

# PHAS2423 Mathematical Methods for Theoretical Physicists

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# Chapter 1

## Introduction

### 1.1 Aims and Syllabus.

Compulsory module for Theoretical Physics students in year 2; optional module for all students in year 3. The course includes 30 lectures, 4 problem solving tutorials (PSTs), and two 1-hour problem based in course assessments (ICAs).

Table 1.1: Timetable.

Week	Lectures (WD & FR)	PST (FR)	ICA (TU/FR)
6	4		
7	4		
8	3	1	
9	4		
10	3	1	
11	Reading week		1
12	4		
13	3	1	
14	4		
15	1	1	
16			1
Total	30	4	2

**Prerequisites** for taking this course are PHAS1245, PHAS1246, PHAS2246

UCL courses, which may be taken concurrently, or their equivalents.

**The Aims** of the course are

- To introduce theoretically-minded students to advanced areas in mathematics, with applications to various problems in physics, particularly in dynamics, and in quantum mechanics, solid mechanics and fluid mechanics.
- To provide a deeper treatment of mathematical methods covered in PHAS2246 Mathematical Methods III.
- To provide mathematical underpinning for Theoretical Physics students taking PHAS2443 Practical Mathematics II in term 2 of year 2.

### Syllabus:

- *Cartesian tensors [5]:*
  - Transformation properties of scalars, vectors and rank-N tensors.
  - Kronecker delta and Levi-Civita symbol.
  - Quotient theorem.
  - Tensor of inertia, stress and strain tensors.
- *Linear ordinary differential equations (ODE) [5]:*
  - 1<sup>st</sup> order ODE, 2<sup>nd</sup> order ODE with constant coefficients. [1]
  - Solution of inhomogeneous ODE using Laplace transform. [1]
  - Solution of inhomogeneous ODE using variation of parameters. [1]
  - Properties of the  $\delta$ -function. [1]
  - Solution of inhomogeneous ODE using Greens functions. [1]
- *Sturm-Liouville theory [4]:*
  - Self-adjoint linear differential operators.
  - Properties of eigenfunctions of Sturm-Liouville equations.
  - Completeness of a basis set.
  - Construction of Greens functions.
  - Representation of the  $\delta$  function.
  - Examples of orthogonal polynomials.
- *Numerical methods for initial value problems [3]:*
  - Tridiagonal matrices.
  - Explicit and implicit Euler method, errors and stability.
  - Advanced methods: predictor-corrector, Runge-Kutta.

- *Integral transforms [3]:*  
Fourier and Laplace transforms.  
Convolution. Inverse Laplace transform.  
Applications in ordinary and partial differential equations.
- *Linear partial differential equations [4]:*  
Categorisation of equations and classes of boundary conditions.  
Eigenfunction representation of solutions.  
Diffusion equation, Laplace/Poisson equation, wave equation.  
Method of characteristics for first order PDEs.
- *Fluid Mechanics [4]:*  
Equations of motion of non-viscous and viscous fluids.  
Euler's equation, irrotational flow, potential flow, Bernoulli's theorem, Navier-Stokes equation, Poiseuille flow, Stokes flow past a sphere.

**Recommended books:**

- Riley, Hobson and Bence, Mathematical Methods for Physics and Engineering, Third Edition (CUP)
- Boas, Mathematical Methods in the Physical Sciences, 3rd Edition (Wiley)
- Tritton, Physical Fluid Dynamics, Second Edition, (Oxford)

## 1.2 Prerequisites.

### Trigonometry

$$\sin(-x) = -\sin x \quad \cos(-x) = \cos x$$

$$\sin^2 x + \cos^2 x = 1$$

$$\sin 2x = 2 \sin x \cos x \quad \cos 2x = \cos^2 x - \sin^2 x$$

$$\cos \alpha \cos \beta = \frac{1}{2} \cos(\alpha + \beta) + \frac{1}{2} \cos(\alpha - \beta)$$

$$\cos \alpha \sin \beta = \frac{1}{2} \sin(\alpha + \beta) - \frac{1}{2} \sin(\alpha - \beta)$$

$$\sin \alpha \sin \beta = \frac{1}{2} \cos(\alpha - \beta) - \frac{1}{2} \cos(\alpha + \beta)$$

$$\begin{aligned}\sin(\alpha \pm \beta) &= \sin \alpha \cos \beta \pm \sin \beta \cos \alpha \\ \cos(\alpha \pm \beta) &= \cos \alpha \cos \beta \mp \sin \alpha \sin \beta\end{aligned}$$

$$\sin x = \frac{e^{ix} - e^{-ix}}{2i} \quad \cos x = \frac{e^{ix} + e^{-ix}}{2}$$

