| > \alpha$ , and let  $b \ge \alpha$ , such that u(x) = 0 for all  $|x| \ge b$ . Then we have u = 0 in  $\mathbb{R}^3$ .

Remark 1.6. Theorem 1.5 holds in a much more general version than we stated here. PROOF. We introduce the scaling parameter  $\varrho = \frac{2b}{\pi}$  and the following function

$$w(x) := e^{\frac{i}{2}x_1 - t\hat{e} \cdot x} u(\varrho x), \quad x \in Q = (-\pi, \pi)^3$$

for some parameter t>0 and now  $\hat{e}=\begin{bmatrix}1\\i\\0\end{bmatrix}\in\mathbb{C}^3$ . Since w(x)=0 for all  $|x|\geq\frac{pi}{2}$  it can be extended to a  $2\pi$ -periodic function by

$$w(2\pi j + x) = w(x), \quad \forall j \in \mathbb{Z}^3, x \in Q,$$

with  $w \in H^1_{per}(Q)$ . It is readily seen that w satisfies

$$\Delta w + \lambda_t \cdot \nabla w + \mu_t w = -\varrho^2 \kappa^2 \tilde{n} w,$$

for

$$\lambda_t \coloneqq 2t\hat{e} - egin{bmatrix} i \ 0 \ 0 \end{bmatrix} \ \mu_t \coloneqq -\left(it + rac{1}{4}
ight)$$

and  $\tilde{n}$  is the periodic function

$$\tilde{n}(x+2\pi j) = n(\varrho x), \quad x \in \bar{Q}, j \in \mathbb{Z}^3$$

(The proof of this is by straightforward differentiation). Lemma 1.4 applies to this situation with  $g := -\varrho^2 \kappa^2 \tilde{n} w$  and yields

$$w = L_t g = -\varrho^2 \kappa^2 L_t(\tilde{n}w)$$

with  $||L_t|| \leq \frac{1}{t}$ . This means that

$$||w||_{L^{2}(Q)} \leq \frac{1}{t} \varrho^{2} \kappa^{2} ||\tilde{n}w||_{L^{2}(Q)}$$
$$\leq \frac{\varrho^{2} \kappa^{2} ||n||_{\infty}}{t} ||w||_{L^{2}(Q)}.$$

This holds for all t > 0. Taking t >> 1 results in  $||w||_{L^2(Q)} = 0$  where w = 0. Thus  $u \equiv 0$ .

#### Theorem 1.7 (Uniqueness)

Problem 1.1 admits at most one solution. That is,  $u^{in} \equiv 0$  implies  $u \equiv 0$ .

PROOF. Let  $u^{in} = 0$ . Recall the formula

$$|a - i\beta|^2 = |a|^2 + |\beta|^2 + 2\operatorname{Im}(\beta \bar{a})$$

(elementary proof). We have

$$O\left(\frac{1}{R^2}\right) = \int_{|x|=R} \left| \frac{\partial u}{\partial r} - i\kappa u \right|^2 dS$$
$$= \int_{|x|=R} \left( \left| \frac{\partial u}{\partial r} \right|^2 + \kappa^2 |u|^2 \right) dS + 2\kappa \operatorname{Im} \int_{|x|=R} u \frac{\partial \bar{u}}{\partial r} dS$$

The divergence-theorem implies

$$2\kappa \operatorname{Im} \int_{|x|=R} u \underbrace{\frac{\partial \bar{u}}{\partial r}}_{\operatorname{normal}} dS = 2\kappa \operatorname{Im} \left[ \int_{|x|< R} \left( u \Delta \bar{u} + \underbrace{|\nabla u|^2}_{\in \mathbb{R}_0^+} \right) dx \right]$$

$$\stackrel{\operatorname{Helmholtz-eq}}{=} 2\kappa \operatorname{Im} \left[ \int_{|x|< R} \left( -\kappa^2 \bar{n} |u|^2 \right) dx \right]$$

$$> 0.$$

Since Im  $n \geq 0$ . Thus we have for large  $R \to \infty$ :

$$0 \le \limsup_{R \to \infty} \int_{|x|=R} \left( \left| \frac{\partial u}{\partial r} \right|^2 + \kappa |u|^2 \right) \, dS \le 0,$$

whence

$$\lim_{R \to \infty} \int_{|x|=R} |u|^2 dS = 0.$$

Theorem 1.2 (Rellich) implies that u(x) = 0 for all |x| > a. By the unique continuation principle we have  $u \equiv 0$  in  $\mathbb{R}^3$ .

We have shown uniqueness. For the existence proof we will construct solutions.

#### **Definition 1.8.** The function

$$\Phi(x,y) := \frac{1}{4\pi|x-y|} e^{i\kappa|x-y|}, \quad x,y \in \mathbb{R}^3, x \neq y$$

is called fundamental solution or free space Green's function.

#### $\Phi$ has the following properties

#### Proposition 1.9 (Properties of the fundamental solution)

- 1.  $\Phi(\cdot,y)$  satisfies the Helmholtz-equation  $\Delta u + \kappa^2 u = 0$  in  $\mathbb{R}^3 \setminus \{y\}$
- 2.  $\Phi$  satisfies the emphradiation condition

$$\frac{x}{|x|} \cdot \nabla_x \Phi(x, y) - i\kappa \Phi(x, y) = O\left(\frac{1}{|x|^2}\right), \quad as \ |x| \to \infty$$

uniformly in  $\hat{x} = \frac{x}{|x|} \in \mathcal{S}^2$  (Sphere)

3.  $\Phi$  has the asymptotic behaviour

$$\Phi(x,y) = \frac{e^{i\kappa|x|}}{4\pi|x|}e^{-i\kappa\hat{x}\cdot y} + O\left(\frac{1}{|x|^2}\right), \quad as \ |x| \to \infty$$

uniformly in  $\hat{x} = \frac{x}{|x|} \in \mathcal{S}^2$  (Sphere)

PROOF. The first 2 properties are easily verified. We prove the third:

We calculate the binomial formula

$$|x - y| - (|x| - \hat{x} \cdot y) = \frac{|x - y|^2 - (|x| - \hat{x} \cdot y)^2}{|x - y| + (|x| - \hat{x} \cdot y)}$$

$$= \frac{|y|^2 - 2x \cdot y + |x|^2 - |x|^2 + 2x \cdot y - (\hat{x} \cdot y)^2}{|x| \left(1 + \left|\hat{x} - \frac{y}{|x|}\right| - \frac{\hat{x} \cdot y}{|x|}\right)}$$

$$\leq \frac{|y|^2}{2|x|\left(1 - \frac{y}{|x|}\right)}.$$

Hence  $|x-y|=|x|-\hat{x}\cdot y+O\left(\frac{1}{|x|}\right)$ . Take the exponential of this to get

$$e^{i\kappa|x-y|} = e^{i\kappa|x|}e^{-i\kappa\hat{x}\cdot y}\left(1 + O\left(\frac{1}{|x|}\right)\right).$$

By the above formula we also have

$$\frac{1}{|x-y|} = \frac{1}{|x|} + \left[ \frac{|x| - |x-y|}{|x-y||x|} \right] = \frac{1}{|x|} + O\left( \frac{1}{|x|^2} \right).$$

So

$$\frac{e^{i\kappa|x-y|}}{|x-y|} = \frac{e^{i\kappa|x-y|}}{|x|} + O\left(\frac{1}{|x|^2}\right)$$
$$= \frac{1}{|x|}e^{i\kappa|x|}e^{-i\kappa\hat{x}\cdot y} + O\left(\frac{1}{|x|^2}\right),$$

as  $|x| \to \infty$ .

Remark 1.10. The previous result states in particular that  $\Phi$  is determined by the function

$$e^{-i\kappa\hat{x}\cdot y}$$

on  $\mathcal{S}^2$  (up to pertubation). We will see that this property holds in a more general context.

With the help of the fundamental solution  $\Phi$  we can create

#### Theorem 1.11

Let  $\Omega \subseteq \mathbb{R}^3$  be bounded. For every  $\phi \in L^2(\Omega)$ , the function

$$v(x) := \int_{\Omega} \phi(y) \Phi(x, y) \, dy, \quad x \in \mathbb{R}^3$$

belongs to  $H^1_{loc}(\mathbb{R}^3)$  and satisfies the Sommerfeld radiation condition. Moreover, v is the only radiating solution (it is the only function in the set of solution that satisfies the Sommerfeld radiation condition) to

$$\Delta v + \kappa^2 v = -\phi$$

in the variational sense

$$\int_{\mathbb{R}^3} \left( \nabla v \cdot \nabla \bar{\Psi} - \kappa^2 v \bar{\Psi} \right) \, dx = \int_{\mathbb{R}^3} \phi \bar{\Psi} \, dx \tag{*}$$

for all  $\Psi \in H^1(\mathbb{R}^3)$  with compact support. For any R > 0 with  $\Omega \subseteq B_R(0) =: K$  we have with  $c = c(R, \kappa, \Omega)$  that

$$||v||_{H^1(K)} \le c||\phi||_{L^2(\Omega)}.$$

In other words, the mapping  $\phi \mapsto v$  is a bounded (continuous linear) operator from  $L^2(\Omega)$  to  $H^1(K)$ .

PROOF. (1) Since  $\frac{1}{r^2}$  is locally integrable in  $\mathbb{R}^3$ , the expression on the right-hand side in Eq. (\*) is well-defined. Provided  $\phi \in C^1(\bar{\Omega})$ , then we can interchange integration and differentiation (possible as we have a majorant, cf. PDE theory) and obtain

$$\Delta v + \kappa^2 v = \begin{cases} -\phi & \text{in } \Omega \\ 0 & \text{in } \mathbb{R}^3 \setminus \bar{\Omega} \end{cases}$$

This means that v solves Eq. (\*) for any  $\kappa \in \mathbb{C}$ .

