



Lecture Notes 5

## Helmholtz Equation and High Frequency Approximations

### 1 The Helmholtz equation

The Helmholtz equation,

$$\Delta u(x) + n(x)^2 \omega^2 u(x) = f(x), \quad x \in \mathbb{R}^d, \quad (1)$$

is a time-independent linear partial differential equation. The interpretation of the unknown  $u(x)$  and the parameters  $n(x)$ ,  $\omega$  and  $f(x)$  depends on what the equation models. The most common areas are wave propagation problems and quantum mechanics, in which case  $u(x)$  is the amplitude of a time-harmonic wave and the orbitals for an energy state, respectively. We will now derive (1) for those two cases.

#### 1.1 Derivation from the wave equation

This derivation starts from the scalar wave equation,

$$v_{tt} = c(x)^2 \Delta v + F(t, x), \quad (2)$$

where  $c(x)$  is the local speed of propagation for waves and  $F(t, x)$  is a source that injects waves into the solution. Suppose we look for solutions with a single angular time frequency  $\omega$ , and that the source generates waves of this type,

$$v(t, x) = u(x)e^{-i\omega t}, \quad F(t, x) = g(x)e^{-i\omega t}. \quad (3)$$

Entering this into (2) we obtain

$$-\omega^2 u(x)e^{-i\omega t} = c(x)^2 \Delta u(x)e^{-i\omega t} + g(x)e^{-i\omega t}.$$

Hence, after dividing by  $e^{-i\omega t}$  and reordering the terms,

$$\Delta u(x) + \frac{\omega^2}{c(x)^2} u(x) = -\frac{g(x)}{c(x)^2}.$$

This is the Helmholtz equation (1) with  $f(x) = -g(x)/c(x)^2$  and

$$n(x) = \frac{1}{c(x)},$$

which is the *index of refraction*, defined as the inverse of the speed of propagation. From (3) we see that in this setting the solution  $u(x)$  represents the amplitude of time-harmonic solutions to (2) at frequency  $\omega$ .

**Remark 1** *The solution in (3) will appear if (2) is solved with zero initial condition over infinite time. One can therefore also think of Helmholtz as a steady state version of the wave equation, even though it is of course just the amplitude that is steady, not the oscillating factor  $\exp(-i\omega t)$ , cf. standing waves.*

## 1.2 Derivation from the Schrödinger equation

The Helmholtz equation can also be obtained from the Schrödinger equation for the wave function  $\psi(t, x)$  of a particle in quantum mechanics,

$$ih\psi_t = -\frac{\hbar^2}{2m}\Delta\psi + V(x)\psi, \quad (4)$$

where  $h$  is Planck's constant,  $m$  is the particle mass and  $V(x)$  is the potential. As before we let  $\psi$  have a fixed oscillation in time,

$$\psi(t, x) = \phi(x)e^{-ikt}.$$

Entering this into (4) gives us

$$-k\hbar e^{ikt}\phi(x)e^{-ikt} = -\frac{\hbar^2}{2m}\Delta\phi(x)e^{-ikt} + V(x)\phi(x)e^{-ikt}.$$

Noting that  $kh = E$ , the total energy in the quantum setting, we get after dividing by  $e^{-ikt}$ ,

$$\frac{\hbar^2}{2m}\Delta\phi - V(x)\phi + E\phi = 0. \quad (5)$$

The function  $\phi(x)$  is called a *stationary state* or *orbital* and  $|\phi(x)|^2$  represents the probability distribution of the spatial location for a particle at a fixed energy  $E$ .

In general only certain quantized values of  $E$  are possible for (5) and the problem becomes a PDE eigenvalue problem: find both  $\phi$  and  $E$  such that (5) holds. A discrete set of such pairs typically exists. These are called *bound states*. For large enough  $E$ , however, there is a solution for every  $E$  and the problem becomes the same as for the wave case, with  $\omega^2 = E$  and  $n(x)^2 = 2m(1 - V(x)/E)/\hbar^2$ . Mathematically, this means that the eigenvalue problem has a continuous spectrum.

## 1.3 Canonical solutions

When the index of refraction is constant  $n(x) \equiv n$  a generic solution of (1) is given by the plane wave

$$u(x) = Ae^{i\omega n\hat{k}\cdot x}, \quad |\hat{k}| = 1,$$

where  $A$  is the amplitude and  $\hat{k}$  is the direction of propagation. Note that in the time-dependent setting this is indeed the usual plane wave,

$$v(t, x) = u(x)e^{-i\omega t} = Ae^{i\omega n(\hat{k}\cdot x - ct)}, \quad c = 1/n.$$

Another typical solution is the circular wave, which is the wave emanating from a point source. In three dimensions it is given by

$$u_c(x) = \frac{e^{i\omega n|x|}}{4\pi|x|}, \quad x \in \mathbb{R}^3.$$

This is also the Green function for Helmholtz, since

$$\Delta u_c + \omega^2 n^2 u_c = \delta(x).$$

In 2D and 1D the corresponding Green functions are  $u_c(x) = iH_0(\omega n|x|)/4$  (the first Hankel function) and  $u_c(x) = i\exp(i\omega n|x|)/2\omega n$ , respectively. The decay rate as  $|x| \rightarrow \infty$  of these, and any solution with a localized source, is  $|x|^{-(d-1)/2}$ , where  $d$  is the dimension.

## 2 Properties of Helmholtz

We will here go through some general properties of solutions to (1). Since they are quite different for interior and exterior problems we divide the discussion accordingly.

### 2.1 Interior problems

In interior problems (1) is set in a *bounded domain*  $\Omega \subset \mathbb{R}^d$ ,

$$\Delta u(x) + n(x)^2 \omega^2 u(x) = f(x), \quad x \in \Omega, \quad (6)$$

with boundary conditions such as

$$\begin{aligned} u(x) &= 0, & x \in \partial\Omega, & \quad (\text{Dirichlet}), \\ \frac{\partial u(x)}{\partial n} &= 0, & x \in \partial\Omega, & \quad (\text{Neumann}). \end{aligned}$$



This formulation of the problem is well-posed for almost all values of  $\omega$ .

However, the problem is *ill-posed* for a discrete set of  $\omega$ , which corresponds to the eigenvalues of the operator

$$-\frac{1}{n(x)^2} \Delta,$$

set on  $\Omega$  with the specified boundary conditions. These  $\omega$  correspond physically to resonance modes of  $\Omega$ . The Helmholtz operator  $\Delta + n(x)^2 \omega^2$  is singular and there is either no solution or an infinite set of solutions to (6).

**Example 1** Consider the constant coefficient 1D case,

$$\begin{aligned} u_{xx} + \omega^2 u &= f, & x \in (0, L), \\ u(0) = u(L) &= 0. \end{aligned}$$

We note that the eigenfunctions of  $-\partial_{xx}$  with these boundary conditions are sin-functions. More precisely, the eigenfunctions  $\phi_k$  and eigenvalues  $\lambda_k$  are

$$\phi_k(x) = \sin\left(\frac{k\pi x}{L}\right), \quad \lambda_k = \left(\frac{k\pi}{L}\right)^2, \quad k = 1, 2, \dots$$

Expanding  $u$  and  $f$  in these eigenfunctions,

$$u(x) = \sum_{k=1}^{\infty} u_k \phi_k(x), \quad f(x) = \sum_{k=1}^{\infty} f_k \phi_k(x).$$

and noting that

$$u_{xx} + \omega^2 u = \sum_{k=1}^{\infty} (-\lambda_k + \omega^2) u_k \phi_k(x).$$

we get

$$u_k = \frac{f_k}{\omega^2 - \lambda_k}.$$

This is only well-defined if  $\omega^2 \neq \lambda_k$  for all  $k$  where  $f_k \neq 0$ . We conclude that the problem

- Has a unique solution if  $\omega^2 \neq \lambda_k$  for all  $k$ ,
- Has no solution if  $\omega^2 = \lambda_k$  for some  $k$  and  $f_k \neq 0$ ,
- Has an infinite set of solutions if  $\omega^2 = \lambda_k$  for some  $k$  and  $f_k = 0$ . (Then we can add  $\phi_k(x)$  to any solution and it is still a solution.)

