PDE-introduction

In quantum physics the time independent *Schrödinger equation* in three dimensions is

$$\frac{-\hbar^2}{2m}\Delta\Psi(x,y,z) + V(x,y,z)\Psi(x,y,z) = E\Psi(x,y,z) \tag{1}$$

Here $\Psi(x,y,z)$ is called the wave function, E is the energy of the particle with mass m, $\hbar$ is Planck's constant and $V(x,y,z)$ is the potential energy. Going from a classical (Newtonian) description of a system to a quantum mechanical the functions are replaced by operators. In the Schrödinger equation kinetic energy corresponds to the operator $\frac{-\hbar^2}{2m}\Delta$.

Sometimes the potential, V, can in a region K to a good approximation be given by

$$\begin{aligned} V(x,y,z) &= 0, \quad \text{inside } K \\ V(x,y,z) &= \infty, \quad \text{outside } K. \end{aligned}$$

Then the Schrödinger equation turns into the *Helmholtz equation*

$$\Delta\Psi(x,y,z) + k^2\Psi(x,y,z) = 0 \tag{2}$$

in K. Here $k^2 = 2mE/\hbar^2$. The *boundary condition* is $\Psi = 0$ at ∂K and then it turns out that only certain k^2-values are possible. See my notes on the square for an example. For a circular disc these *eigenvalues* are given by zeros of Bessel functions (see chapter 5) and we will solve this problem at the end of the course.

For more complicated geometries *only* numerical solutions exist. An example in two dimensions is Helmholtz equation inside a domain D with ∂D given by

$$\begin{aligned} u &= cos\ \phi + \lambda cos\ 2\phi, \\ v &= sin\ \phi + \lambda sin\ 2\phi. \end{aligned}$$

Here $0 \leq \phi < 2\pi$ and the parameter λ lies between 0 and $\frac{1}{2}$. $\lambda = 0$ is the circle, $\lambda = 0.5$ a cardioid (heart shape). Except for the circle only numerical solutions exist. The domain D is a mapping of the unit disc, $x^2 + y^2 \leq 1$, in the following way

$$\begin{aligned} u = x &+ \lambda(x^2 - y^2), \\ v = y &+ \lambda 2xy. \end{aligned}$$

In the (x,y) coordinates Helmholtz equation becomes

$$\frac{1}{1 + 4\lambda x + 4\lambda^2(x^2 + y^2)}\Delta\Psi(x,y) = -k^2\Psi(x,y), \tag{3}$$

that is a more complicated operator than Δ but a niceer geometry (circle). On the other hand with the (u, v) coordinates we have a simple operator, Δ, but a more complicated geometry. There is no free lunch!

Now some words about PDE's generally. The Laplace operator appears very often in the PDEs. The reason is that in the derivations a divergence of a gradient of a scalar field ϕ is taken, $\Delta\phi = \nabla \cdot \nabla\phi$. There are three classes of linear PDE:

Hyperbolic. The classical example is the wave equation

$$\frac{1}{c^2}\frac{\partial^2 u}{\partial t^2} - \Delta u = 0 \tag{4}$$

For derivation see appendix B in chapter 10. u denotes a displacement (amplitude) for example for a drum skin. c is the propagation speed of the wave.

Parabolic. For example the heat equation,

$$\frac{1}{a}\frac{\partial u}{\partial t} - \Delta u = f(x, y, z, t). \tag{5}$$

u is the temperature, a thermal diffusivity and f is a source of heat.

Elliptic. Laplace equation

$$\Delta u = 0 \tag{6}$$

belongs to this class. u can be the electric potential. If charges are present a source term, $\rho(x, y, z)$, is included in the right hand side and we get Poisson equation.

$$\Delta u = -\rho \tag{7}$$

Example of a PDE problem: A boiling spherical potatoe with radius R. The PDE is the heat equation above, without any source term. The **boundary value** (BV) is

$$u(\mathbf{r}, t) = 100, \qquad \mid \mathbf{r} \mid = R \tag{8}$$

and for the **initial value** (IV) we take

$$u(\mathbf{r}, 0) = 20, \qquad \mid \mathbf{r} \mid \leq R \tag{9}$$

Observe, this is a mathematical model not the reality.

As for ODEs non-linear problems can appear in PDEs and they are also difficult to handle. An example is in fluid mechanics where an operator acting on the velocity field $\mathbf{u}(x, y, z, t)$ has the following expression

$$\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla)\mathbf{u} \tag{10}$$

in a famous PDE called Navier-Stokes equation. Can you see where the non-linearity comes from? In this course we work with linear PDEs and that means that a linear combination of two solutions is again a solution.

When dealing with a PDE problem some important questions arise:

i)**Does a solution exist?** A hard question generally. A construction of a solution needed.
ii)**Is the solution unique?** That depends on the BV and IV.
iii)**Which are the properties of the solution?** For example, how will the solution behave for very large times.
iv)**How can we construct a solution?** There are a lot of methods and theories like: Integral transforms, Integral equations, Conformal maps, Green functions and Distribution theory. In this course we will say something about Green functions but the other techniques will be studied in other courses. We will mainly be occupied with **Fouriers method** or the method of separation of variables. The idea is to assume that the function $u(x, y, z)$ in the PDE can be decomposed into a product of functions, one for each coordinate like $u(x, y, z) = X(x) \cdot Y(y) \cdot Z(z)$ in a rectangular box or $u(x, y) = u(r, \theta) = f(r) \cdot g(\theta)$ on a circular disc. This ansatz works well for simple geometries like square, box, disc and sphere and leads to a couple of ODE's to solve. These problems are studied in chapter 11.

A PDE problem is said to be **well-posed** if
$*$ Solution exists
$*$ The solution is unique
$*$ The solution is continous with respect to variation of physical parameters