(2) We cannot directly evaluate  $L^2$ -integrals of the gradient  $\nabla_x \Phi$ . To prove stability, we first consider the special case  $\kappa = i$  and  $\phi \in C^1(\bar{\Omega})$ . Then, the fundamental solution

$$\Phi_i(x,y) = \frac{1}{4\pi|x-y|} e^{-|x-y|}$$

decays exponentially for  $|x| \to \infty$ , ad by approximation arguments Eq. (\*) holds for any  $\Psi \in H^1(\mathbb{R}^3)$ .

Taking  $\Psi = v$  we obtain

$$||v||_{H^1(\mathbb{R}^3)}^2 = \int_{\Omega} \phi \bar{v} \le ||\phi||_{L^2(\Omega)} ||v||_{H^1(\mathbb{R}^3)}$$

(note that Eq. (\*) with  $\kappa=i$  becomes the  $H^1$ -Norm). By density, this defines a continuous operator

$$\phi \mapsto v \quad \text{from } L^2(\Omega) \text{ to } H^1(K).$$

(3) Let k > 0. We define

$$\Psi(x,y) := \Phi_k(x,y) - \Phi_i(x,y) = \frac{1}{4\pi|x-y|} \left[ e^{i\kappa|x-y|} - e^{-|x-y|} \right]$$

It is easy to prove that  $\Psi$  and  $\nabla_x \Psi$  belong to  $L^2(K \times \Omega)$ . We sketch the crucial part. We calculate

$$4\pi |\nabla_x \Psi(x,y)| = \underbrace{\left| \frac{i\kappa e^{i\kappa|x-y|} - e^{-|x-y|}}{|x-y|}}_{O\left(\frac{1}{|x-y|}\right)} + \underbrace{\frac{e^{i\kappa|x-y|} - e^{-|x-y|}}{|x-y|^3}}_{leqO\left(\frac{1}{|x-y|}\right) \text{ for small } |x-y|}$$

\*: The denominator of the right fraction is in O(|x-y|)

Thus,

$$\|\nabla_x \Psi\|_{L^2(K \times \Omega)} \le C \int_K \int_{\Omega} \frac{1}{|x - y|^2} \, dy \, dx < \infty.$$

(4) With (3) we see that the mapping

$$\varphi \mapsto \int_{\Omega} \varphi(y) \Psi(\cdot, y) \, dy$$

is bounded from  $L^2(\Omega)$  to  $H^1(K)$ , because

$$\begin{split} \int_{K} \left| \nabla_{x} \int_{\Omega} \varphi(y) \Psi(x,y) \, dy \right|^{2} \, dx &= \int_{k} \left[ \int_{\Omega} \left| \varphi(y) \nabla_{x} \Psi(x,y) \right| \, dy \right]^{2} \, dx \\ &\leq \int_{K} \left\| \varphi \right\|_{L^{2}(\Omega)}^{2} \left\| \nabla_{x} \Psi(x,\cdot) \right\|_{L^{2}(\Omega)}^{2} \, dx \\ &\leq \left\| \varphi \right\|_{L^{2}(\Omega)}^{2} \underbrace{\left\| \nabla_{x} \Psi \right\|_{L^{2}(K \times \Omega)}^{2}}_{(3)}. \end{split}$$

This and (2) show that  $\varphi \mapsto v$  is also bounded from  $L^2(\Omega)$  to  $H^1(K)$  for  $\kappa > 0$ .

(5) The radiation condition follows from the radiation condition of  $\Phi$ :

$$\frac{\partial v}{\partial \nu} - i\kappa v = \int_{\Omega} \varphi(y) \left( \frac{\partial}{\partial \nu} - i\kappa \right) \Phi(x, y) \, dy$$
$$\leq \|\varphi\|_{L^{2}(\Omega)} O\left( \frac{1}{r} \right)^{2}.$$

Uniqueness follows from (2).

Remark 1.12. **Proof of Theorem 1.11** (1).

To prove that  $\Delta v(x) + \kappa^2 v(x) = -\varphi(x)$ , for  $x \in \Omega$ , it satisfies to verify

$$(\Delta + \kappa^2) \int_{B_{\varepsilon}(x)} \varphi(y) \Phi(x, y) \, dy = -\varphi(x),$$

for small  $\varepsilon > 0$ .

1) We readily see that

$$\kappa^2 \left| \int_{B_{\varepsilon}(x)} \varphi(y) \Phi(x, y) \, dy \right| \le \frac{\kappa^2}{4\pi} \left| \int_{B_{\varepsilon}(x)} \frac{e^{i\kappa |y - x|}}{|x - y|} \, dy \right|$$

and the expression on the right tends to 0 for  $\varepsilon \to 0$ .

2) Since  $\Delta_x \Phi(x,y) = \Delta_y \phi(x,y)$ , we see

$$\begin{split} \Delta_y \int_{B_{\varepsilon}(x)} \varphi(y) \phi(x,y) \, dy &= \int_{B_{\varepsilon}(x)} \phi(y) \Delta_y \Phi(x,y) \, dy \\ &= \underbrace{-\int_{B_{\varepsilon}(x)} \nabla \varphi(y) \cdot \nabla \Phi(x,y)}_{=:A} + \underbrace{\int_{|y-x|=\varepsilon} \varphi(y) \frac{\partial \Phi(x,y)}{\partial \nu} \, dS(y)}_{=:B}. \end{split}$$

We have that

$$\nabla_y \Phi(x, y) = \frac{1}{4\pi} e^{i\kappa|x-y|} \left( \frac{1}{|x-y|^2} - \frac{1}{|x-y|^3} \right) (x-y),$$

and thus

$$A \leq \|\nabla \varphi\|_{L^{\infty}} \int_{B_{\varepsilon}(x)} |\nabla_y \Phi(x,y)| \, dy \to 0, \text{ as } \varepsilon \to 0.$$

We stay with B:

$$B = \frac{1}{4\pi} \int_{\partial B_{\varepsilon}(x)} e^{i\kappa\varepsilon} \left(\frac{1}{\varepsilon} - \frac{1}{\varepsilon^2}\right) \varphi(y) \, dS(y)$$
$$= \underbrace{\frac{1}{4\pi} e^{i\kappa\varepsilon} \left(\frac{1}{\varepsilon} - \frac{1}{\varepsilon^2}\right) 4\pi\varepsilon^2}_{=e^{i\kappa\varepsilon} (\varepsilon + \varepsilon^{-1}) \to -1, \text{ as } \varepsilon \to 0} \underbrace{\int B_{\varepsilon}(x) \varphi(y) \, dS(y)}_{\to \varphi(x), \text{ as } \varepsilon \to 0}$$

#### Theorem 1.13 (Lippmann Schwinger integral equation)

Let  $\alpha > 0$  and  $K = B_{\alpha}(0)$ . If  $u \in H^1$  solves the Problem 1.1, then  $u_{|K} \in L^2(K)$  satisfies the Lippmann Schwinger equation

$$u(x) = u^{i} n(x) - \kappa^{2} \int_{|y| < \alpha} (1 - n(y)) \Phi(x, y) u(y) \, dy$$
 (LS)

for almost all  $x \in K$ .

Conversely, if  $u \in L^2(K)$  satisfies Eq. (LS), then it can be extended by the right-hand side of Eq. (LS) to the solution  $u \in H^1_{loc}(\mathbb{R}^3)$  of Problem 1.1.

PROOF. Let u satisfy Problem 1.1 and define

$$v = \int_K \varphi(y) \Phi(\cdot, y) \, dy$$

for  $\varphi = \kappa^2 (1-n)u \in L^2(K)$ . Theorem 1.11 states that  $v \in H^1_{loc}(\mathbb{R}^3)$  satisfies  $\Delta v + \kappa^2 v = -\varphi$ . Since

$$\Delta u + \kappa^2 u = \kappa^2 (1 - n) u$$

and

$$\Delta u^{in} + \kappa u^{in} = 0.$$

we have (addition of previous equations)

$$\Delta(v + u^s) + \kappa^2(v + u^s) = 0.$$

The uniqueness from Theorem 1.7 shows that  $v + u^s = 0$ . Therefore

$$u = u^{in} + u^s = u^{in} - v.$$

For the converse direction let  $u \in L^2(K)$  satisfy Eq. (LS). Define v as above, such that  $u = u^{in} - v$  in K (in the  $L^2$ -sense). By Theorem 1.11 we know that  $v \in H^1_{loc}(\mathbb{R}^3)$  by extending it to  $\mathbb{R}^3$ , and that  $\Delta v + \kappa v = -\varphi$ . This implies  $u \in H^1_{loc}(\mathbb{R}^3)$ . Furthermore

$$\Delta u + \kappa^2 u = \varphi = \kappa^2 (1 - n) u,$$

that is

$$\Delta u + \kappa^2 n u = 0.$$

This implies that  $u^s = -v$ . The radiation condition follows again from Theorem 1.11. We now can derive existence for Problem 1.1.

#### Theorem 1.14 (Existence of solutions for Problem 1.1)

Let  $\kappa, n, \theta$  be as assumed previously. Then, the Lippmann Schwinger equation (LS), and thus Problem 1.1, is uniquely solvable.

PROOF. Define the following operator  $T: L^2(B_{\alpha}(0)) \to L^2(B_{\alpha}(0))$  by

$$(Tu)(x) = \kappa^2 \int_{|y| < \alpha} (1 - n(y)) \Phi(x, y) u(y) \, dy, \text{ for } |x| < \alpha.$$

Theorem 1.11 shows that T is bounded from  $L^2(B_{\alpha}(0))$  to  $H^1(B_{\alpha}(0))$ , and by the compact embedding  $H^1(B_{\alpha}(0)) \hookrightarrow L^2(B_{\alpha}(0))$ , the operator T is compact from  $L^2(B_{\alpha}(0))$  into itself. The Lippmann Schwinger equation reads

$$u + Tu = u^{in}$$

and by the Riesz theory (Fredholm alternative) for compact operators, the uniqueness of u (Theorems 1.7 and 1.13) implies its existence.