In many cases when (6) models a physical situation with waves inside a bounded domain there is in fact also some damping or absorption in the material which makes the solution well-defined also at the resonant frequencies. Mathematically, it is therefore natural to regularize (6) by adding a damping term,

$$i\omega\alpha u(x) + \Delta u(x) + n(x)^2\omega^2 u(x) = f(x), \quad x \in \Omega, \quad (7)$$

where  $\alpha > 0$  is the damping coefficient. This formulation is well-posed for all  $\omega$ . There are no resonances, since the eigenvalues of  $(i\omega\alpha + \Delta)/n^2$  have an imaginary part.

The effect of the damping term is that waves eventually die off when they travel long distances, and energy is thus dissipating. For instance, the canonical plane wave solution is now

$$u(x) = Ae^{i\tilde{\omega}n\hat{k}\cdot x}e^{-\tilde{\alpha}x/2}, \quad |\hat{k}| = 1,$$

where  $\tilde{\omega} \approx \omega$  and  $\tilde{\alpha} \approx \alpha$  for small  $\alpha$ . (More precisely,  $\tilde{\omega} = \beta\omega$ ,  $\tilde{\alpha} = \alpha/\beta$  and  $\beta^2 = (1 + \sqrt{1 + \alpha^2/\omega^2})/2$ .)

**Remark 2** *The problem with resonances in general becomes worse at higher frequencies.*

*First, for large (non-resonant)  $\omega$  a given  $\Omega$  is geometrically closer to being resonant than for a small  $\omega$ . Consider for example the constant coefficient 1D problem above. If  $\omega$  is non-resonant for the domain size  $L$ , then for some  $k$ ,*

$$\frac{\pi k}{L} = \sqrt{\lambda_k} < \omega < \sqrt{\lambda_{k+1}} = \frac{\pi(k+1)}{L},$$

so that, for some  $r \in (0, 1)$ ,

$$\omega = \frac{\pi(k+r)}{L} = \frac{\pi(k+1)}{L\left(1 + \frac{1-r}{k+r}\right)} = \frac{\pi(k+1)}{L + \delta L}, \quad \delta L = \frac{1-r}{k+r}L.$$

The  $\omega$  will, hence, be resonant for the nearby domain size,  $L + \delta L$ , where

$$\delta L \leq \frac{L}{k} \leq \frac{2L}{k+1} \leq \frac{2\pi}{\omega},$$

showing that for large  $\omega$  a smaller perturbation of  $L$  is sufficient to become resonant.

Second, according to a fundamental theorem on elliptic operators (see e.g. Weyl and Carleman), in higher dimensions the eigenvalues become denser and denser as the size of them increases. More precisely, let  $N(\lambda)$  be the number of eigenvalues (counting multiplicities) smaller than  $\lambda$ . According to the theorem  $N(\lambda) = c\lambda^{d/2} + \text{higher order terms}$ , where  $d$  is the dimension. (In the 1D case above, for instance,  $N(\lambda) \sim L\sqrt{\lambda}/\pi$ .) It follows that the number of resonant frequencies in the range  $(\omega_0, \omega_0 + \Delta\omega)$  is

$$N((\omega_0 + \Delta\omega)^2) - N(\omega_0^2) \sim c((\omega_0 + \Delta\omega)^d - \omega_0^d) \sim \Delta\omega\omega_0^{d-1}.$$

This shows that in two and higher dimensions the resonant frequencies are denser and denser for higher frequencies, making it increasingly likely that a given  $\omega$  is close to a resonant value.

## 2.2 Exterior problems

In exterior problems (1) is set in an *unbounded domain*. The most common example is the *scattering problem* and we will focus on that here. Then the domain of the solution is outside a bounded open set  $\Omega \subset \mathbb{R}^d$ , describing the *scatterer*. The equation is

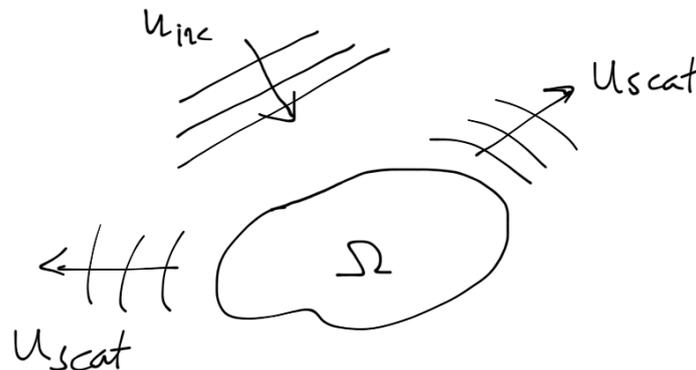
$$\Delta u(x) + \omega^2 u(x) = 0, \quad x \notin \bar{\Omega}, \quad (8)$$

with inhomogeneous boundary conditions on  $\Omega$  of Dirichlet or Neumann type:

$$\begin{aligned} u(x) &= g(x), & x \in \partial\Omega, & \quad (\text{Dirichlet}), & (9) \\ \frac{\partial u(x)}{\partial n} &= h(x), & x \in \partial\Omega, & \quad (\text{Neumann}). \end{aligned}$$

Note that  $n(x)$  is constant in (8). In another version of the scattering problem (8) is set in all of  $\mathbb{R}^d$  but  $n(x)$  is allowed to vary inside a compact set. Also note that there is no source,  $f(x) = 0$ , and the waves are instead generated by the inhomogeneous boundary conditions  $g(x)$  or  $h(x)$ .

**Example 2** In the scattering problem the objective is to find the wave that is scattered off  $\Omega$  from an incident plane wave  $u_{\text{inc}}(x) = e^{i\omega \hat{k} \cdot x}$  coming in from infinity.



We let  $u_{\text{tot}}$  be the sum of the known incident wave  $u_{\text{inc}}$  and the unknown scattered wave  $u_{\text{scat}}$ . The total field  $u_{\text{tot}} = u_{\text{inc}} + u_{\text{scat}}$  satisfies (8) with homogeneous boundary conditions on  $\partial\Omega$ , either Dirichlet with  $g = 0$  or Neumann with  $h = 0$  depending on the physics of the waves considered. Since  $u_{\text{inc}}$  clearly also satisfy (8), so does  $u_{\text{scat}}$  and on the boundary  $u_{\text{inc}}(x) + u_{\text{scat}}(x) = 0$ . Consequently, we have

$$\Delta u_{\text{scat}} + \omega^2 u_{\text{scat}} = 0, \quad x \notin \bar{\Omega}, \quad (10)$$

and one of

$$\begin{aligned} u_{\text{scat}}(x) &= -u_{\text{inc}}(x), & x \in \partial\Omega, & \quad (\text{Dirichlet}), & (11) \\ \frac{\partial u_{\text{scat}}(x)}{\partial n} &= -\frac{\partial u_{\text{inc}}(x)}{\partial n}, & x \in \partial\Omega, & \quad (\text{Neumann}). \end{aligned}$$

The problems (8, 9) and, equivalently, (10, 11) are well-posed if additional boundary conditions are given at infinity, namely

$$\lim_{|x| \rightarrow \infty} |x|^{\frac{d-1}{2}} \left( \frac{\partial u}{\partial r} - i\omega u \right) = 0, \quad (12)$$

where  $\partial/\partial r$  is differentiation in the radial direction and  $d$  is the dimension. This is called the *Sommerfeld radiation condition* or simply the *outgoing condition*. Without this condition the solution is not uniquely determined. The point of (12) is to filter out waves that are propagating inwards from infinity, such as a plane wave or an incoming circular wave,

$$u_c(x) = \frac{e^{-i\omega n|x|}}{4\pi|x|}, \quad x \in \mathbb{R}^3,$$

(note the negative sign in the exponent) which would never satisfy (12). The solutions of (8) with (9) and (12) are thus "outgoing", i.e. they are made up of waves that propagate outwards to infinity.

An alternative way to get uniqueness of the solution is to add damping as in the interior problem, i.e. to replace (8) by

$$i\omega\alpha u(x) + \Delta u(x) + \omega^2 u(x) = 0, \quad x \notin \bar{\Omega}, \quad (13)$$

for some  $\alpha > 0$ . Then (12) is not needed. What is more, if  $u_\alpha(x)$  is the solution of (13) with  $\alpha$ , then one can show that  $u_0(x) = \lim_{\alpha \rightarrow 0^+} u_\alpha(x)$  is the same outgoing solution that one obtains using the Sommerfeld condition. This is called the *limiting absorption principle*, cf. the equivalence between the entropy solution and the vanishing viscosity solution in hyperbolic conservation laws.