### Vectors and Matrices

$$\mathbf{a} = a_x \mathbf{i} + a_y \mathbf{j} + a_z \mathbf{k}$$

$$\lambda(\mathbf{a} + \mathbf{b}) = \lambda \mathbf{a} + \lambda \mathbf{b} = \lambda(a_x + b_x)\mathbf{i} + \lambda(a_y + b_y)\mathbf{j} + \lambda(a_z + b_z)\mathbf{k}$$

$$\mathbf{a} \cdot \mathbf{b} = \mathbf{b} \cdot \mathbf{a} = \mathbf{b} \mathbf{a} = a_x b_x + a_y b_y + a_z b_z = |\mathbf{a}| |\mathbf{b}| \cos \theta$$

$$\mathbf{a} \times \mathbf{b} = (a_y b_z - a_z b_y)\mathbf{i} + (a_z b_x - a_x b_z)\mathbf{j} + (a_x b_y - a_y b_x)\mathbf{k}$$

$$\mathbf{a} \cdot (\mathbf{b} + \mathbf{c}) = \mathbf{a} \cdot \mathbf{b} + \mathbf{a} \cdot \mathbf{c}$$

$$\mathbf{a} \times (\mathbf{b} + \mathbf{c}) = \mathbf{a} \times \mathbf{b} + \mathbf{a} \times \mathbf{c}$$

Determinant of a matrix  $A$ :

$$\det(A) = |A_{ij}| = \begin{vmatrix} A_{11} & A_{12} & \dots & A_{1N} \\ A_{21} & A_{22} & \dots & A_{2N} \\ \dots & \dots & \dots & \dots \\ A_{N1} & A_{N2} & \dots & A_{NN} \end{vmatrix} = \sum_{n=1}^{N!} (-1)^{P_n} A_{1\alpha} A_{2\beta} \dots A_{N\omega}$$

$$\mathbf{a} \times \mathbf{b} = \begin{vmatrix} \mathbf{i} & \mathbf{j} & \mathbf{k} \\ a_x & a_y & a_z \\ b_x & b_y & b_z \end{vmatrix} = -\mathbf{b} \times \mathbf{a}$$

For  $N \times N$  matrices  $A$  and  $B$ :

$$\det(AB) = \det(A)\det(B).$$

Trace of a matrix  $A$ :

$$\text{tr}(A) = A_{11} + A_{22} + \dots + A_{NN} = \sum_{i=1}^N A_{ii} = \text{Sp}(A)$$

Transpose of a matrix  $A$ :

$$A^T = [A_{ij}]^T = [A_{ji}].$$

If matrix  $S$  is such that  $\det(S) \neq 0$ , it is possible to define inverse matrix  $S^{-1}$ :

$$S S^{-1} = S^{-1} S = I,$$

where  $I$  is a unity matrix. (Notation  $E$  is also used for unity matrices.)

If an  $N \times N$  matrix  $S$  is such that its rows are orthogonal and its columns are orthogonal, i.e.,

$$\sum_{i=1}^N S_{ij} S_{ik} = \sum_{i=1}^N S_{ji} S_{ki} = \delta_{jk},$$

where  $\delta_{jk}=1$  if  $j=k$  and  $\delta_{jk}=0$  if  $j \neq k$ , then  $S$  is called *orthogonal* and

$$S^{-1} = S^T,$$

i.e.,

$$S_{ij} = (S^T)_{ji} = (S^{-1})_{ji}.$$

**Differential calculus** Derivative of a function of a single argument:

$$\frac{df(x)}{dx} = f'(x) = \lim_{\Delta x \rightarrow 0} \frac{f(x + \Delta x) - f(x)}{\Delta x}$$