#### Theorem 1.15 (Far-field pattern)

Let u solve Problem 1.1. Then we have

$$u(x) = u^{in}(x) + \frac{e^{i\kappa|x|}}{|x|} u_{\infty}(\hat{x}) + O\left(\frac{1}{|x|^2}\right), \text{ as } |x| \to \infty,$$

uniformly in  $\hat{x} = \frac{x}{|x|}$  (direction of x). The function  $u_{\infty}(\hat{x})$  is given by

$$u_{\infty}(\hat{x}) = \frac{\kappa^2}{4\pi} \int_{|y| < \alpha} (n(y) - 1)e^{-i\kappa \hat{x} \cdot y} u(y) dy$$

is called far-field pattern or scattering amplitude

$$u_{\infty}: \underbrace{\mathcal{S}^2}_{Sphere} \to \mathbb{C}$$

is analytic on  $S^2$  and determines  $u^s$  of uside  $B_{\alpha}(0)$  uniquely  $(u_{\infty} = 0 \Leftrightarrow u^s(x) = 0 \text{ for } |x| > \alpha).$ 

The formula for u(x) follows from Proposition 1.9 (iii):

$$\Phi(x,y) = \frac{e^{i\kappa|x|}}{|x|}e^{-i\kappa\hat{x}\cdot y} + O\left(\frac{1}{|x|^2}\right).$$

By Theorem 1.2 (Rellich) we have

$$\lim_{R \to 0} \int_{|x|=R} |u(x)|^2 dS(x) = 0, \text{ for } |x| > \alpha$$

and this implies uniqueness. The analyticity follows from the formula (calculate derivate w.r.t  $\hat{x}$ ).

Remark 1.16. 1. The concept of far-field pattern is <u>fundamental</u> to inverse scattering theory.

2. The analyticity of  $u_{\infty}$  shows that the inverse scattering problem is ill-posed (little pertubations of  $u_{\infty}$  can destroy analyticity of the function!).

#### Theorem 1.17 (Green's representation theorem)

(i) Any  $y \in C^2(\Omega) \cap C^1(\overline{\Omega})$  satisfies for any  $x \in \Omega$ 

$$u(x) = \int_{\partial\Omega} \left[ \Phi(x,y) \frac{\partial u(y)}{\partial \nu} - u(y) \frac{\partial \Phi}{\partial \nu(y)} \right] dS(y) - \int_{\Omega} \Phi(x,y) (\kappa^2 u(y) + \Delta u(y)) dy$$

(where  $\nu$  denotes the outer normal of  $\Omega$ ).

(ii) Let  $\Omega^c := \mathbb{R}^3 \setminus \Omega$  and let  $u \in H^1_{loc}(\mathbb{R}^3)$  satisfy the Sommerfeld radiation condition, and solve

$$\Delta u + \kappa^2 u = 0, \quad in \ \Omega^c.$$

Then, the Green's formula holds:

$$u(x) = \int_{\partial\Omega} \left[ u(y) \frac{\partial \Phi(x,y)}{\partial \nu(y)} - \Phi(x,y) \frac{\partial}{\partial \nu} u(y) \right] dy, \quad x \in \mathbb{R}^3 \setminus \overline{\Omega}.$$

(iii) In the situation of (ii), the far-field pattern of u reads for  $\hat{x} = \frac{x}{|x|} \in \mathcal{S}^2$ 

$$u_{\infty}(\hat{x}) = \frac{1}{4\pi} \int_{\partial \Omega} \left[ u(y) \frac{\partial}{\partial \nu(y)} e^{-i\kappa \hat{x} \cdot y} - e^{-i\kappa \hat{x} \cdot y} \frac{\partial u}{\partial \nu}(y) \right] dS(y).$$

PROOF. (i) we know from Theorem 1.11 (see addendum) that

$$-u(x) = \int_{\Omega} u(y)(\kappa^2 + \Delta_y)\Phi(x,y) \, dy.$$

The assertion follows from integrating by parts.

(ii) Let R > 0 and  $K = B_R(0)$ , with  $\overline{\Omega} \subseteq K$ . Define  $D = K \setminus \overline{\Omega}$ . Apply (i) to D and obtain, for  $x \in D$ ,

$$u(x) = \int_{\partial\Omega} + \left[ \int_{\partial K} \right] \left[ \Phi(x, y) \frac{\partial u}{\partial \nu}(y) - u(y) \frac{\partial}{\partial \nu(y)} \Phi(x, y) \right] dS(y).$$

We want to show, that the  $\int_{\partial K}$ -integral vanishes for large  $R \to \infty$ . From the proof of Theorem 1.7 we know, that  $\int_{\partial K} |u|^2 dS \leq O(1)$  as  $R \to \infty$ . From the Sommerfeld radiation condition of u and  $\Phi$ , we obtain with the Cauchy-Schwarz inequality

$$\int_{\partial K} \dots dS = \int_{\partial K} \Phi(x,y) \left[ \frac{\partial u}{\partial \nu}(y) - i\kappa u(y) \right] + u(y) \left[ i\kappa \Phi(x,y) - \frac{\partial}{\partial \nu(y)} \Phi(x,y) \right] dS(y)$$

$$\stackrel{C.S.}{\leq} \underbrace{\|\Phi\|_{L^2(\partial K, dy)} O\left(\frac{1}{r^2}\right) + \|u\|_{L^2(\partial K)} O\left(\frac{1}{r^2}\right)}_{\to 0, \text{ as } R \to \infty}.$$

From Proposition 1.9 we know  $(\hat{x} = \frac{x}{|x|})$ :

$$\Phi(x,y) = \frac{1}{4\pi|x|} e^{i\kappa|x|} e^{-i\kappa\hat{x}\cdot y} + O\left(\frac{1}{|x|^2}\right).$$

We plug this into the formula of (ii) and obtain for |x| >> 1:

$$u(x) = \frac{1}{4\pi} e^{i\kappa w} \int_{\partial\Omega} \left[ u(y) \frac{\partial}{\partial\nu(y)} e^{-i\kappa \hat{x}\cdot y} - e^{-i\kappa \hat{x}\cdot y} \frac{\partial}{\partial\nu} u(y) \right] \, dy + O\left(\frac{1}{|x|^2}\right).$$

Uniqueness of the far-field pattern proves (iii).

#### 1.3 Density results

In this section we collect some density results, useful in the labour study of inverse scattering. Recall: The refraction index n satisfies |n(x)| = 1 for  $|x| > \alpha$ .

#### Lemma 1.18

Let  $\beta > \alpha$ ,  $K := B_{\beta}(0)$ . Then there exist constants M > 0, C > 0, such that for any  $z \in \mathbb{C}^3$  with  $z \cdot z = 0$  and  $|z| \geq M$  there exists a solution  $u_z \in H^1(K)$  to the equation

$$\Delta u_z + \kappa^2 n u_z = 0, \quad in \ K,$$

of the form

$$u_z(x) = e^{z \cdot x} (1 + v_z(x)), \quad x \in K,$$

and  $v_z$  satisfies

$$||v_z||_{L^2(K)} \le \frac{C}{|z|}.$$

PROOF. The technical lemma will be proven later.

#### Theorem 1.19 (1st density theorem)

Let  $\Omega \subseteq \mathbb{R}^3$  be bounded and let  $n_1, n_2 \in L^{\infty}(\Omega)$  such that  $(n_1 - 1)$  and  $(n_2 - 1)$  have a compact support in  $\Omega$ . Then, the following linear hall of products is dense in  $L^2$ :

$$X \coloneqq span\{u1u2: \forall j = 1, 2\,u_j \in H^1(\Omega) \text{ solves } \Delta u_j + \kappa^2 n_j u_j = 0 \text{ in } \Omega\}$$

PROOF. Let  $\beta > 0$  such that  $\overline{\Omega} \subseteq B_{\beta}(0)$  and let  $g \in L^{2}(\Omega)$  be  $L^{2}(\Omega)$ -Orthogonal to the set X. We have to show, that g is zero. Then X is dense.

Fix  $y \in \mathbb{R}^3 \setminus \{0\}$  and choose a unit vector  $\hat{a} \in \mathbb{R}^3$  (\*means unit length) and some  $b \in \mathbb{R}^3$  with  $|b|^2 = |y|^2 + s^2$  such that  $\{y, \hat{x}, b\}$  is an orthogonal system in  $\mathbb{R}^3$  and some s > 0 (real).

Define the following elements of  $\mathbb{C}^3$ :

$$z^{1} \coloneqq \frac{1}{2}b - \frac{i}{2}(y + s\hat{a})$$
$$z^{2} \coloneqq -\frac{1}{2}b - \frac{i}{2}(y - s\hat{a}).$$

Then  $z^1 \cdot z^1 = 0 = z^2 \cdot z^2$ . We have

$$|z^1|^2 = |z^2|^2 = \frac{1}{4} \left[ |b|^2 + |y|^2 + s^2 \right] \ge \frac{1}{4} s^2.$$

Furthermore  $z^1 + z^2 = -iy$ . From Lemma 1.18 we obtain solutions to  $\Delta u_j + \kappa^2 n_j u_j = 0$  in  $B_{\beta}(0)$  with

$$u_j(x) = e^{z^j \cdot x} \left[ 1 + v_{z_j}(x) \right].$$

These are in particular solutions when restricted to the smaller domain  $\Omega$ . The orthogonal property of g yields

$$0 = \int_{\Omega} e^{(z^1 + z^2)x} [1 + v_{z_1}^2 + v_{z_2}^2 + v_{z_1}v_{z_2}] g \, dx.$$

From Lemma 1.18 we obtain

$$||v_j||_{L^2(\Omega)} \le \frac{C}{|z_j|} \le \frac{2C}{s}.$$

Last inequality follows from a previous equation. From Cauchy's inequality and the limit  $s \to 0$  that

$$0 = \int_{\Omega} e^{-iy \cdot x} g(x) \, dx, \quad \forall y \in \mathbb{R}^3 \setminus \{0\}.$$

So, the Fourier-Transform of g vanishes (it is defined like in our equation). Thus g = 0.