### 2.3 Dealing with infinite domains

In the exterior problem the infinite size of the solution domain is a difficulty when approximating the problem numerically. It is of course then not possible, for instance, to discretize the entire domain. There are two common approaches to get around this complication, which we describe briefly below.

#### 1. Rewrite as an integral equation

When the exterior of  $\Omega$  has constant index of refraction, as we have assumed, it is possible to rewrite the PDE (8) as an integral equation which is set on the *boundary* of  $\Omega$ . The infinite domain  $\Omega^c$  is thus replaced by a finite domain  $\partial\Omega$ . We show how this works for the Dirichlet case, with  $g(x) = -u_{\text{inc}}(x)$ .

Let  $G(x)$  be the Green's function for Helmholtz in  $d$  dimensions, e.g.

$$G(x) = \begin{cases} \frac{i}{4} H_0(\omega|x|), & d = 2, \\ \frac{e^{i\omega|x|}}{4\pi|x|}, & d = 3. \end{cases}$$

Then, we can solve the *single layer potential* integral equation

$$\int_{\partial\Omega} G(x-y)\psi(y)dy = -u_{\text{inc}}(x), \quad x \in \partial\Omega, \quad (14)$$

for  $\psi(x)$ ,  $x \in \partial\Omega$ . The scattered solution outside  $\Omega$  is subsequently given by evaluating the integral

$$u(x) = \int_{\partial\Omega} G(x-y)\psi(y)dy, \quad x \in \bar{\Omega}^c.$$

Alternatively, we can solve the *double layer potential* integral equation

$$\frac{1}{2}\psi(x) - \int_{\partial\Omega} \frac{\partial G}{\partial n}(x-y)\psi(y)dy = -u_{\text{inc}}(x), \quad x \in \partial\Omega. \quad (15)$$

In this case the scattered solution outside  $\Omega$  is given by

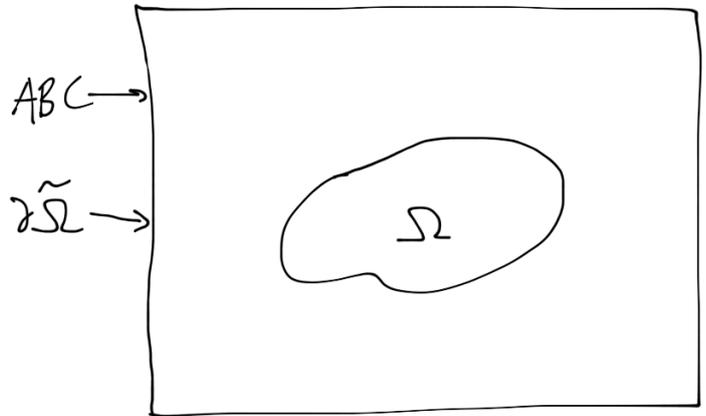
$$u(x) = - \int_{\partial\Omega} \frac{\partial G}{\partial n}(x-y)\psi(y)dy, \quad x \in \bar{\Omega}^c.$$

Upon discretizing the boundary  $\partial\Omega$ , both (14) and (15) lead to full linear systems of equations for an approximation of the potential  $\psi$ .

**Remark 3** *Both the single and double layer formulation have resonances as in the interior case. The equations are not well-posed for certain  $\omega$ . However, by taking a linear combination of the two integral equations one avoids this problem. This is an important technique when solving high frequency scattering problems.*

## 2. Absorbing boundary conditions

In this approach one simply cuts off the infinite domain and add an artificial absorbing boundary condition (ABC) at the new boundary,  $\partial\tilde{\Omega}$ , which models the effect of the rest of the domain. The principle of the ABC is to allow no incoming waves into the domain, and let all outgoing waves leave the domain without any reflections at the artificial boundary. This can be done in many different ways and we will discuss it further in the numerical section below.



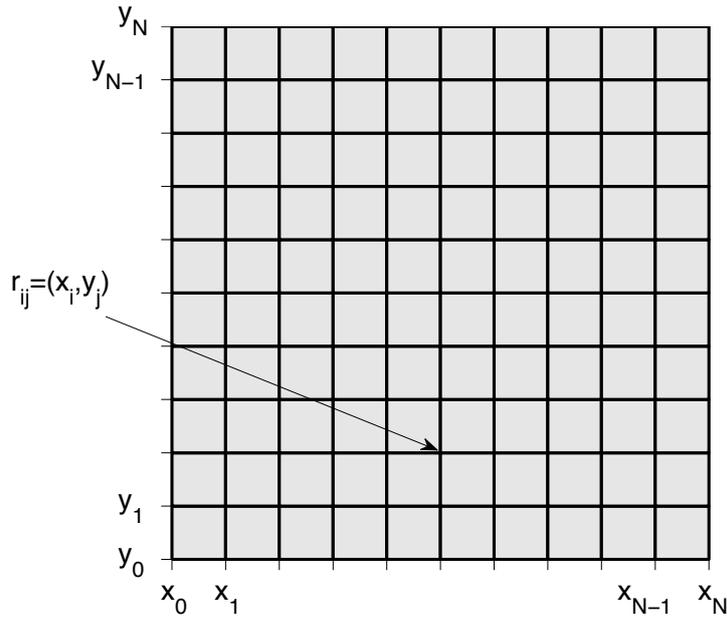
## 3 Numerical methods for Helmholtz

We will here describe the simplest approximation of Helmholtz equation by the finite difference method. To fix ideas we consider the interior problem on the unit square in two dimensions,  $\Omega = [0, 1]^2$ .

### 3.1 Discretization

We discretize the unit square with a uniform grid size. We let  $N$  be the number of grid cells in each coordinate direction and set

$$r_{ij} = (x_i, y_j), \quad x_i = ih, \quad y_j = jh, \quad h = 1/N.$$



We then let  $u_{ij}$  approximate the exact solution in each grid point

$$u_{ij} \approx u(r_{ij}).$$

Note that we now approximate  $u(x)$  *pointwise* in  $r_{ij}$ , not its local average as in finite volume methods. The Laplace operator is approximated by the standard 5-point formula,

$$\Delta u(r_{ij}) \approx \frac{u_{i+1,j} + u_{i-1,j} + u_{i,j+1} + u_{i,j-1} - 4u_{ij}}{h^2}, \quad (16)$$

which is second order accurate. Higher order approximations can be obtained by further Taylor approximation of  $u$ . It leads to wider stencils. The full approximation of (1) for the inner points of  $\Omega$  using (16) is

$$\frac{u_{i+1,j} + u_{i-1,j} + u_{i,j+1} + u_{i,j-1} - 4u_{ij}}{h^2} + n(r_{ij})^2 \omega^2 u_{ij} = f(r_{ij}), \quad r_{ij} \in \Omega, \quad r_{ij} \notin \partial\Omega. \quad (17)$$

Boundary conditions determine the approximation when  $r_{ij} \in \partial\Omega$ . For instance, with the Dirichlet conditions  $u(x) = g(x)$  on  $\partial\Omega$  we simply have

$$u_{0,j} = g(r_{0,j}), \quad u_{N,j} = g(r_{N,j}), \quad u_{i,0} = g(r_{i,0}), \quad u_{i,N} = g(r_{i,N}). \quad (18)$$

Together (17) and (18) lead to a linear system of equations for the unknowns  $u_{ij}$  in the interior of  $\Omega$ , i.e. for  $i, j = 1, \dots, N-1$ ,

$$A\mathbf{u} = \mathbf{b}, \quad \mathbf{u}, \mathbf{b} \in \mathbb{R}^{(N-1)^2}, \quad A \in \mathbb{R}^{(N-1)^2 \times (N-1)^2}, \quad (19)$$

where  $\mathbf{u}$  contains all the  $\{u_{ij}\}$  and  $\mathbf{b}$  contains the source values  $\{f(r_{ij})\}$  and the boundary conditions  $\{g(r_{ij})\}$ .