Examples:

$$\begin{aligned}(x^n)' &= nx^{n-1} & (a^x)' &= a^x \ln a \\(e^{kx})' &= ke^{kx} & (\ln x)' &= \frac{1}{x} \\(\cos x)' &= -\sin x & (\sin x)' &= \cos x \\(\arcsin x)' &= \frac{1}{\sqrt{1-x^2}} & (\arctan x)' &= \frac{1}{1+x^2}\end{aligned}$$

Differentiation rules:

$$\begin{aligned}(c_1 f(x) + c_2 g(x))' &= c_1 f'(x) + c_2 g'(x) \\(f(x)g(x))' &= f'(x)g(x) + f(x)g'(x) \\\left(\frac{f(x)}{g(x)}\right)' &= \frac{f'(x)g(x) - f(x)g'(x)}{g(x)^2}\end{aligned}$$

If  $y = f(x)$  and  $x = g(u)$ , then

$$\frac{dy}{du} = f'(x)g'(u) = \frac{df(x)}{dx} \frac{dx}{du}.$$

Partial derivative of a function of several arguments:

$$\frac{\partial f(x_1, x_2, \dots, x_N)}{\partial x_i} = \lim_{\Delta x_i \rightarrow 0} \frac{f(x_1, \dots, x_i + \Delta x_i, \dots, x_N) - f(x_1, \dots, x_i, \dots, x_N)}{\Delta x_i}$$

Full differential:

$$df = \frac{\partial f(x_1, x_2, \dots, x_N)}{\partial x_1} dx_1 + \frac{\partial f(x_1, x_2, \dots, x_N)}{\partial x_2} dx_2 + \dots + \frac{\partial f(x_1, x_2, \dots, x_N)}{\partial x_N} dx_N$$

## Complex variables

$$z = x + iy$$

$$z^* = x - iy$$

$$|z|^2 = zz^* = (x + iy)(x - iy) = x^2 + y^2$$

$$z = |z| \left( \frac{x}{\sqrt{x^2 + y^2}} + i \frac{y}{\sqrt{x^2 + y^2}} \right) = |z| (\cos \alpha + i \sin \alpha) = |z| e^{i\alpha}$$

# Chapter 2

## Cartesian tensors

### 2.1 Definitions.

Physical properties are described using one or several independent variables. For example, volume  $V$  of a cake (see Fig. 2.1a) is described using only one variable. Such properties are called *scalars*. Three *independent* variables are needed to describe velocity of the champaign cork (Fig. 2.1b). Such properties are called *vectors*. We can use  $\mathbf{v}$  or  $(v_x, v_y, v_z)$  or  $x_1, x_2, x_3$  to represent the vector of velocity.

How many independent variables are needed to describe response of a solid to the external stress? This property should reflect the direction and magnitude of the force, applied to each point, and the direction and magnitude of the displacement of each point. Hence, nine independent variables are needed. Thus, in general, physical properties are described using  $N$  independent variables.

In this Chapter, we will consider how representation of these properties changes upon transformation from one coordinate system to another. We will consider *real* variables only and focus on *three-dimensional Euclidean* space. Some of the definitions will be given for  $N$ -dimensional space.