The second density theorem is the following.

#### Theorem 1.20 (2nd density theorem)

Let  $n \in L^{\infty}(\mathbb{R}^3)$  with n(x) = 1 for  $|x| > \alpha$ . Let  $\beta > \alpha$  and define

$$H := \left\{ v \in H^1(B_{\beta}(0)) | \Delta v + \kappa^2 n v = 0 \text{ in } B_{\beta}(0) \right\}$$

the set of Helmholtz-solutions. Let for any  $\hat{\theta} \in S^2$ ,  $u(\cdot, \hat{\theta})$  denote the total field corresponding to the incident plain wave  $e^{i\kappa\hat{\theta}\cdot x}$  (plain wave from direction  $\hat{\theta}$ ). Then, the span of all plain wave solutions,

$$span\{u(\cdot,\hat{\theta}): \hat{\theta} \in \mathcal{S}^2\},\$$

is dense

$$H|_{B_{\alpha}(0)}$$
 in  $L^2(B_{\alpha}(0))$  - norm.

PROOF. Let  $K = B_{\alpha}(0)$  and  $\langle v, w \rangle$  the  $L^2$  product over K, so

$$\langle v, w \rangle := \int_K v \overline{w} \, dx.$$

Let v be in the closure of H with the following property:

$$\langle v, u(\cdot, \hat{\theta}) \rangle = 0$$

for all  $\hat{\theta} \in \mathcal{S}^2$ . Recall the operator

$$T: v \mapsto \kappa^2 \int_{|x| < \alpha} (1 - n(y)) \Phi(x, y) w(y) \, dy$$

and the Lippmann-Schwinger equation

$$u(\cdot, \theta) = (1+T)^{-1}u^{in}(\cdot, \theta).$$

With the adjoint operator  $T^*$ , that satisfies

$$\langle T^*v, w \rangle = \langle v, Tw \rangle, \quad \forall v, w \in X,$$

and the fact that

$$[[1+T]^{-1}]^* = (1+T^*)^{-1},$$

we obtain that

$$0 = \langle v, (1+T)^{-1} u^{in}(\cdot, \hat{\theta})$$
  
=  $\langle (1+T^*)^{-1} v, u^{in}(\cdot, \hat{\theta}),$ 

for all  $\hat{\theta} \in \mathcal{S}^2$ . We compute  $T^*$ : Since, for all  $w_1, w_1 \in L^2(K)$  we have

$$\begin{split} \frac{1}{\kappa^2} \langle T^* w_1, w_2 \rangle &= \frac{1}{\kappa^2} \langle w_1, T w_2 \rangle \\ &= \int_K \int_K w_1(x) \overline{(1 - n(y))} \Phi(x, y) w_2(y) \, dy \, dx \\ &= \langle (1 - \overline{n}) \int_K w_1(x) \overline{\Phi(x, \cdot)} \, dx, w_2 \rangle, \end{split}$$

we have

$$T^*w_1 = \kappa^2 \overline{(1-n)} \int_K w_1(y) \overline{\Phi(\cdot, y)} \, dy.$$

Thus  $w := (1 + T^*)^{-1}v$  satisfies

$$v(x) = w(x) + \kappa^2 (1 - \overline{n(x)}) \int_K \overline{\Phi(x, y)} w(y) \, dy.$$

We now set

$$\tilde{w}(x) := \int_K \overline{w(y)} \Phi(x, y) \, dy, \quad x \in \mathbb{R}^3.$$

Then,  $\tilde{w}$  is a volume potential for  $\bar{w}$  in the sense of Theorem 1.11:  $w \in H^1_{loc}(\mathbb{R}^3)$  and

$$\int_{\mathbb{R}^3} \left( \nabla \tilde{w} \cdot \nabla \overline{\Psi} - \kappa^2 \tilde{w} \overline{\Psi} \right) \, dx = \int_K \overline{w} \overline{\Psi} \, dx, \quad \forall \Psi \in H^1(\mathbb{R}^3) \text{ with compact support.}$$

The far-field pattern  $\tilde{w}_{\infty}$  vanishes. Indeed, as Theorem 1.17 (iii) and the divergence theorem imply for any  $\hat{\Theta} \in \mathcal{S}^2$ :

$$\overline{\tilde{w}_{\infty}(\hat{\theta})} = \int_{K} w(y) e^{i\kappa \hat{\theta} \cdot y} \, dy = 0,$$

since w is orthogonal to the plain waves. Rellichs theorem implies then, that  $\tilde{w} = 0$  outside of K! Consider a sequence  $v_i \in H$  with  $v_i \to v$  in  $L^2(H)$  as  $j \to \infty$ . From

$$v = w + \overline{\kappa^2 (1 - n)\tilde{w}}$$

we get

$$\int_{K} \overline{v}v_{j} dx = \int_{K} \overline{w}v_{j} dx + \kappa^{2} \int_{K} (1 - n)\tilde{w}v_{j} dx. \tag{*}$$

Since  $\tilde{w}$  vanishes outside K, we obtain from  $v_i \in H$ 

$$\int_{|x|<\beta} (\nabla v_j \cdot \nabla \tilde{w} - \kappa^2 v_j \cdot \tilde{w}) \, dx = -\kappa^2 \int_K (1-n) v_j \tilde{w} \, dx.$$

We extend  $v_j$  to a  $H^1(\mathbb{R}^3)$  function with compact support. The property of  $\tilde{w}$  implies

$$\int_{|x|<\beta} (\nabla \tilde{w} \cdot \nabla v_j - \kappa^2 \tilde{w} \cdot v_j) \, dx = \int_K (1-n) v_j \tilde{w} \, dx.$$

The previous formulas imply

$$-\kappa^2 \int_K (1-n)v_j \tilde{w} \, dx = \int_K \overline{w} v_j \, dx.$$

This and Eq. (\*) give

$$\int_K \overline{v}v_j = 0, \quad \forall j \in \mathbb{N}.$$

In the limit  $j \to \infty$  we obtain

$$||v||_{L^2(K)} = 0 \Longleftrightarrow v = 0.$$

This proves density.

### Chapter 2

# Discretization of the direct scattering problem

#### 2.1 Dealing with infinite domains

Recall the direct scattering Problem 1.1 from Chapter 1: Given some incident wave  $u^{in}(x)$  of plain-wave type, i.e.

$$u^{in}(x) = ce^{i\kappa\hat{\theta}\cdot x},$$

with direction  $\hat{\theta} \in \mathcal{S}^{d-1}$  (unit sphere in  $\mathbb{R}^d$ ) and (real) frequency  $\kappa > 0$ , find the total field  $u \in H^1_{loc}(\mathbb{R}^d)$  such that for all  $\Psi \in H^1(\mathbb{R}^d)$  with compact support it holds that

$$\int_{\mathbb{R}^d} (\nabla u \cdot \nabla \overline{\Psi} - \kappa^2 n u \overline{\Psi}) \, dx = 0,$$

where  $n \in L^{\infty}(\Omega)$  function with  $\Re n, \Im n \geq 0$ . Additionally the scattered field  $u^s := u - u^{in}$  should solve the Sommerfeld radiation condition

$$\frac{\partial u^s(x)}{\partial r} - i\kappa u^s(x) = O\left(\frac{1-d}{2}\right),\,$$

for  $|x| = r \to \infty$  uniformly in  $\hat{x} = \frac{x}{|x|} \in \mathcal{S}^{d-1}$ .

The scattering problem is an infinite-dimensional variational problem on an infinite (unbounded) domain.

**Aim of this chapter:** Approximate Problem 1.1 in a finite computational complexity and time.

This section deals with the restriction / truncation to bounded domains.

Common approach: Simply replace  $\mathbb{R}^d$  by some bounded domain  $\Omega$  and put some artificial absorbing boundary condition on  $\partial\Omega$ . The principle is to allow all waves to leave the domain without any artifical scattering (i.e. the initial wave, that may be scattered by some objects in  $\Omega$ , should be able to leave the domain without any harm). At the boundary of the domain, nothing that's leaving should be scattered inside again (as  $\Omega$  is just used for being able to compute something).

Reference: Lecture-notes of Olof Runborg, KTH Stockholm.

#### 2.1.1 One-dimensional illustration

In 1d (and only in 1d), it is possible to design exact local absorbing boundary conditions. W.l.o.g. let the artificial domain  $\Omega = B_L(0)$  be clutered and let  $\overline{B_{\alpha}(0)} \subseteq B_L(0)$  ( $L > \alpha$ , where  $\alpha$  is the parameter from Chapter 1,  $n|_{B_{\alpha}(0)^c} = 1$ ). Close to  $\partial\Omega = \{-L, L\}$ , the medium is homogeneous and hence the scattered wave  $u^s := u - u^{in}$  satisfies the Helmholtz-equation

$$u_{rr}^s - \kappa^2 u^s = 0,$$

for  $|x \pm L|$  sufficiently small.