**Remark 4** *In general the solution  $u$  will be complex because of complex valued source or boundary conditions. Hence,*

$$A\mathbf{u} = \mathbf{b}, \quad \mathbf{u}, \mathbf{b} \in \mathbb{C}^{(N-1)^2}, \quad A \in \mathbb{C}^{(N-1)^2 \times (N-1)^2}.$$

### 3.2 Errors

The errors in standard discretizations of Helmholtz are dominated by dispersion errors rather than dissipative errors. This means that waves in a numerical solution travel at a slightly wrong speed.

To understand how this error depends on the grid size  $h$  and the frequency  $\omega$  we consider the simplest possible case: 1D constant coefficients and the standard second order discretization, i.e.

$$u_{xx} + n^2\omega^2u = 0 \quad \text{and} \quad \frac{u_{j+1} - 2u_j + u_{j-1}}{h^2} + n^2\omega^2u_j = 0,$$

where  $u_j \approx u(x_j)$  and  $x_j = jh$ . In the continuous equation an exact solution is the plane wave

$$u(x) = e^{i\omega nx}.$$

The speed of propagation for this wave is  $c = 1/n$ , for all  $\omega$ . We shall now show that the discrete equation has a similar solution, namely

$$u_j = e^{i\omega\tilde{n}x_j}, \tag{20}$$

for a perturbed  $\tilde{n} = n + O((h\omega)^2)$ , which corresponds to a perturbed speed of propagation  $\tilde{c} = 1/\tilde{n} = c + O((h\omega)^2)$ . Indeed, since with (20)

$$u_{j+1} - 2u_j + u_{j-1} = e^{i\omega\tilde{n}x_j} \left( e^{i\omega\tilde{n}h} - 2 + e^{-i\omega\tilde{n}h} \right) = 2 [\cos(\omega\tilde{n}h) - 1] e^{i\omega\tilde{n}x_j},$$

we see that (20) solves the discrete equation if  $\tilde{n}$  is a solution to

$$2 \frac{\cos(\omega\tilde{n}h) - 1}{h^2} + n^2\omega^2 = 0.$$

Taylor expanding  $\cos(x) = 1 - x^2/2 + O(x^4)$  for small  $x$  we obtain

$$-(\omega\tilde{n})^2 + O(h^2\omega^4) + n^2\omega^2 = 0,$$

which, after division by  $\omega^2$ , shows that

$$\tilde{n}^2 = n^2 + O(h^2\omega^2) \quad \Rightarrow \quad \tilde{n} = n + O(h^2\omega^2) \quad \Rightarrow \quad \tilde{c} = 1/\tilde{n} = c + O(h^2\omega^2).$$

Hence, the numerical speed of propagation  $\tilde{c}$  differ from the exact speed of propagation  $c$  by an error of size  $O((h\omega)^2)$ . The total error in this second order approximation of a plane wave is then

$$\text{error} = |e^{i\omega nx_j} - e^{i\omega\tilde{n}x_j}| = \left| 1 - e^{i\omega(\tilde{n}-n)x_j} \right| \leq C\omega|\tilde{n} - n| \leq Ch^2\omega^3.$$

This error is often interpreted as follows. The error when the wave travels one wave length (period) is the error in the speed =  $O((h\omega)^2)$ . The total error is the error for one wave length multiplied by the total number of wave lengths the wave travels inside the domain. Since the wave length is given by  $\lambda = 2\pi/(n\omega)$  this number is proportional to  $\omega$ . Hence, the total error is of order  $O(h^2\omega^3)$ . This extra factor of  $\omega$  is called the "pollution error".

The result above for the one-dimensional constant coefficient case is very typical for numerical approximations of Helmholtz. In general, for a  $p$ -th order method we have the error

$$\text{error} \sim h^p\omega^{p+1}. \tag{21}$$

The same form of the error is also true for the time-dependent wave equation (for a semi-discretization) and higher dimensions.

**Remark 5** In higher dimensions the error  $\tilde{n} - n$  also depends on the direction  $\hat{k}$  of the plane wave. This means that the numerical speed of propagation is slightly anisotropic, i.e. different in different directions, and numerical solutions depend on the orientation of the grid.

The implication of (21) on the choice of grid sizes can be understood as follows. We note first that

$$h\omega = \frac{2\pi h}{n\lambda} = \frac{2\pi}{nM},$$

where

$$M = \frac{\lambda}{h} = \frac{\#\text{grid points}}{\text{wave length}}.$$

The total error therefore scales as

$$\text{error} \sim h^p \omega^{p+1} \sim M^{-p} \omega.$$

Hence, to get an accurate solution we need to take a sizable number of grid points per wave length  $M$ . Moreover, to maintain a constant small error as the frequency  $\omega$  grows, we would need to increase  $M$  as

$$M \sim \omega^{1/p}.$$

**Remark 6** Conventional wisdom dictates that 10-20 grid points per wave length is needed for a second order method at moderate frequencies.

### 3.3 Computational costs

To obtain the approximate solution of Helmholtz one needs to solve the linear system (19). In  $d$  dimensions we have

$$A\mathbf{u} = \mathbf{b}, \quad \mathbf{u}, \mathbf{b} \in \mathbb{C}^{(N-1)^d}, \quad A \in \mathbb{C}^{(N-1)^d \times (N-1)^d}.$$

The computational cost of such problems depend on the structure and properties of the system matrix  $A$ . For Helmholtz we have

- $A$  is symmetric but indefinite — it has both positive and negative eigenvalues
- $A$  can be arbitrarily ill-conditioned for interior problems, when  $\omega$  is close to a resonance
- $A$  is sparse: there are  $O(1)$  elements per row, hence  $O(N^d)$  elements in total,
- $A$ 's bandwidth is of size  $O(N^{d-1})$ , but with appropriate reordering it can be reduced to  $O(N^{d-3/2})$  for  $d \geq 2$ .

Recall that the computational cost for a direct solution by gaussian elimination of a banded system is  $O(\text{bandwidth}^2 \times \text{size})$ . Here we therefore get

$$\text{Direct solver cost} : O(N^{2d-3} \times N^d) = O(N^{3d-3}),$$

for  $d \geq 2$ . On the other hand, the cost of an iterative solver is  $O(\#\text{iterations} \times \#\text{elements in matrix})$ . The number of iterations needed can depend strongly on problem type and method, but we can safely assume it is at least  $N$ . Then

$$\text{Iterative solver cost} : O(N \times N^d) = O(N^{d+1}).$$

This analysis explains why direct solvers are usually used for 1D and 2D problems. (Although we have the same formal complexity in 2D, direct methods are usually faster and more robust.) In 3D, however, iterative methods are preferred (direct solver  $O(N^6)$ , iterative  $O(N^4)$ ).

**Remark 7** Getting the number of iterations needed to be  $O(N)$  is not easy. Standard fast methods (like multigrid) and preconditioners (like incomplete LU) fail to give fast convergence for discretizations of Helmholtz equation, in particular for the high frequency case when  $N$  increases, while  $M \sim N/\omega$  is held constant. Finding good preconditioners for Helmholtz is an active research area.<sup>1</sup>

**Remark 8** As we saw in the previous section we need to take  $N \sim \omega M \sim \omega^{1+1/p}$  to get an accurate solution when  $\omega$  grows. Since the computational cost is always greater than  $O(N^d)$  (the number of unknowns) the cost in terms of frequency grows at least as

$$\text{Cost} \sim O(\omega^d).$$

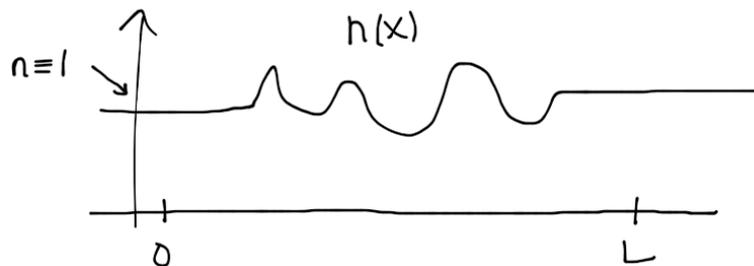
This shows why high frequency problems are very computationally expensive.