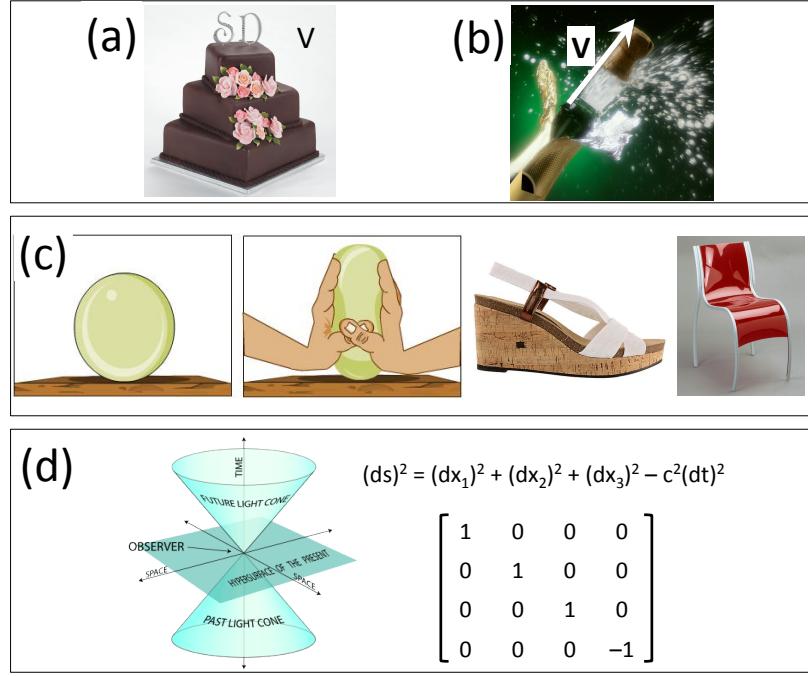


Figure 2.1: Examples of (a) scalar: volume of a cake; (b) vector: velocity of a champaign cork; (c) relation between directions of forces and displacements of each point in a solid; (d) metric of Minkowski space.

**$N$ -dimensional space.** Consider a set of  $N$  real independent variables  $x_1, x_2, \dots, x_i, \dots, x_N$ . These values will be called coordinates of a point. All the points corresponding to all the possible values of the coordinates form the  $N$  dimensional space. This space will be denoted as  $V_N$ .

Note the difference between a coordinate system defined by  $x_1, x_2, \dots, x_i, \dots, x_N$  and a point given by a specific realisation of the coordinates  $x_1, x_2, \dots, x_i, \dots, x_N$ .

**Curve in  $N$ -dimensional space.** If there are  $N$  equations

$$x_i = f_i(u), \quad (i = 1, 2, \dots, N),$$

where  $u$  is a parameter and  $f_i(u)$  are functions of  $u$ , the collection of points which satisfy these equations defines a *curve* in  $V_N$ .

**Subspace in  $N$ -dimensional space.** In general, if there are  $N$  equations

$$x_i = f_i(u_1, u_2, \dots, u_M), \quad (i = 1, 2, \dots, N \text{ and } M < N),$$

where  $u_1, u_2, \dots, u_M$  are parameters and  $f_i(u_1, \dots, u_M)$  are functions of these parameters, the collection of all points which satisfy these equations defines an  $M$ -dimensional *subspace*  $V_M$  in  $V_N$ . If  $M=N-1$ , the subspace  $V_M$  is called *hypersurface* of  $V_N$ .

**Kronecker  $\delta$  (delta) symbol:**

$$\delta_{ij} = \begin{cases} 1 & \text{if } i = j \\ 0 & \text{if } i \neq j \end{cases}$$

**Summation convention.** In order to simplify equations, we will use two conventions regarding the indices.

1. Indices will take *all values* from 1 to  $N$ , unless otherwise is stated explicitly.
2. If an index appears *twice* in any single term, a summation with respect to this index is implied. The summation goes over the range from 1 to  $N$  (convention 1).

For example, in 3D space ( $N=3$ ):

$$a_i x_i = a_1 x_1 + a_2 x_2 + a_3 x_3$$

$$a_{ij} b_{jk} = a_{i1} b_{1k} + a_{i2} b_{2k} + a_{i3} b_{3k} \quad \text{the sum depends on } i \text{ and } k$$

$$a_{ij} b_{jk} c_{kmn} = \sum_{j=1}^3 \sum_{k=1}^3 a_{ij} b_{jk} c_{kmn} \quad \text{the sum depends on } i, m \text{ and } n$$

$$\frac{\partial^2 \phi}{\partial x_i \partial x_i} = \frac{\partial^2 \phi}{\partial x_1^2} + \frac{\partial^2 \phi}{\partial x_2^2} + \frac{\partial^2 \phi}{\partial x_3^2}.$$