Therefore

$$u^{s}(x) = \underbrace{c_{0}e^{-i\kappa x}}_{A} + \underbrace{c_{1}e^{i\kappa x}}_{B}, \tag{2.1}$$

with  $c_0, c_1 \in \mathbb{R}$  and x close to  $\pm L$ . The part A of the solutions travels to the left of the interval, the part B travels to the right of the interval. As stated above: If we were sitting on the boundary, we would like to be able to allow waves to pass the boundary from the inside. If a wave comes from the outside, we don't let it pass. Therefore we want to design the absorbing boundary condition at -L such that it accepts any  $c_0$ , but prevents  $c_1 \neq 0$ . This is archieved by applying the operator  $\frac{\partial}{\partial x} + i\kappa$ . Why this? Because:

$$\left(\frac{\partial}{\partial x} + i\kappa\right)u^s = -c_0i\kappa e^{-i\kappa x} + c_1i\kappa e^{i\kappa x} + c_0i\kappa e^{-i\kappa x} + c_1i\kappa e^{i\kappa x}$$
$$= 2c_1i\kappa e^{i\kappa x},$$

and this shows that  $\left(\frac{\partial}{\partial x} + i\kappa\right)$  doesn't 'see' waves leaving  $\Omega$  (i.e. the  $c_0$  part of the solution), and incoming waves can be avoided by the boundary condition

$$\left(\frac{\partial}{\partial x}u^s + i\kappa u^s\right)(-L) = 0.$$

Similarly, at x = +L we impose

$$\left(\frac{\partial}{\partial x}u^s - i\kappa u^s\right)(+L) = 0$$

(calculation shows this again). Introducing the concept of an outer normal  $\nu$ , i.e.  $\nu(\pm L) = \pm 1$ , we can rewrite both conditions as

$$\frac{\partial u^s}{\partial \nu}(x) - i\kappa u^s(x) = 0,$$

for  $x \in \partial\Omega = \{-L, L\}$ . This leads to the following inhomogeneous boundary condition for the total wave  $u = u^s + u^{in}$ :

$$\left(\frac{\partial u}{\partial \nu} - i\kappa u\right)(x) = \left(\frac{\partial u^{in}}{\partial \nu} - i\kappa u^{in}\right)(x), \quad x \in \partial\Omega = \{-L, L\}.$$
 (2.2)

#### Example.

 $u^{in}=e^{-i\kappa x}$  is a wave travelling from right to left. Then the absorbing boundary condition reads

$$\left(\frac{\partial u}{\partial \nu} - i\kappa u\right)(-L) = 0,$$

$$\left(\frac{\partial u}{\partial \nu} - i\kappa u\right)(L) = 2i\kappa u^{in}(L).$$

We shall emphasize that the scattering problem on  $\Omega$  with absorbing boundary condition Eq. (2.2),

$$\begin{array}{ll} \Delta u + i \kappa n u = 0, & \text{in } \Omega \\ \frac{\partial u}{\partial \nu} - i \kappa u = \frac{\partial u^{in}}{\partial \nu} - i \kappa u^{in}, & \text{on } \partial \Omega, \end{array}$$

reproduces the solution of Problem 1.1 in  $\Omega$ .

#### 2.1.2 Multi-dimensional case

In higher dimensions, there is no simple form like Eq. (\*) for this scattered wave close to the artificial boundary  $\partial\Omega$ . Exact absorbing boundary conditions will be necessarily non-local and computationally demanding.

A cheaper and popular approach is the following:

Assume that the scattered wave in the full problem is close to a spherical wave in a vicinity of the artificial boundary. If we choose  $\Omega = B_L(0)$ , then the 1d-arguments can be applied. If  $u^s(x) \approx e^{i\kappa|x|}$  (i.e. the wave is approximately spherical; spherical waves have no angular dependence) close to  $\partial\Omega$ , then  $\frac{\partial u^s}{\partial\nu} - i\kappa u^s \approx i\kappa e^{i\kappa|x|} - i\kappa e^{i\kappa|x|} = 0$  on  $\partial\Omega$ 

This motivates the simplest absorbing bc in 2 and 3 dimensions:

$$\frac{\partial u}{\partial \nu} - i\kappa u = \frac{\partial u^{in}}{\partial \nu} - i\kappa u^{in}, \quad \text{on } \partial\Omega.$$
 (2.3)

We have seen in Theorem 1.15 that  $u^s$  is actually spherical, up to some perturbation of order  $O\left(\frac{1}{|x|^2}\right)$ :

$$u^{s}(x) = \frac{e^{i\kappa|x|}}{|x|} u_{\infty}(\hat{x}) + O\left(\frac{1}{|x|^{2}}\right), \text{ as } |x| \to \infty,$$

i.e. 'the scattered wave is spherical if we are far enough away from all obstacles'. Hence, for sufficiently large L ( $\Omega = B_L(0)$ ), is absorbing boundary condition (2.3) appears reasonable.

For the remaining part of this chapter, our model problem reads

#### Problem 2.1.

$$\begin{split} \Delta u + \kappa^2 n u &= 0, \text{ in } \Omega \\ \frac{\partial u}{\partial \nu} - i \kappa u &= \frac{\partial u^{in}}{\partial \nu} - i \kappa u^{in}, texton \partial \Omega. \end{split}$$

Remark 2.1. The absorbing boundary condition (2.3) can be seen as applying the Sommerfeld radiation condition at  $\partial B_L(0)$  instead of  $\infty$ .

Note, that the choice of the boundary condition we made was just the easiest one. There are many alternatives. The most popular approach is the so called *Perfectly Matched Layer* (PML). In this approach no bc on  $\partial\Omega$  are imposed. The idea is to put around  $\Omega$  some thin layer of artificial material (by changing n / making it imaginary). This can also be used to absorb outgoing waves.

## 2.2 Well-posedness of the scattering problem in bounded domains

Recall the scattering problem

$$\Delta u + \kappa^2 n u = 0, \quad \text{in } \Omega$$

$$\frac{\partial u^s}{\partial \nu} - i\kappa u^s = 0, \quad \text{on } \partial\Omega$$
(2.4)

in a boudned domain  $\Omega \supseteq B_{\alpha}(0) \supseteq \text{supp}(1-n)$  with absorbing boundary condition Eq. (2.3) for the scattered wave  $u^s := u - u^{in}$ . W.l.o.g. we assume that  $\Omega \subseteq \mathbb{R}^3$  as in Chapter 1. To be compatible with linear finite elements, we assume that  $\Omega$  is polyhedral. Moreover we choose  $\Omega$  to be convex, which seems to be reasonable with regard to the desired absorption properties (in this way no inner boundaries may reflect incoming waves).

Since it is easier for the numerical analysis of finite element methods, we will now switch to the equivalent problem of finding the scattered wave, i.e. **Problem 2.2.** Given the incident wave  $u^{in} \in H^1(\Omega)$ , we seek  $u^s \in H^1(\Omega)$  such that

$$\Delta u^{s} + \kappa^{2} n u^{s} = \overbrace{-\Delta u^{in} - \kappa^{2} n u^{in}}^{\text{known data}}, \text{ in } \Omega$$

$$\frac{\partial u^{s}}{\partial \nu} - i \kappa u^{2} = 0, \text{ on } \partial \Omega.$$
(2.5)

For  $u^{in} = ce^{i\kappa\hat{\Theta}\cdot x}$ ,  $\hat{\Theta} \in \mathcal{S}^2(\mathbb{R}^3)$  the right hand side of the first equation becodes  $\kappa^2(1-n)u^{in}$  (in  $\Omega$ ).

The weak formulation of Problem 2.2 (and also the concept of a weak solution) is based on the sesquilinearform

$$a: H^{1}(\Omega) \times H^{1}(\Omega) \to \mathbb{C}$$

$$(u,v) \mapsto \int_{\Omega} \nabla u \cdot \nabla \overline{v} \, dx - \kappa^{2} \int_{\Omega} nu \overline{v} \, dx + i\kappa \int_{\partial \Omega} u \overline{v} \, dS_{x} \qquad (2.6)$$

and the anti-linear form

$$F: H^{1}(\Omega) \to \mathbb{C}$$

$$v \mapsto \kappa^{2} \int_{\Omega} (1-n)u^{in}\overline{v} dx \qquad (2.7)$$

(satisfies  $F(\lambda v) = \overline{\lambda}F(v)$ ).

The weak formulation reads: Given  $F \in (H^1(\Omega))'$  (space of bounded anti-linear functionals), e.g. the particular F of Section 2.2, seek  $u^s \in H^1(\Omega)$  such that

$$a(u^s, v) = F(v), \quad \forall v \in H^1(\Omega).$$
 (2.8)

We call any solution  $u^s$  of Eq. (2.8) a weak solution of Problem 2.2 and  $u = u^{in} + u^s$  weak solution of Section 2.2.

The sesquilinear form a is bounded:

$$|a(u,v)| < C||u||_{\kappa}||v||_{\kappa}$$

with respect to the  $\kappa$ -dependent norm

$$\|\cdot\|_{\kappa} \coloneqq \sqrt{\|\nabla\cdot\|_{L^2(\Omega)}^2 + \kappa^2 \|n^{\frac{1}{2}}\cdot\|_{L^2(\Omega)}^2},$$

which is equivalent to the classical  $H^1$ -norm. The boundedness follows from Cauchy-Schwarz inequality and the trace inequality

$$||v||_{L^2(\partial\Omega)}^2 \le C'(\Omega)||v||_{L^2(\Omega)}||v||_{H^1(\Omega)}.$$

The constant  $C'(\Omega)$  (and also the constant  $C(\Omega)$ ) are independent of  $\kappa \geq 1$ . The regime  $\kappa \to 0$  would requiere special treatment here and in what follows. Since this is not our regime of interest, we shall assumme that  $\kappa$  is sufficiently large, i.e.  $\kappa \geq 1$ . All results remain valid for  $0 < \kappa < 1$ . However, constants may blow up with  $\kappa \to 0$ .

More explanation: When  $\kappa \to 0$  we are mainly killing the  $\kappa^2 nu$  term of our equation, and also the  $\kappa$  term in the boundary condition. This leads to the Laplace-Problem with Neumann-B.C. However, there is more than one solution (e.g. the constant function is a solution).

The sesquilinear form a is symetric:  $a(u,v) = a(v,u), \forall u,v \in H^1(\Omega,\mathbb{R})$ . However, it is <u>not</u> hermitian in general:

$$a(u,v) \neq \overline{a(u,v)}$$
.