### 3.4 Absorbing boundary conditions

As discussed above, absorbing boundary conditions (ABCs) are used when the computational domain is infinite or too large to discretize numerically. The domain is cut down to a manageable size and an artificial boundary  $\partial\tilde{\Omega}$  is introduced. The ABCs are applied at this boundary. The goal is that the reduced problem should have the same solutions as the solutions of the full problem (restricted to the smaller domain). In wave problems, this means that all outgoing waves should be allowed to pass the artificial boundary unaffected, in particular without being reflected, and no waves should be allowed to enter the domain from the outside.

#### 3.4.1 One dimension

We consider the one dimensional case and derive exact absorbing boundary conditions. Let  $n(x)$  be constant one outside the domain  $(0, L)$  and varying in a compact subset of  $(0, L)$ .



Also suppose  $f(x)$  is compactly supported in  $(0, L)$ . We want to solve Helmholtz in this bounded interval

$$u_{xx} + n(x)^2 \omega^2 u = f(x), \quad x \in (0, L), \quad (22)$$

and to construct ABCs at  $x = 0$  and  $x = L$ . In a neighborhood of  $x = 0$  the index of refraction is constant one and  $f(x)$  is identically zero so  $u(x)$  solves

$$u_{xx} + \omega^2 u = 0, \quad x \approx 0.$$

Therefore,

$$u(x \approx 0) = \underbrace{c_0 e^{-i\omega x}}_{\text{leftgoing}} + \underbrace{c_1 e^{i\omega x}}_{\text{rightgoing}} \quad (23)$$

<sup>1</sup>See e.g. O. Ernst and M. Gander, *Why it is difficult to solve Helmholtz problems with classical iterative methods*. In I. Graham, T. Hou, O. Lakkis, and R. Scheichl, editors, Numerical Analysis of Multiscale Problems, LNCSE volume 83, page 325–361. Springer-Verlag, Berlin Heidelberg, 2011.

for some constants  $c_0$  and  $c_1$ , i.e. a linear combination of the fundamental solutions of the ODE. We want the ABC to accept any value of  $c_0$  but disallow a non-zero  $c_1$ . We note that

$$u_x + i\omega u = -c_0 i\omega e^{-i\omega x} + c_1 i\omega e^{i\omega x} + c_0 i\omega e^{-i\omega x} + c_1 i\omega e^{i\omega x} = 2c_1 i\omega e^{i\omega x}. \quad (24)$$

Applying this at  $x = 0$  and setting  $c_1 = 0$  we get

$$\boxed{u_x + i\omega u = 0, \quad x = 0.} \quad (25)$$

Similarly, at  $x = L$  the boundary condition should force  $c_0 = 0$  and accept any  $c_1$ . We get as above

$$u_x - i\omega u = -2c_0 i\omega e^{i\omega x}.$$

Therefore, the boundary condition is

$$\boxed{u_x - i\omega u = 0, \quad x = L.} \quad (26)$$

We stress that (25, 26) are exact in the sense that we would get the same solution in  $(0, L)$  if (22) was solved over all of  $\mathbb{R}$  without (25, 26).

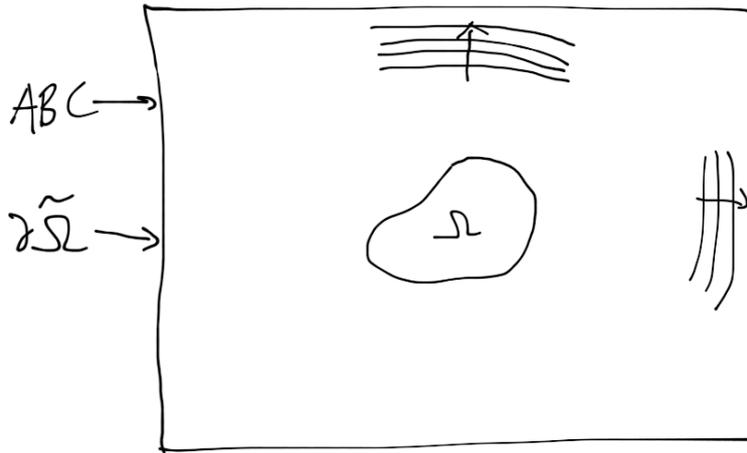
**Remark 9** *In (22) waves were generated by the source  $f(x)$ . Instead one often wants to solve the problem where there is an incoming wave from infinity rather than a source, for instance in the scattering problem. The boundary condition should then both model this incoming wave and act as an absorbing boundary condition, while  $f(x)$  is set to zero. The result is an inhomogeneous version of the ABC. For instance, from (24) we see that if the incoming wave has amplitude  $A_{\text{in}}$ , instead of setting  $c_1$  to zero, we should set it to  $A_{\text{in}}$ . Applying (24) at  $x = 0$  then gives the inhomogeneous boundary condition*

$$\boxed{u_x + i\omega u = 2i\omega A_{\text{in}}, \quad x = 0.} \quad (27)$$

### 3.4.2 Two dimensions

In higher dimensions there is no simple form like (23) for the solution close to the artificial boundary, even if the index of refraction is constant. In general, there will be waves propagating in every direction at each boundary point. An *exact* absorbing boundary condition, of the type we derived in one dimension must therefore necessarily be nonlocal, e.g. expressed via an integral over the boundary, cf. the integral equation formulation. Applying such nonlocal conditions numerically is expensive. Instead, one uses various approximate ABC which are local. Since they are not exact, they will in general cause, small, artificially reflected waves when a wave hits the artificial boundary.

One common approach is to assume that the solution of the full problem, close to the artificial boundary, can be approximated by a plane wave that propagates in a direction normal to the boundary. Then the same argument as in one dimension can be used.



Indeed if

$$u(x) \approx C e^{i\omega \hat{n} \cdot x},$$

where  $\hat{n}$  is the normal of the boundary, then

$$\frac{\partial u}{\partial n} - i\omega u \approx i\omega C e^{i\omega \hat{n} \cdot x} \frac{\partial(\hat{n} \cdot x)}{\partial n} - i\omega C e^{i\omega \hat{n} \cdot x} = 0.$$

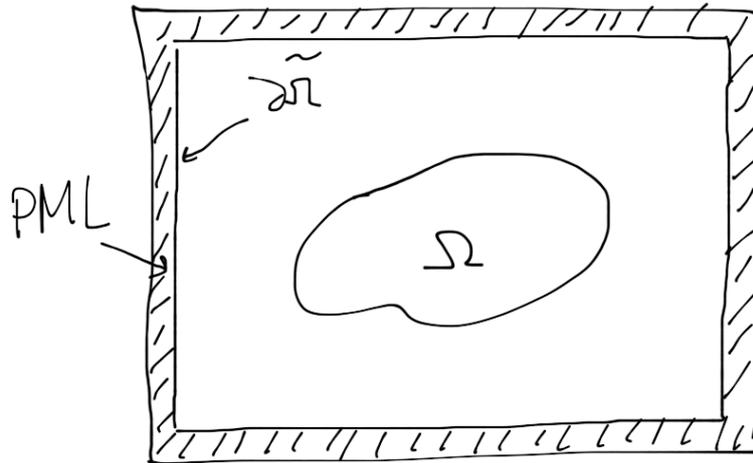
This motivates the simplest ABC in two dimensions:

$$\boxed{\frac{\partial u}{\partial n} - i\omega u = 0, \quad x \in \partial\tilde{\Omega}.} \quad (28)$$

**Remark 10** A wave generated by a localized source function, or from inhomogeneous boundary conditions on a bounded scatterer, will propagate outwards from the source/scatterer and eventually, as the distance increases, it will assume the form of a circular wave coming from an (anisotropic) point source. A circular wave with a large radius looks locally like a plane wave propagating in the radial direction. Hence, at a distance from the source/scatterer an ABC of the type (28) on a circular artificial boundary  $\partial\tilde{\Omega} = \{|x| = \text{constant}\}$  will be very accurate. For this choice of  $\partial\tilde{\Omega}$ , using (28) can also be thought of as applying the Sommerfeld radiation condition (12) at a finite distance from the center, instead of at infinity. In fact, another way to interpret the Sommerfeld radiation condition is as an ABC at infinity, just that as  $x \rightarrow \infty$  the wave itself decays as  $1/|x|^{(d-1)/2}$ , and the quantity in the left hand side of (28) must be appropriately scaled when  $|x|$  becomes large.