Similarly, in  $N$ -dimensional space,

$$\sum_{i=1}^N a_i x_i + \sum_{j=1}^N b_j x_j = a_i x_i + b_j x_j.$$

Note that no summation is implied in

$$a_i + x_i + b_j + x_j.$$

The summation index is called a *dummy* index; it can be replaced by any other index as long as it does not conflict with other indices used in equations. For example, if  $\bar{x}_i$  is defined by the function  $\phi_i$  as

$$\bar{x}_i = \phi_i(x_1, x_2, \dots, x_N),$$

then differential of  $\bar{x}_i$  can be written as

$$d\bar{x}_i = \sum_j^N \frac{\partial \phi_i}{\partial x_j} dx_j = \frac{\partial \phi_i}{\partial x_j} dx_j = \frac{\partial \phi_i}{\partial x_r} dx_r.$$

In order to avoid confusion, the same index should not be used more than twice in one term. For example,

$$d\bar{x}_j = \frac{\partial \phi_j}{\partial x_i} dx_i \quad \text{but not} \quad d\bar{x}_j = \frac{\partial \phi_j}{\partial x_j} dx_j$$

and

$$\left( \sum_{i=1}^N a_i x_i \right)^2 = (a_i x_i)^2 = (a_i x_i)(a_j x_j) = a_i a_j x_i x_j \quad \text{but not} \quad a_i x_i a_i x_i.$$

In order to demonstrate the effect of the Kronecker symbol:

$$\begin{aligned} b_j \delta_{ij} &= b_i \\ a_{ij} \delta_{jk} &= a_{ik} \\ a_{ij} b_{jk} \delta_{ki} &= a_{ij} b_{ji} = a_{kj} b_{jk}. \end{aligned}$$


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**Exercise.** Show that

$$\delta_{ij} \delta_{jk} = \delta_{ik}$$

and

$$\delta_{ii} = N$$


---

## 2.2 Change of basis.

**Transformation of coordinates in 3-dimensional space.** Let us introduce a set of *independent* basis vectors in a 3D space:  $\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3$ . Then, any vector  $\mathbf{x}$  can be represented as

$$\mathbf{x} = x_1 \mathbf{e}_1 + x_2 \mathbf{e}_2 + x_3 \mathbf{e}_3 = x_k \mathbf{e}_k$$

where  $x_1, x_2, x_3$  are called components of the vector  $\mathbf{x}$ . Consider a new basis set  $\mathbf{e}'_1, \mathbf{e}'_2, \mathbf{e}'_3$  related to the old one by

$$\begin{aligned}\mathbf{e}'_1 &= S_{11} \mathbf{e}_1 + S_{21} \mathbf{e}_2 + S_{31} \mathbf{e}_3 = S_{k1} \mathbf{e}_k \\ \mathbf{e}'_2 &= S_{12} \mathbf{e}_1 + S_{22} \mathbf{e}_2 + S_{32} \mathbf{e}_3 = S_{k2} \mathbf{e}_k \\ \mathbf{e}'_3 &= S_{13} \mathbf{e}_1 + S_{23} \mathbf{e}_2 + S_{33} \mathbf{e}_3 = S_{k3} \mathbf{e}_k\end{aligned}$$

or

$$\mathbf{e}'_j = S_{kj} \mathbf{e}_k,$$

where  $S_{ij}$  are elements of a matrix  $S$ . In the new basis set vector  $\mathbf{x}$  can be written as

$$\mathbf{x} = x'_1 \mathbf{e}'_1 + x'_2 \mathbf{e}'_2 + x'_3 \mathbf{e}'_3 = x'_k \mathbf{e}'_k.$$

Substitution of the expressions for  $\mathbf{e}'_1, \mathbf{e}'_2, \mathbf{e}'_3$  into this equation gives:

$$\begin{aligned}\mathbf{x} &= x'_1 (S_{11} \mathbf{e}_1 + S_{21} \mathbf{e}_2 + S_{31} \mathbf{e}_3) + \\ &\quad x'_2 (S_{12} \mathbf{e}_1 + S_{22} \mathbf{e}_2 + S_{32} \mathbf{e}_3) + \\ &\quad x'_3 (S_{13} \mathbf{e}_1 + S_{23} \mathbf{e}_2 + S_{33} \mathbf{e}_3) \\ &= x'_1 (S_{k1} \mathbf{e}_k) + x'_2 (S_{k2} \mathbf{e}_k) + x'_3 (S_{k3} \mathbf{e}_k) \\ &= x'_j (S_{kj} \mathbf{e}_k)\end{aligned}$$