Moreover a is not coercive (that is, a is far away from being a scalar product), but a satisfies

$$\underbrace{\operatorname{Re} a(u,u) + 2\kappa^2 \|n^{\frac{1}{2}}u\|_{L^2(\Omega)}^2 = \|u\|_{\kappa}^2, \quad \forall u \in H^1(\Omega).}_{\text{'Garding's inequality}}$$

due to the compactness of the embedding  $H^1(\Omega) \subseteq L^2(\Omega)$ .

The sesquilinear form a can be cast in the form "coercive + compact perturbation". Hence, the well-posedness of Eq. (2.8) follows from uniqueness by Fredholm's alternative.

To show uniqueness, assume that  $u \in H^1(\Omega)$  satisfies Eq. (2.8) with right-hand side F = 0, i.e.

$$a(u, v) = 0, \quad \forall v \in H^1(\Omega).$$

Choosing v = u yields

$$\operatorname{Im} a(u, u) = \kappa \|u\|_{L^2(\partial\Omega)}^2 = 0,$$

i.e.  $u \in H_0^1(\Omega)$ . Hence we can extend u to whole  $\mathbb{R}^d$ , and the extension

$$\tilde{u}(x) \coloneqq \begin{cases} u(x) & x \in \Omega \\ 0 & \text{elsewhere} \end{cases}$$

is in  $H^1_{loc}(\mathbb{R}^d)$  and satisfies the assumptions of Theorem 1.5 (unique continuation principle). Hence

$$\Delta u + \kappa n u = 0$$
$$u(x) = 0, \quad \forall |x| \ge \beta \ge \alpha$$

implies  $u \equiv 0$ .

This proves that for any  $F \in (H^1(\Omega))'$  there exists a unique solution  $u^s \in H^1(\Omega)$  of Eq. (2.8) and

$$||u^s||_{\kappa} \leq C_{st}(\Omega, n, \kappa) ||F||_{(H^1(\Omega))'},$$

with some generic (st = stability) constant  $C_{st}(\Omega, n, \kappa)$ , that only depends on  $\Omega, n, \kappa$  and especially <u>not</u> on  $F, u^s$ ! For the particular F of Section 2.2, this implies

$$||u^s||_{\kappa} \le C_{st}(\Omega, n, \kappa)||1 - n||_{L^{\infty}(\Omega)}||u^{in}||_{\kappa, \text{supp}(1-n)}$$

(the scattered wave is bounded by the incident wave).

The dependence of  $C_{st}$  on |kappa| is not known in general. Actually, very little is known. With regard to [Bet] an exponential growth w.r. to  $\kappa$  is possible for non generic coefficients n.

If this is the case, then numerical approximation will hardly be reliable (there is no theoretical evidence in our methods), because perturbations caused e.g. by the Galerkin method, or quadrature errors, or numerical linear algebra (precision of arithmetics), etc. may be amplified by  $C_{st}$ . There is really not much that we can do apart from "hoping" that our computations reflect the true solution. In order to analyse the numerical method, we will assume a moderate growth.

#### Assumption 2.2 (Polynomial-in- $\kappa$ stability)

Given  $n \in L^{\infty}(\Omega)$  with  $\operatorname{supp}(1-n) \subseteq B_{\alpha}(0) \subseteq \Omega$ , we assume that there are constants  $C(\Omega, n)$  and  $\beta(\Omega, n)$  such that for all  $k \ge 1$  and  $F \in (H^1(\Omega))'$ , the unique solution  $u^s \in H^1(\Omega)$  of Eq. (2.8) satisfies

$$||u^s||_{\kappa} \underbrace{C(\Omega, n)}_{C_{st}(\Omega, n, k)} k^{\beta(\Omega, n)} ||F||_{(H^1(\Omega))'}.$$

#### Recall that $\Omega$ is convex!

Remark 2.3. For constant n, it is known that Assumption 2.2 is satisfied with  $C(\Omega, n)$  and  $\beta(\Omega, n) = 1$ . However, for the particular F of Section 2.2, this is not relevant, because n = const implies  $u^s = 0$ . For non-constant coefficients, almost no results are available in literature.

See the literature for a broader overview on regularity estimates. LITERATUR FEHLT!!!!!!!!

Assumption 2.2 will allow us to quantify rates of convergence of the Galerkin method as the mesh-size tends to zero. As usual, the accuracy of the methods depends on the

regularity of  $u^s$ . If the right-han side functional of Eq. (2.8) is in  $L^2$ , then the classical regularity theory for  $-\Delta$  shows that  $u^s \in H^2(\Omega)$  and

$$||D^2 u^s||_{L^2(\Omega)} \le C(\Omega) \left( ||\Delta u^s||_{L^2(\Omega)} + ||\frac{\partial u^s}{\partial \nu}||_{H^{\frac{1}{2}}(\partial \Omega)} \right)$$

and we can use that  $\|\Delta u^s = -\kappa^2 u^s + F$  and  $\frac{\partial u^s}{\partial \nu} = i\kappa u^s$ . Therefore we can estimate

$$||D^{2}u^{s}||_{L^{2}(\Omega)} \leq C(\Omega) \left( ||\Delta u^{s}||_{L^{2}(\Omega)} + ||\frac{\partial u^{s}}{\partial \nu}||_{H^{\frac{1}{2}}(\partial \Omega)} \right)$$

$$\leq C(\Omega, n) \left( ||F||_{L^{2}(\Omega)} + \underbrace{k^{2}||u^{s}||_{L^{2}(\Omega)}}_{=\kappa||u^{s}||_{\kappa}} + \kappa ||u^{s}||_{\kappa} \right)$$

$$\leq C(\Omega, n) \left( ||F||_{L^{2}(\Omega)} + \kappa^{\beta(\Omega, n) + 1} \underbrace{||F||_{(H^{1}(\Omega))}}_{\leq c(n)\kappa^{-1}||F||_{L^{2}(\Omega)}} \right)$$

so in the end

$$||D^2 u||_{L^2(\Omega)} \le C(\Omega, n) \kappa^{\beta(\Omega, n)} ||F||_{L^2(\Omega)}.$$
 (2.9)

#### 2.3 Finite element discretization

We study the FE discretization of the model variational problem Eq. (2.8). Recall that  $\Omega$  is assumed to be polyhedral. Let  $\{\mathcal{T}_h\}_{h>0}$  be a family of regular subdivisions of  $\Omega$  into tetrahedra. For the sake of simplicity, we consider only quasi-uniform triagulations and shape-regular families of triangulations, that is there are constants c, C > 0 such that

$$\forall h > 0 \,\forall T \in \mathcal{T}_h: \quad ch^d \le |T| \le Ch^d,$$
 (2.10)

where  $h := \max_{T \in \mathcal{T}_h} \operatorname{diam} T$ .

Remark 2.4. Regular means, that any 2 distinct elements of  $\mathcal{T}_h$  are either disjoint or share exactly one node, or one face.

We consider linear finite elements, i.e. we are seeking an approximation of the unknown scattered wave  $u^s$  in the subspace

$$V_h := \left\{ v_h \in C^0(\Omega) | \forall T \in \mathcal{T}_h : v_h|_T \text{ is affine} \right\} \subseteq H^1(\Omega),$$

of continuous, piecewise affine functions.

The approximate scattered field  $u_h^s \in V_h$  is selected by Galerkin projection: Find  $u_h^s \in V_h$  such that

$$a(u_h^s, v_h) = F(v_h), \quad \forall v_h \in V_h \tag{2.11}$$

Note that the well-posedness of the discrete problem is not guaranteed for a general mesh-size h.

The clear condition

$$h \lesssim \kappa^{-1} \tag{2.12}$$

**is not sufficient!** The well-posedness of the standard FEM requires a stronger condition (resolution condition) of the form

$$h \le \kappa^{-(\beta(\Omega,n)+1)}$$

where  $\beta$  is the exponent from Assumption 2.2. We will decude the (conditional) stability / well-posedness of the method from the following error estimate:

#### Theorem 2.5 (Quasi-optimality of Galerkin FEM)

Let  $\Omega$  and n are chosen s.t. Assumption 2.2 holds true. Furthermore let  $\kappa^{\beta(\Omega,n)+1}h \leq 1$  and sufficiently small. Then there is a constant  $C(\Omega,n)$  such that the solution  $u^s \in H^1(\Omega)$  and its galerkin approximation  $u^s \in V_h$  satisfy

$$||u^s - u_h^s||_{\kappa} \le C(\Omega, n) \min_{v_h \in V_h} ||u^s - v_h||_{\kappa}$$
 (2.13)

PROOF. Define  $e := u^s - u_h^s \in H^1(\Omega)$  and the following auxiliary problem of finding  $z \in H^1(\Omega)$  such that

$$a(z,w) = \underbrace{\kappa^2 \int_{\Omega} n\bar{e}\bar{w} \, dS}_{\in L^2(\Omega)}, \quad \forall w \in H^1(\Omega).$$

As we know from the end of Section 2.2, Eq. (2.9),  $z \in H^2(\Omega)$  and

$$||D^2z||_{L^2(\Omega)} + ||z||_{\kappa} \le C(\Omega, n)\kappa^{\beta(\Omega, n) + 1}||e||_{\kappa},$$

where  $\beta(\Omega, n)$  is the exponent in Assumption 2.2, and  $C(\Omega, n)$  is some generic constant independent of  $\kappa$ . This shows that

$$\kappa^2 \|n^{\frac{1}{2}}e\|_{L^2(\Omega)}^2 = a(z,\bar{e}) = a(e,\bar{z}) \overset{\text{Galerkin property } a(e,\bar{z_h})=0}{=} a(e,\bar{z}-\bar{z_h}).$$

Choosing  $z_h = I_h z$ , the nodal interpolation, then

$$||z - z_h||_{\kappa} \le C(\Omega, n) h \kappa^{\beta(\Omega, n) + 1} ||e||_{\kappa}.$$

In this estimate we are using that  $h\kappa^{\beta(\Omega,h)+1} \leq 1$ . Hence,

$$\kappa^2 \| n^{\frac{1}{2}} e \|_{L^2(\Omega)}^2 \le C(\Omega, n) h \kappa^{\beta(\Omega, n) + 1} \| e \|_{\kappa}^2.$$

Using the Galerkin property once more yields, for any  $v_h \in V_h$ 

$$||e||_{\kappa}^{2} = \operatorname{Re} a(e, e) + 2\kappa^{2} ||n^{\frac{1}{2}}e||_{L^{2}(\Omega)}^{2}$$

$$= \operatorname{Re} a(e, u^{s} - y_{h}^{s} - v_{h}) + 2\kappa^{2} ||n^{\frac{1}{2}}e||_{L^{2}(\Omega)}^{2}$$

$$\leq C(\Omega, n)||e||_{\kappa} ||u^{s} - v_{h}||_{\kappa} + \tilde{C}(\Omega, n)h\kappa^{\beta(\Omega, n) + 1}||e||_{\kappa}^{2}.$$

for sufficiently small h, i.e.  $h \leq \kappa^{\beta(\Omega,n)+1}$ . This proves the assertion.