**Remark 11** When a plane wave hits the boundary at an oblique angle, with direction  $\hat{k} \neq \hat{n}$  the ABC (28) will give an error (an artificially reflected wave) whose size is proportional to the difference  $|\hat{k} - \hat{n}|$  for small deviations. It is thus a first order method in the difference. It is possible to also derive higher order ABCs in this difference, which produce much smaller artificial reflections.

Perfectly matched layers (PML) is another popular type of ABC for 2D and 3D problems. In this approach a thin layer is added around the artificial boundary  $\partial\tilde{\Omega}$ . Inside the layer the PDE is altered such that 1) waves are damped rapidly and 2) no reflections are introduced at  $\partial\tilde{\Omega}$ . At the outer end of the layer any boundary condition can be used, for instant homogeneous Dirichlet  $u = 0$ . The change in the PDE must be done carefully so that the effective material felt by the waves is matched at  $\partial\tilde{\Omega}$ ; otherwise artificial reflections are introduced.



A typical example is as follows. Let the reduced domain be the square in two dimensions  $\tilde{\Omega} = [-1, 1]^2$  and let  $n(x) \equiv 1$ . Suppose the support of  $f(x)$  is inside  $\tilde{\Omega}$ . One then solves the modified PDE

$$\frac{\partial S(y)}{\partial x} \frac{\partial}{\partial x} u + \frac{\partial S(x)}{\partial y} \frac{\partial}{\partial y} u + \omega^2 S(x)S(y)u = f(x, y), \quad (29)$$

where

$$S(x) = 1 + \frac{\sigma(x)}{i\omega}, \quad \sigma(x) = \begin{cases} 0, & |x| \leq 1, \\ (|x| - 1)^2, & |x| > 1. \end{cases}$$

On the outer boundary one can use Dirichlet conditions,

$$u(1 + \delta, y) = u(1 - \delta, y) = u(x, 1 + \delta) = u(x, 1 - \delta) = 0,$$

where  $\delta$  is the thickness of the PML. Note that inside  $\tilde{\Omega}$  the parameter  $\sigma$  is identically equal to zero, so that (29) reduces to just Helmholtz equation with  $n \equiv 1$ .

#### 4 High frequency Helmholtz equation

As noted above, methods based on a direct discretization of the Helmholtz equation become very expensive when the frequency  $\omega$  is large. The cost grows at least as  $O(\omega^d)$  in  $d$  dimensions. In this section we will discuss how one can approximate such high frequency solutions in other ways.

We start by looking at the plane and circular wave solution in 3D with constant coefficients  $n(x) \equiv 1$  as introduced in Section 1.3,

$$u_{\text{plane}}(x) = Ae^{i\omega \hat{k} \cdot x}, \quad u_{\text{circ}}(x) = \frac{A}{4\pi|x|} e^{i\omega|x|}.$$

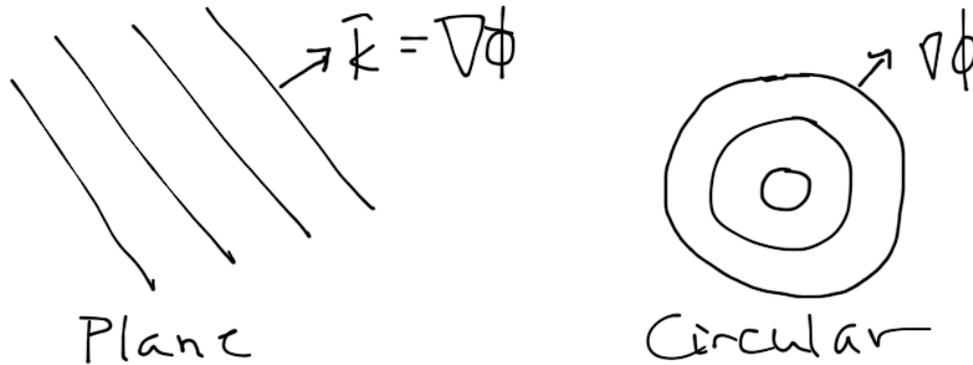
Both these solutions are of the form of a *simple wave*,

$$u(x) = A(x)e^{i\omega\phi(x)}, \quad (30)$$

where  $A(x)$  is the *amplitude* function and  $\phi(x)$  is the *phase* function. For the plane and circular wave,

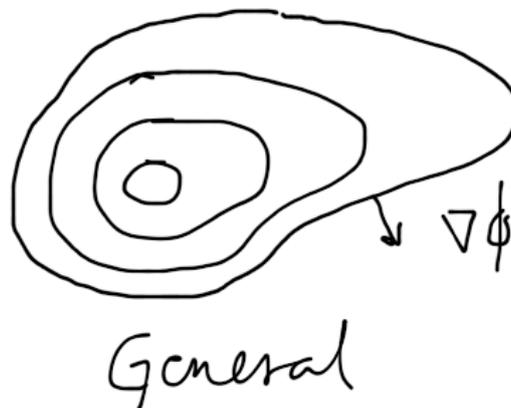
$$A_{\text{plane}}(x) = A, \quad A_{\text{circ}}(x) = \frac{A}{4\pi|x|}, \quad \phi_{\text{plane}}(x) = \hat{k} \cdot x, \quad \phi_{\text{circ}}(x) = |x|.$$

The contour lines of  $\phi(x)$  for these two cases look like this:



One often interprets these constant phase lines as *wave fronts* of a propagating wave. The gradient  $\nabla\phi(x)$  is then orthogonal to the wave fronts and represents the *direction* of the wave. For instance,  $\nabla\phi_{\text{plane}}(x) = \hat{k}$  and  $\nabla\phi_{\text{circ}}(x) = x/|x|$ , as expected.

An important observation here is that the expressions for the solutions above are valid for all  $\omega$ , in particular also when  $\omega \rightarrow \infty$  (given that the same boundary data/source data is used). Hence, the amplitude and phase functions remain smooth and non-oscillatory as  $\omega \rightarrow \infty$ , even though  $u(x)$  becomes increasingly oscillatory. The only place  $\omega$  appears in the solution is where it multiplies  $\phi(x)$  in the exponential. For high frequencies this is approximately true also in much more general situations. Even for variable  $n(x)$  and other types of sources (30) is a good ansatz for solutions. The amplitude  $A(x)$  will then depend mildly on  $\omega$ , but less and less as  $\omega \rightarrow \infty$ . Of course,  $\phi(x)$  and  $A(x)$  will be more complicated functions in general. The interpretation of the contour lines of  $\phi$  as wave fronts are still valid though.



The idea in high frequency methods is to compute the amplitude  $A(x)$  and the phase  $\phi(x)$  numerically, instead of the full solution  $u(x)$ . Since  $A$  and  $\phi$  do not oscillate, and do not change much with  $\omega$ , the number of grid points needed to approximate them accurately is virtually independent of  $\omega$  as  $\omega \rightarrow \infty$ . At high frequencies the numerical computations are therefore much less expensive than in direct methods where  $u(x)$  is approximated.

**Remark 12** *There are of course many situations where (30) is not sufficient to describe the solution. It only describes one wave. In general there are many crossing waves, all depending on boundary conditions and sources. In general a sum of simple waves, each with different amplitude*

and phase, describes the solution better

$$u(x) = \sum_j A_j(x) e^{i\omega\phi_j(x)}. \quad (31)$$

This description essentially only breaks down at a small set of points, where waves focus. In these notes, however, we concentrate on how to compute one of the waves.

#### 4.1 Eikonal and transport equations

In this section we derive PDEs for the amplitude  $A(x)$  and phase  $\phi(x)$  in the limit as  $\omega \rightarrow \infty$ . Upon entering (30) into the Helmholtz equation (1) with  $f = 0$  we obtain

$$\begin{aligned} 0 &= \Delta(Ae^{i\omega\phi}) + n^2\omega^2 Ae^{i\omega\phi} \\ &= [(A(n(x)^2 - |\nabla\phi|^2)\omega^2 + (2\nabla A \cdot \nabla\phi + A\Delta\phi)i\omega + \Delta A)] e^{i\omega\phi}. \end{aligned}$$

When  $\omega \gg 1$  the first two terms must vanish. This gives the two PDEs for  $\phi$  and  $A$ , the eikonal and transport equations

$$|\nabla\phi| = n(x), \quad \text{"eikonal equation"} \quad (32)$$

$$2\nabla A \cdot \nabla\phi + A\Delta\phi = 0, \quad \text{"transport equation"}. \quad (33)$$

If (32) and (33) hold for  $\phi$  and  $A$  one can show that the exact solution  $u(x)$  is well approximated by (30) at high frequencies,

$$u(x) = A(x)e^{i\omega\phi(x)} + O(1/\omega).$$

The eikonal equation is a nonlinear time-independent PDE which belongs to a class of PDEs called Hamilton–Jacobi equations. The transport equation, on the other hand, is a linear equation with variable coefficients given by  $\phi(x)$ . Both equations are hyperbolic.