Hence, components of the vector  $\mathbf{x}$  in the old and new basis sets are related as

$$\begin{aligned}x_1 &= S_{11} x'_1 + S_{12} x'_2 + S_{13} x'_3 = S_{1k} x'_k \\ x_2 &= S_{21} x'_1 + S_{22} x'_2 + S_{23} x'_3 = S_{2k} x'_k \\ x_3 &= S_{31} x'_1 + S_{32} x'_2 + S_{33} x'_3 = S_{3k} x'_k\end{aligned}$$

or

$$x_i = S_{ik} x'_k,$$

i.e.  $x_i$  are *functions* of  $x'_i$  and components of the transformation matrix  $S$  are given by

$$S_{ik} = \frac{\partial x_i}{\partial x'_k}.$$

The system of equations  $x_i = S_{ij}x'_j$  can be resolved with respect to  $x'_i$  if  $\det(S) \neq 0$ . In this case, it is possible to define inverse of the matrix  $S$ , which transforms components of  $\boldsymbol{x}$  from the old basis to the new one:

$$x'_i = (S^{-1})_{ij}x_j.$$

**Rotation.** If the transformation defined by the matrix  $S$  is a *rotation*, i.e.,  $S$  is orthogonal ( $S^{-1} = S^T$ ), then

$$x'_i = (S^T)_{ij}x_j = S_{ji}x_j.$$

**Transformation of coordinates in  $N$ -dimensional space.** Consider a space  $V_N$  and a coordinate system  $x_1, x_2, \dots, x_N$ . If there are  $N$  equations

$$x'_i = \phi_i(x_1, x_2, \dots, x_N) \quad (i = 1, 2, \dots, N),$$

where  $\phi_i$  are *independent* single-valued continuous and differentiable functions of coordinates, these equations are said to define *transformation* of coordinate system  $x_1, x_2, \dots, x_N$  into a new coordinate system  $x'_1, x'_2, \dots, x'_N$ .

A necessary and sufficient condition for independency of the functions  $\phi_i$  is that determinant of the  $N \times N$  matrix formed by the derivatives

$$\frac{\partial x'_i}{\partial x_j} = \frac{\partial \phi_i(x_1, \dots, x_N)}{\partial x_j} \quad (i, j \in 1, \dots, N),$$

(and denoted as  $S$ ) is not equal to zero:

$$\det([S_{ji}]) = \det\left(\left[\frac{\partial \phi_i(x_1, \dots, x_N)}{\partial x_j}\right]\right) \neq 0.$$

Under this condition, the above equations can be solved with respect to  $x_i$ , i.e., one can find functions  $\psi_i$  which express old coordinates  $x_i$  in terms of new coordinates  $x'_j$ :

$$x_i = \psi_i(x'_1, x'_2, \dots, x'_N) \quad (i = 1, 2, \dots, N).$$

## 2.3 Rotations of Cartesian coordinate systems.

Investigate how *components* of a vector are changed by a rotation of the Cartesian coordinate system. For convenience, introduce transformation matrix  $L=S^{-1}$ , where matrix  $S$  defines the rotation of the *basis set* vectors. Then,

$$x'_i = L_{ij}x_j$$

and

$$x_i = L_{ji}x'_j.$$

Orthogonality of  $L$  means that

$$L_{ik}L_{jk} = \delta_{ij} \quad (\text{orthogonality of rows})$$

and

$$L_{ki}L_{kj} = \delta_{ij} \quad (\text{orthogonality of columns}).$$

(In the following we always assume that matrix  $L$  is orthogonal.)

Since we defined new basis  $\mathbf{e}'_j$  ( $j=1,2,3$ ) as

$$\mathbf{e}'_j = S_{ij}\mathbf{e}_i = (L^{-1})_{ij}\mathbf{e}_i,$$

For orthonormal vectors  $\mathbf{e}_k$  ( $k=1,2,3$ ) and rotation  $L$

$$\mathbf{e}_k \cdot \mathbf{e}'_j = S_{ij}\mathbf{e}_k \cdot \mathbf{e}_i = S_{ij}\delta_{ki} = S_{kj} = (L^{-1})_{kj} = (L^T)_{kj} = L_{jk},$$

i. e. elements of the transformation matrix  $L$  are *defined* by the scalar products of the old and new basis vectors.