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Remark 2.6 (Resolution condition and stability). Theorem 2.5 states quasi-optimality and stability of the Finite Element Method, provided

$$h\kappa^{\beta(\Omega,n)+1} \le C(\Omega,n)$$

is sufficiently small. In particular, we have stability in the followiung sense

$$||u_h||_{\kappa} \le C(\Omega, n)||u||_{\kappa} \le C(\Omega, n)\kappa^{\beta(\Omega, n) + 1}||F||_{H^1(\Omega)}.$$

While this resolution condition is rather sharp for quasi-optimality, it can be relaxed if we are merely interested in existence. However, the natural resolution condition

$$\kappa h \le C$$

is by no means sufficient for stability of quasi-optimality. There is even a proof that

$$\frac{\|u - u_h\|_{\kappa}}{\min_{v_h \in V_h} \|u - v_h\|_{\kappa}} \stackrel{\kappa \to \infty}{\to} \infty.$$

This is referred to as the pollution effect.

Reference: Babuska, Sauter, SIAM Rev 2000.

Remark 2.7. Under the resolution condition ?? and  $H^2$  regularity of u, the approximation properties of  $V_h$  show that

$$||u - u_h||_{\kappa} \lesssim h\kappa ||F||_{L^2(\Omega)}.$$

In particular, for F from Section 2.2, we have

$$||u - u_h||_{\kappa} \lesssim h\kappa ||u^{in}||_{\kappa.\mathrm{SUDD}(n)}.$$

### Chapter 3

### Inverse Problems

#### 3.1 Basic concepts and examples

In many mathematical problems, one is interested in determing a solution of some problem Px = f, for given f. This is referred to as the <u>forward</u> or <u>direct problem</u>. The <u>inverse problem</u> is to reconstruct f from given solution x. This "definition" is rather vague. Consider the following examples.

#### Example.

Forward problem (FP): Find the zeros  $(x_1,...,x_n)$  of a given polynomial p of degree n Inverse problem (IP): Determine p with zeros  $(x_1,...,x_n)$ 

 $\overline{\Rightarrow The \ solution \ of \ (IP)}$  is given by  $p(x) = \prod_{i=1}^{n} (x - x_i)$ . Here (IP) is easier than (FP). Example (Lagrange interpolation).

(FP): Evaluate a polynomial p at  $(x_1,...,x_n)$ 

(IP): Find a polynomial p of degree n with prescribed values  $(y_1,...,y_n)$  at  $(x_1,...,x_n)$ .

Example (Inverse scattering).

(FP): Given  $\kappa$ , the refractive index n and a plane wave  $u^{in} = e^{-i\kappa\Theta \cdot x}$ , compute the far field patterns  $\hat{u}_{\infty}$ 

(IP): Given far-field patterns  $\hat{u}_{\infty}(\hat{\Theta})$  for direction(s)  $\hat{\Theta} \in \mathcal{S}^2$ , reconstruct the refractive index n

We have already seen, that  $\hat{u}_{\infty}$  is analytic and, hence, the inverse scattering problem is "ill-posed".

A problem is referred to as well-posed, if it has a unique solution, which depends continuously on the data.

**Definition 3.1 (Well-posedness and ill-posedness).** Let X, Y be normed spaces with a mapping  $K: X \to Y$ . The equation Kx = y is well-posed, if

- 1. For every  $y \in Y$  there exists  $x \in X$  with Kx = y ("existence")
- 2. For every  $y \in Y$  there exists at most one  $x \in X$  with Kx = y ("uniqueness")
- 3. For every sequence  $\{x_n\} \in X^{\mathbb{N}}$  with  $Kx_n \to Kx$  as  $n \to \infty$ , it holds that  $x_n \to x$  as  $n \to \infty$  ("Stability")

If one of the properties does not hold, then the problem is *ill-posed*.

Remark 3.2. The first 2 conditions are algebraic conditions. The last states continuity of  $K^{-1}$  and, therefore, depends on the topologies on X, Y.

#### Example (Hadamard, 1923).

We want to solve  $\Delta u = 0$  in  $\mathbb{R} \times [0, \infty)$ , subject to u(x, 0) = f(x),  $\frac{\partial u}{\partial y}(x, 0) = g(x)$   $(x \in \mathbb{R})$ . Let f = 0 and  $g(x) = \frac{1}{n}\sin(nx)$ . Then the unique solution is

$$u(x,y) = \frac{1}{n^2}\sin(nx)\sinh(ny), \quad (x,y) \in \mathbb{R} \times [0,\infty).$$

*Therefore* 

$$\sup_{x \in \mathbb{R}} \{ |f(x)|, |g(x)| \} = \frac{1}{n} \stackrel{n \to \infty}{\to} 0,$$

but  $\sup_{x\in\mathbb{R}} |u(x,y)| = \frac{1}{h^2}\sin(ny) \to \infty$ , as  $n \to \infty$ . Therefore, this "initial value problem" is ill-posed.

#### Example (Differentiation).

Let X = Y = C([0,1]) with max-norm  $\|\cdot\|_{\infty}$ .

(FP) Given  $x \in X$ , find the antiderivative  $y \in Y$  with y(0) = 0. This is, compute

$$y(t) = \int_0^t x(t) dt, \quad \forall t \in [0, 1].$$

 $\underline{(IP)}$  Given some  $y \in Y$  with y(0) = 0, determine the derivative x = y'. This means: Solve the integral equation Kx = y where

$$(Kx)(t) = \int_0^t x(t) dt, \quad t \in [0, 1].$$

To see, that (IP) is ill-posed, consider a continuous and differentiable  $y \in Y$ , with x = y'. For the perturbation  $\delta$  define

$$\tilde{y}(t) \coloneqq y + \delta \sin\left(\frac{t}{\delta^2}\right).$$

(We would expect that the difference between the derivatives of y and  $\tilde{y}$  is small, for small  $\delta$ )

We have  $||y - \tilde{y}||_{\infty} = \delta$ . But since

$$\tilde{x}(t) = x(t) = \frac{1}{\delta} \cos\left(\frac{t}{\delta^2}\right)$$

solves  $K\tilde{x} = \tilde{y}$ , and

$$||x - \tilde{x}||_{\infty} = \mathcal{O}\left(\frac{1}{\delta}\right),$$

so the problem is ill-posed.

If we now let

$$Y = \{y \in C^1[0,1] : y(0) = 0\} \text{ with } ||y||_{C^1} = ||y'||_{\infty},$$

the problem is well-posed. Indeed

$$||x - \tilde{x}||_{\infty} = ||y'\tilde{y}'||_{C^1}.$$

The previous example shows, that the "worst-case error" for some given tolerance  $\delta$  may be  $\infty$ . Let now

$$z \coloneqq \tilde{y} - y$$

and for simplicity assume that z(0) = 0 = z'(0) and  $tildez \ge 0$ . Then

$$|x(t) - \tilde{x}(t)|^2 = |z'(t)|^2$$

$$= \int_0^2 \frac{d}{ds} (z'(s))^2 ds$$

$$= 2 \int_0^t z'(s) z''(s) ds$$

$$\leq 2||z''||_{\infty} z(t)$$

$$\leq 2||y''\tilde{y}''|| ||\tilde{y} - y||_{\infty}.$$

This means, under additional information

$$\max\{\|y''\|_{\infty}, \|\tilde{y}''\|_{\infty}\} \le E,$$

we have the following bound

$$||x - \tilde{x}||_{\infty} \le 4E||y\tilde{y}||_{\infty}.$$

This leads to the following concept

**Definition 3.3 (Worst-case error).** Let  $K: X \to Y$  be a linear bounded operator between Banach spaces X, Y, and let  $X_1 \subseteq X$  be a subspace of X, with a stronger "stronger" norm  $\|\cdot\|_1$ , i.e.

$$\|\cdot\| \le c\|\cdot\|_1,$$

for some C>0. We define the worst-case error for the error $\delta$  in the data and the a priori information

$$||x||_1 \leq E$$

by

$$\mathcal{F}(\delta, E, \|\cdot\|_1) := \sup \{ \|x\|_X : x \in X_1, \|Kx\| \le \delta, \|x\|_1 \le E \}.$$

In practical examples, K is often compact. This leads typically to ill-posed problems (inversion of compact operators leads to ill-posed problems). In particular we have the following two results

#### Theorem 3.4

Let  $K: X \to Y$  be a linear, bounded, compact operator between Banach spaces X, Y, with the property

$$\dim\left[X_{|_{\ker(K)}}\right]=\infty$$

(quotient space).

Then there exists a sequence  $\{x_n\} \in X^{\mathbb{N}}$  such that  $Kx_n \to 0$ , but  $||x_n|| \to \infty$  as  $n \to \infty$ . In particular, if K is injective, the inverse  $K^{-1} : \operatorname{Im}(K) \to X$  is unbounded.