We note that solving the pair (32) and (33) does not involve  $\omega$  at all. The cost of computing  $A(x)e^{i\omega\phi} \approx u(x)$  is therefore independent of  $\omega$  and for sufficiently large  $\omega$  it is a more efficient approach than a direct solver. This is also the regime where it is accurate; the error is proportional to  $1/\omega$ .

**Example 3** For constant coefficients  $n(x) = 1$  we saw that the phase of a circular wave was  $\phi(x) = |x|$ . This solves the eikonal equation since

$$|\nabla|x|| = \left| \frac{x}{|x|} \right| = 1 = n(x).$$

##### 4.1.1 Boundary conditions for $\phi(x)$

For high frequency wave problems it is natural to prescribe a *wave front*  $\Gamma$  of the simple wave in (30). This will then be a boundary of the problem. Since  $\phi(x) = \text{constant}$  defines wave fronts, we set

$$\phi(x) = 0, \quad x \in \Gamma.$$

For example, if we want to find a solution where a plane wave comes in from infinity we would use a linear  $\Gamma$ , corresponding to one fixed wave front of the plane wave. If the wave propagates in the direction of the  $x$ -axis this would be  $\Gamma = \{(x, y) : x = 0\}$  and the boundary condition would be

$$\phi(0, y) = 0.$$

If we are looking for a wave emanating from a point source, then  $\Gamma$  is just a point. If the source is in the origin we would use

$$\phi(0, 0) = 0.$$

Note that in infinite domain problems there is no need for complicated ABCs as for Helmholtz, since the characteristics of the eikonal equation would be outgoing, meaning that no boundary condition should be prescribed at the artificial boundary.

## 4.2 Rays

One way to solve the eikonal equation (32) is with the method of characteristics. The characteristics<sup>2</sup> for the eikonal equation are given by the ODEs

$$\frac{dx(t)}{dt} = \frac{1}{n(x(t))^2} p(t), \quad (34)$$

$$\frac{dp(t)}{dt} = \frac{\nabla n(x(t))}{n(x(t))}. \quad (35)$$

Here  $x, p \in \mathbb{R}^d$  in  $d$  dimensions. The curve  $x(t) \subset \mathbb{R}^d$  is called a *ray* as it corresponds to a ray of light when Helmholtz models the high frequency Maxwell equations (electromagnetic waves). The vector  $p(t)$  is called the *slowness*. It has length  $1/c(x) = n(x)$  (see below) and points in the direction of the ray — it is parallel to  $dx/dt$  by (34). The rays originate from the initial wave front  $\Gamma$ , and start in a direction orthogonal to it, giving the initial data

$$x(0) \in \Gamma, \quad p(0) \perp \Gamma, \quad |p(0)| = n(x(0)).$$

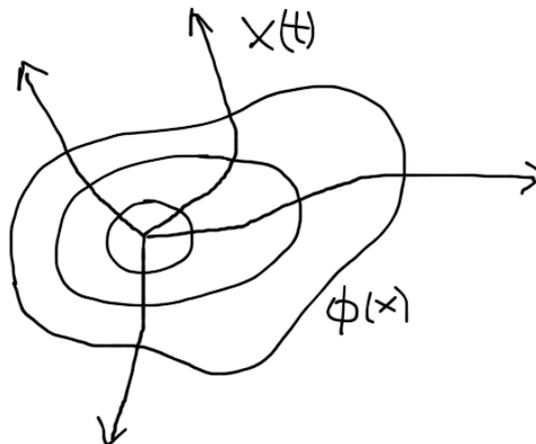
The most important property of the rays are that

$$\phi(x(t)) = t \quad \text{if } \phi(x) = 0 \text{ on } \Gamma. \quad (36)$$

Hence, by solving the ray equations (34) and (35) one obtains the value of  $\phi$  along the ray. Another property is that

$$p(t) = \nabla \phi(x(t)). \quad (37)$$

Since  $p$  points in the direction of the ray, this shows that the rays are always orthogonal to the iso-phase lines, i.e. to the wave fronts.



<sup>2</sup>In the context of Hamilton–Jacobi equations like the eikonal equation they are actually called bi-characteristics.

Moreover, together (32) and (37) show that  $|p(t)| = n(x(t))$  and then by (34),

$$\left| \frac{dx}{dt} \right| = \frac{1}{n(x)^2} |p| = \frac{1}{n(x)} = c(x),$$

which shows that the speed of the ray is precisely the speed of propagation of the waves.

Let us now derive (36) and (37). By taking the gradient of the eikonal equation (32) we get

$$\nabla|\nabla\phi| = \nabla n(x) \quad \Rightarrow \quad D^2\phi \frac{\nabla\phi}{|\nabla\phi|} \quad \Rightarrow \quad D^2\phi \frac{\nabla\phi}{n(x)} = \nabla n(x).$$

Then, upon also using (34) and (35),

$$\frac{d}{dt}(\nabla\phi(x(t)) - p(t)) = D^2\phi \frac{dx}{dt} - \frac{\nabla n}{n} = D^2\phi \frac{p}{n^2} - \frac{D^2\phi \nabla\phi}{n^2} = -\frac{D^2\phi}{n^2}(\nabla\phi(x(t)) - p(t)).$$

Since  $p(t) = \nabla\phi(x(t))$  is true at  $t = 0$  it follows that it is true for all  $t > 0$  by the uniqueness of solutions to ODEs. This shows (37). Finally, (36) holds since

$$\frac{d\phi(x(t))}{dt} = \nabla\phi(x(t)) \cdot \frac{dx(t)}{dt} = \frac{1}{n(x(t))^2} p(t) \cdot p(t) = \frac{|p(t)|^2}{n(x(t))^2} = 1.$$

### 4.3 Alternative interpretation of $\phi$

Suppose  $\phi$  solves the eikonal equation

$$|\nabla\phi| = \frac{1}{c(x)}, \quad \phi(x) = 0, \quad x \in \Gamma. \quad (38)$$

As we have seen,  $\phi$  can then be interpreted as the phase of a high frequency wave with initial wave front  $\Gamma$ . Another interpretation is as follows:

$\phi(x)$  is the shortest travel time to the boundary  $\Gamma$  from  $x$  if the local speed is  $c(x)$ .

The rays in (34) and (35) correspond to the optimal paths to  $\Gamma$  which have the shortest travel time. With this interpretation there are many other applications for the eikonal equation in areas like path planning, visibility detection, optimal control, shape from shading and general front propagation.