PROOF. We write  $\mathcal{N} := \ker(K)$ . Since  $\mathcal{N}$  is closed, we can build  $X_{|\mathcal{N}}$ , which is a normed space:

$$||[x]|| \coloneqq \inf_{z \in \mathcal{N}} ||x + z||.$$

The induced operator  $\tilde{K}: X_{|\mathcal{N}} \to Y$ , with  $\tilde{K}([x]) \coloneqq K(x)$   $(x \in X)$ , is injective and compact. Since  $X_{|\mathcal{N}}$  is infinite-dimensional, the identity  $id: X_{|\mathcal{N}} \to X_{|\mathcal{N}}$  cannot be compact. But since  $id = \tilde{K}^{-1}\tilde{K}$  and  $\tilde{K}$  is compact,  $\tilde{K}^{-1}$  cannot be continuous. Otherwise the identity would be compact as composition of continuous and compact operators. Since  $\tilde{K}^{-1}$  is unbounded, there exists a sequence  $\{[z_n]\} \in (X_{|\mathcal{N}})^{\mathbb{N}}$  with  $\|[z_n]\| = 1$  and  $Kz_n \to 0$  as  $n \to \infty$ . By shifting with  $v_n \in \mathcal{N}$  such that  $\|z_n + v_n\| \ge \frac{1}{2}$ , and defining

$$x_n \coloneqq \frac{z_n + v_n}{\sqrt{\|Kz_n\|}},$$

we obtain

$$||Kx_n|| = \frac{||Kz_n||}{\sqrt{||Kz_n||}} \to 0 \quad \text{and} \quad ||x_n|| \to \infty.$$

Recall the worst-case error

$$\mathcal{F}(\delta, E, \|\cdot\|_1) = \sup\{\|x\| : \|Kx\| \le \delta, \|x\|_1 \le E, x \in X_1\}.$$

#### Lemma 3.5

Let  $K: X \to Y$  be linear, compact and continuous, and assume that  $X_{|\ker(K)|}$  to be infinite-dimensional. Then, for every a priori information E > 0 there exists a constant c > 0 and a tolerance  $\delta_0 > 0$  such that

$$\mathcal{F}(E, \delta, \|\cdot\|) \ge c, \quad \forall 0 < \delta \le \delta_0.$$

PROOF. For contradiction assume that there is a sequence  $\{\delta_n\}$ ,  $\delta_n \to 0$ , such that  $\mathcal{F}(E, \delta_n, \|\cdot\|) \to 0$  as  $n \to \infty$ . Consider again

$$\tilde{K}: X_{|\ker K} \to Y$$

and let  $\{x_m\} \subset X^{\mathbb{N}}$  with  $Kx_m \to 0$  as  $m \to \infty$ . Then there exists a subsequence  $\{x_{m_n}\}_n$  with

$$||Kx_{m_n}|| \leq \delta_n, \quad \forall n.$$

Define

$$z_n := \begin{cases} x_{m_n}, & ||x_{m_n}|| \le E \\ E||x_{m_n}||^{-1}x_{m_n}, & ||x_{m_n}|| > E \end{cases}$$

Then  $||z_n|| \leq E$  for all n, and  $||Kz_n|| \leq \delta_n$ . Since the worst-case error converges to zero, also  $||z_n|| \to 0$  has to hold for  $n \to \infty$ . Moreover, by definition we have  $z_n = x_{m_n}$ , if n >> 1 (sufficiently large). (If we are in the second case, the norm is always E. Therefore sooner or later we will get into the first case, as  $||z_n|| \to 0$ ). This procedure cannot only be applied to  $\{x_m\}$ , but also to any subsequence. Hence  $x_m \to 0$  as  $m \to \infty$ . This implies that  $\tilde{K}^{-1}$  is continuous, which contradicts Theorem 3.4.

#### 3.2 Regularizing filters

In this section, we study one (of many possible) regularization strategy. Throughout this section, let  $K: X \to Y$  be linear, bounded, compact operator between Hilbert spaces X, Y and assume that K is injective. We assume that for  $y \in Y$  there is a (unique) solution  $x \in X$  with Kx = y, that is  $y \in \text{Im } K$ . In practice, one has perturbed data  $y^{\delta}$  with

$$||y - y^{\delta}|| \le \delta.$$

We have seen that  $Kx^{\delta} = y^{\delta}$  may not be solvable. The aim is to determine at least some approximation  $x^{\delta} \in X$  such that  $||x - x^{\delta}||$  is comparable to the worst-case error. We seek a bounded approximation

$$R: Y \to X$$
, of  $K^{-1}$ ,  $\mathcal{R}(K) \to X$ .

**Definition 3.6.** A family of linear and bounded operators  $(R_{\alpha})_{\alpha>0}$  such that  $\lim_{\alpha\to 0} R_{\alpha}K(x)\to x$ , for all  $x\in X$ , is called a *regularization strategy*.

Remark 3.7. Definition 3.6 states <u>pointwise</u> convergence towards the identity. It can be shown that uniform convergence cannot be expected in general.

Let now  $y^{\delta} \in Y$  be "measured data" with  $\|y - y^{\delta}\| < \delta$  and define

$$x^{\alpha,\delta} := R_{\alpha} y^{\delta}.$$

Then

$$||x^{\alpha,\delta} - x|| \le ||R_{\alpha}y^{\delta} - R_{\alpha}y|| + ||R_{\alpha}y - x|| \le ||R_{\alpha}|| \underbrace{||y^{\delta} - y||}_{\le \delta} + ||R_{\alpha}y - x||$$

SO

$$||x^{\alpha,\delta} - x|| \le ||R_{\alpha}||\delta + ||R_{\alpha}y - x||.$$
 (3.1)

We expect that  $||R_{\alpha}|| \to \infty$  as  $\alpha \to 0$ . Therefore we need a stratety for minimizing the RHS of Eq. (3.1).

**Definition 3.8.** A regularization strategy  $\alpha = \alpha(\delta)$  is *admissible*, if for  $\delta \to 0$  we have  $\alpha \to 0$  and

$$\sup\{\|R_{\alpha(\delta)}y^{\delta} - x\| : y^{\delta} \in Y \text{ with } \|Kx - y^{\delta}\| < \delta\} \to 0$$

for every  $x \in X$ .

We now briefly recall the *singular value decomposition (SVD)* in Hilbert spaces. Here  $J \subseteq \mathbb{N}$  be an index set (finite or infinite).

Let  $K: X \to Y$  be linear and compact with  $K^*: Y \to X$ . Then  $K^*K: X \to X$  is self-adjoint, compact, and has real nonnegative eigenvalues  $(\lambda_j)_{j \in J}$ . The numbers

$$\mu_j \coloneqq \sqrt{\lambda_j}$$

are called the **singular values** of K. They can be ordered:

$$\mu_1 \ge \mu_2 \ge \dots \ge 0.$$

The SVD states:

#### Theorem 3.9 (Singular-value decomposition)

There exist orthonormal systems  $(x_j)_{j\in J} \in X^J$  and  $\{y_j\}_{j\in J} \in Y^J$  such that

$$Kx_j = \mu_j y_j, \quad \forall j \in J,$$

and  $K^*y_j = \mu_j x_j$ . We call  $(\mu_j, x_j, y_j)_j$  a singular system for K. Every  $x \in X$  has the singular value decomposition

$$x = x_0 + \sum_{j \in J} (x, x_j) x_j$$
, for some  $x_0 \in \ker K$ 

 $((\cdot,\cdot))$  denotes the scalar product), and

$$Kx = \sum_{j \in J} \mu_j(x, x_j) x_j.$$

If kx = y is solvable, then

$$x = \sum_{j \in J} \frac{1}{\mu_j} (y, y_j) x_j.$$

Proof. See Functional Analysis I.

By damping the factors  $\frac{1}{\mu_j}$  we obtain a class of regularization strategies.

#### Theorem 3.10 (Regularizing filter)

Let  $K: X \to Y$  be linear and compact, with singular system  $(x_j, y_j, \mu_j)_{j \in J}$  and let

$$q:(0,\infty)\times(0,\|K\|)\to\mathbb{R}$$

be a function satisfying

- (i)  $q(\alpha, \mu) \le 1$  for all  $(\alpha, \mu) \in (0, \infty) \times (0, ||K||)$
- (ii) For any  $\alpha > 0$  there exists a constant  $c(\alpha) > 0$  such that

$$|q(\alpha, \mu)| \le c(\alpha)\mu, \quad \forall 0 < \mu \le ||K||$$

(iii)  $\lim_{\alpha\to 0} q(\alpha,\mu) \to 1$  pointwise, for every  $0 < \mu \le ||K||$ 

Then  $R_{\alpha}: Y \to X$  defined by

$$R_{\alpha}(y) = \sum_{j \in J} \frac{q(\alpha, \mu_j)}{\mu_j} (y, y_j) x_j$$

for  $y \in Y$  is a regularization strategy with

$$||R_{\alpha}|| \le c(\alpha).$$

The strategy  $\alpha = \alpha(\delta)$  is admissible if  $\alpha(\delta) \to 0$  and  $\delta c(\alpha(\delta)) \to 0$  as  $\delta \to 0$ . If in addition, for some  $c_1 > 0$ , we have

(iv) 
$$|q(\alpha,\mu)| \le c_1 \frac{\sqrt{\alpha}}{\mu}$$
, for all  $\alpha > 0$  and  $0 < \mu \le ||K||$  then

$$||R_{\alpha}Kx - x|| \le c_1 \sqrt{\alpha} ||z||$$

provided  $x \in \mathcal{R}(K^*)$  with  $x = K^*z$ .

## Bibliography

[Bet] Graham Langdon Lindner Betcke, Chandler-Wilde, Condition number estimates, num. meth. pdes.