To understand this interpretation suppose  $\phi(x)$  is smooth at  $x$ . Moreover assume  $x(s)$  is an optimal path from  $\Gamma$  and  $s$  is the arc length parameterization. Then since the local speed is  $c(x)$ ,

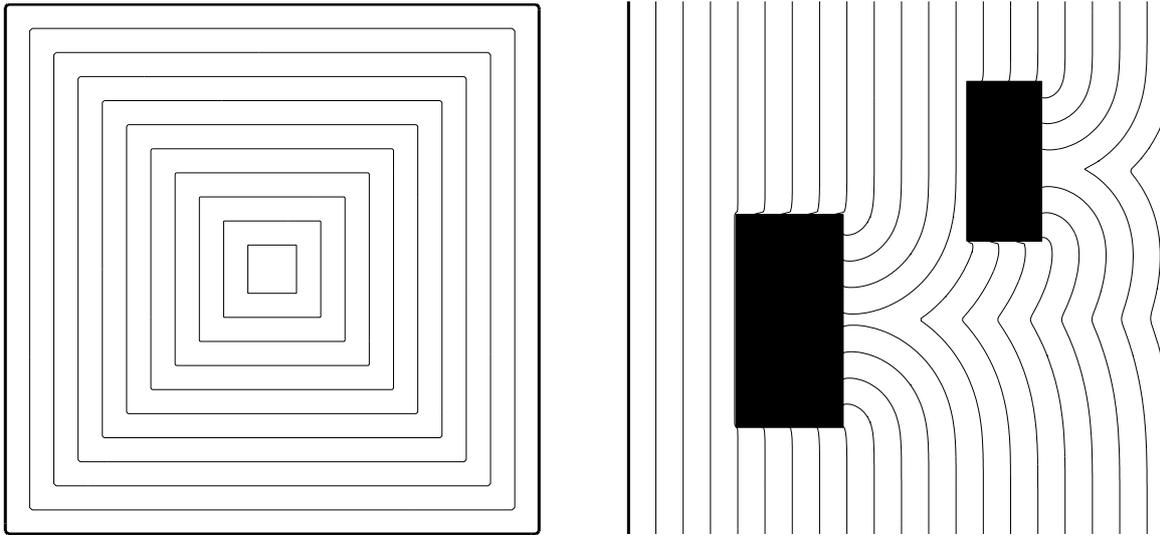
$$\frac{1}{c(x(s))} = \frac{d}{ds}\phi(x(s)) = \nabla\phi(x(s)) \cdot \frac{dx}{ds} = |\nabla\phi(x(s))| \cos(\theta),$$

for some angle  $\theta$ . Hence,

$$|\nabla\phi(x)| \geq \frac{1}{c(x)}. \quad (39)$$

On the other hand, if  $\phi(x)$  is the shortest travel time from  $x$  then the shortest travel time from  $x + \Delta x$  is at most  $\phi(x)$  plus the time to travel along a straight line between  $x$  and  $x + \Delta x$ ,

$$\phi(x + \Delta x) \leq \phi(x) + |\Delta x| \int_0^1 \frac{1}{c(x + s\Delta x)} ds = \phi(x) + \frac{|\Delta x|}{c(x)} + O(|\Delta x|^2).$$



**Figure 1.** Two examples of solutions to the eikonal equation: a square and two obstacles. Isolines of  $\phi(x)$  plotted; bold line indicates  $\Gamma$ .

This holds for all  $\Delta x = \varepsilon \hat{s}$  where  $|\hat{s}| = 1$ . Hence,

$$\sup_{|\hat{s}|=1} \frac{\phi(x + \varepsilon \hat{s}) - \phi(x)}{\varepsilon} \leq \frac{1}{c(x)} + O(\varepsilon),$$

and upon taking the limit  $\varepsilon \rightarrow 0$ ,

$$\frac{1}{c(x)} \geq \sup_{|\hat{s}|=1} \hat{s} \cdot \nabla \phi(x) = |\nabla \phi(x)|.$$

Together with (39) this shows that  $\phi$  must satisfy the eikonal equation (38).

**Example 4** Consider the example in Figure 1, left. Here  $\Gamma$  is the boundary of the square  $[0, 1]^2$  and we seek  $\phi$  inside the domain. The local speed is constant  $c \equiv 1$ . The fastest paths to  $\Gamma$  are obviously straight lines orthogonal to the nearest side. The shortest travel time is the distance of these paths. On the diagonals of the square there are two optimal paths and in the center of the square there are four optimal paths. Everywhere, however, the shortest travel time is well-defined, namely

$$\phi(x, y) = \min(x, 1 - x, y, 1 - y).$$

This means that  $\phi(x)$  is continuous but  $\nabla \phi(x)$  is not continuous, and the solution has "kinks" along the diagonals. Note that that  $|\nabla \phi| = 1$  and  $\phi(x, y) = 0$  on  $\Gamma$ .

**Example 5** A more complicated example is shown in Figure 1, right. Here  $\Gamma$  is the bold line  $\{x = 0\}$  on the left side. The speed  $c(x)$  is equal to one everywhere, except in the black boxes where it is zero (or very small). The fastest path to  $\Gamma$  from a point unobstructed by boxes is again a straight line orthogonal to  $\Gamma$ . The optimal path from a point behind one of the boxes is different, however. The initial part of that path is a straight line to the nearest box corner, hence the curved iso lines. If the point behind the box is precisely in between the two corners, there are two equally fast paths, and therefore, again,  $\phi(x)$  has a kink, and  $\nabla \phi$  has a discontinuity.

The kinks in the examples above are in fact a generic feature of solutions to the eikonal equation. Even for smooth data and  $\Gamma$  the gradient  $\nabla\phi$  will in general develop discontinuities ("shocks") in finite time. In the wave setting these kinks means that the exact solution is no longer a simple wave of the form (30) but should rather be written as a sum of simple waves like (31). Hence, the model in (30) breaks down. This happens typically when a wave which starts out as a simple wave is refracted and focused.

#### 4.4 Numerical methods for eikonal equation

We discuss three different ways to solve the eikonal equation.

##### 4.4.1 Ray tracing

Ray tracing means solving the ray equations (34) and (35). Any numerical ODE-method can be used. The phase is then given by the relation (36). Pros and cons:

- + Simple.
- + Gives relevant solutions also for multivalued phases like in (31), where the eikonal equation breaks down.
- Only gives  $\phi(x)$  along the ray, not on a uniform grid.

##### 4.4.2 Fast marching method

In the fast marching method the eikonal equation is discretized on a grid. In two dimensions we can take

$$r_{ij} = (x_i, y_j), \quad x_i = ih, \quad y_j = jh, \quad h = 1/N,$$

and let  $\phi_{ij}$  approximate the exact solution in each grid point

$$\phi_{ij} \approx \phi(r_{ij}).$$

The grid is considered as a graph, where the grid points are nodes which are connected by edges to their closest neighbors. Each edge is assigned a travel time value based on the local speed  $c(x)$ . The fast marching method then uses the Dijkstra algorithm from computer science to find the shortest path in this graph. (Recall that  $\phi(x)$  is precisely the shortest travel time to the boundary.) For details see

[http://math.berkeley.edu/~sethian/2006/Explanations/fast\\_marching\\_explain.html](http://math.berkeley.edu/~sethian/2006/Explanations/fast_marching_explain.html)

Pros and cons:

- + Efficient. The computational cost is  $O(N^d \log N)$  if there are  $N$  grid points in each coordinate direction. Because of this it is something of an industry standard for solving problems involving the eikonal equation.
- Complicated to implement.
- Standard version is only first order accurate. Higher order methods possible but are even more complicated.

#### 4.4.3 Time-dependent version

A third approach to solving (32) is to first convert it to a time-dependent problem

$$|\nabla\phi| = n(x) \quad \Rightarrow \quad \phi_t + |\nabla\phi| = n(x).$$

Then use numerical methods for time-dependent Hamilton–Jacobi equations and solve it to steady state,  $\phi_t = 0$ . The simplest such scheme is the Hamilton–Jacobi version of the Lax–Friedrichs scheme. In two dimensions, let  $\phi_{ij}^n$  approximate the time-dependent phase  $\phi(t, x, y)$ ,

$$\phi_{ij}^n \approx \phi(t_n, x_i, y_j), \quad t_n = n\Delta t.$$

The Lax–Friedrichs scheme is then

$$\phi_{ij}^{n+1} = \frac{1}{4} (\phi_{i+1,j}^n + \phi_{i-1,j}^n + \phi_{i,j+1}^n + \phi_{i,j-1}^n) - \Delta t H \left( x_i, y_j, \frac{\phi_{i+1,j}^n - \phi_{i-1,j}^n}{2h}, \frac{\phi_{i,j+1}^n - \phi_{i,j-1}^n}{2h} \right),$$

where

$$H(x, y, \phi_x, \phi_y) = \sqrt{\phi_x^2 + \phi_y^2} - n(x, y).$$

The time to reach steady state is  $O(1)$  which means that the number of time steps is  $O(1/\Delta t) = O(N)$ , with a fixed CFL number  $h = \lambda\Delta t$ . Then the total cost is  $O(N^{d+1})$ , since each step involves  $O(N^d)$  operations. Pros and cons:

- + Easy to implement.
- + Quite straightforward to do higher order.
- Inefficient – the complexity is much higher than for fast marching.
- There is no guarantee that  $\phi(t, x)$  always converges to the time-independent solution as  $t \rightarrow \infty$ .