---

**Exercise.** Show that the transformation matrix  $L$  for a rotation of the coordinate system by an angle  $\theta$  about  $\mathbf{e}_3$  axis is

$$\mathbf{L} = \begin{pmatrix} \cos \theta & \sin \theta & 0 \\ -\sin \theta & \cos \theta & 0 \\ 0 & 0 & 1 \end{pmatrix}$$


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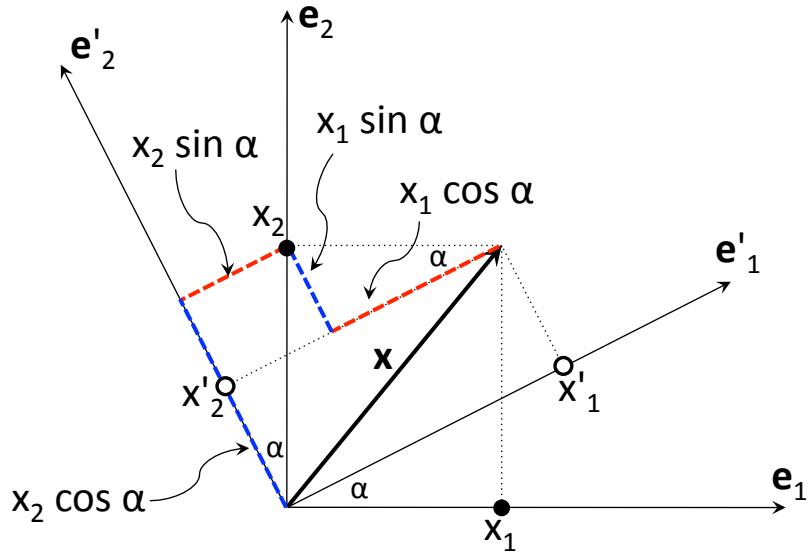


Figure 2.2: Rotation of Cartesian axes by an angle  $\alpha$  about the  $x_3$  axis. Note that the rotation of the axes changes *components* of the vector  $\mathbf{x}$  but not the vector itself.

**Exercise.** Show that two consecutive rotations of the coordinate system by an angle  $\theta$  about  $e_3$  axis is also a rotation with the value of the rotation angle of  $2\theta$ .

In general, the product of two rotations is also a rotation, i.e. if

$$x'_i = L_{ij}x_j$$

and

$$x''_i = M_{ij}x'_j$$

then

$$x''_i = M_{ij}x'_j = M_{ij}(L_{jk}x_k) = (M_{ij}L_{jk})x_k = (ML)_{ik}x_k.$$

**Transformation of vectors.** Consider a set of quantities  $v_i$  ( $i=1,\dots,N$ ;  $N=3$ ), which are **functions** of coordinates  $x_j$  ( $j=1,\dots,N$ ;  $N=3$ ), i.e.

$$v_i = v_i(x_1, x_2, x_3),$$

and investigate how their values are changed by a rotation of the Cartesian axes. We already know that coordinates transform as

$$x'_i = L_{ij}x_j.$$

If a set of new quantities  $v'_i$  can be obtained from the set of  $v_i$  by the same transformation:

$$v'_i = L_{ij}v_j,$$

then  $v_i$  form the components of a *vector* or *1st-order Cartesian tensor*. According to this definition:

$$v'_k \mathbf{e}'_k = (L_{kj}v_j)(S_{nk}\mathbf{e}_n) = (S_{nk}L_{kj})v_j\mathbf{e}_n = S_{nk}(S^{-1})_{kj}v_j\mathbf{e}_n = \delta_{nj}v_j\mathbf{e}_n = v_n\mathbf{e}_n,$$

i.e.,

$$\mathbf{v} = v_i\mathbf{e}_i = v'_j\mathbf{e}'_j.$$


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### Review:

1.  $N$ -dimensional space: variables  $x_1, x_2, \dots, x_N$ , ( $x_i \in \mathbb{R}$ ).
  2. The summation convention:  $\sum a_i b_i = a_i b_i$ .
  3. Basis set  $\mathbf{e}_i$ , rotation of the coordinate system  $\mathbf{e}'_j = S_{ij}\mathbf{e}_i$  and the corresponding transformation of coordinates  $x'_i = (S^{-1})_{ij}x_j$ .
  4. 1st-order Cartesian tensors  $\mathbf{v} = (v_1, v_2, v_3)$ :  $v'_i = (S^{-1})_{ij}v_j = L_{ij}v_j$ .
- 

Clearly (by definition),  $\mathbf{v}$  is a vector if

$$v_1 = x_1 \quad v_2 = x_2 \quad v_3 = x_3,$$

i.e.,  $\mathbf{v} = (x_1, x_2, x_3)$ . Consider other sets of  $v_i$  in 2D space. Which of these functions are scalars, vectors, or neither?

$$\begin{aligned} \mathbf{v}(x_1, x_2) &= (v_1) = x_1 + x_2 \\ \mathbf{v}(x_1, x_2) &= (v_1) = (x_1)^2 + (x_2)^2 \\ \mathbf{v}(x_1, x_2) &= (v_1, v_2) = (x_1, x_2) \\ \mathbf{v}(x_1, x_2) &= (v_1, v_2) = (x_2, -x_1) \\ \mathbf{v}(x_1, x_2) &= (v_1, v_2) = (x_2, x_1) \end{aligned}$$


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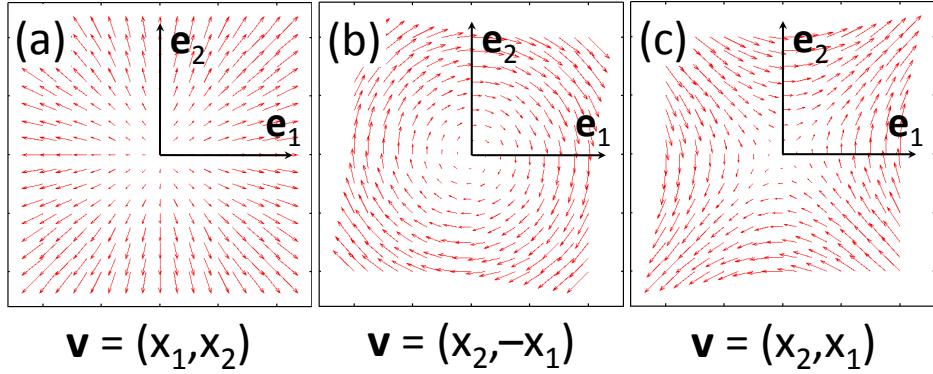


Figure 2.3: Examples of functions in 2D case: (a)  $\mathbf{v}(x_1, x_2) = x_1\mathbf{e}_1 + x_2\mathbf{e}_2$ ; (b)  $\mathbf{v}(x_1, x_2) = x_2\mathbf{e}_1 - x_1\mathbf{e}_2$ ; (c)  $\mathbf{v}(x_1, x_2) = x_2\mathbf{e}_1 + x_1\mathbf{e}_2$

**Exercise.** For the case of a two-dimensional space, show that  $\mathbf{v} = (x_2, -x_1)$  transforms as a vector under rotation of the coordinate system and  $\mathbf{v} = (x_2, x_1)$  – does not.

---

**Transformation of scalars.** Scalars or  $0^{\text{th}}$  order tensors have only one component, which is invariant with respect to the rotation of the coordinate system. Are  $x_1^2 + x_2^2$  and  $x_1^2 + x_2^2 + x_3^2$  scalars in the three-dimensional Cartesian space?

Examples of scalars include  $\mathbf{F} \cdot d\mathbf{r}$ ,  $e\mathbf{E} \cdot d\mathbf{r}$ ,  $\mathbf{B} \cdot \mathbf{B}$  and many others.

---

**Exercise.** Show that scalar product of vectors  $\mathbf{a}$  and  $\mathbf{b}$  is, indeed, a scalar, then demonstrate it for  $\nabla \cdot \mathbf{v}$ , where  $\mathbf{v}$  is a vector.

---

**Example.** Let  $\phi(x_1, x_2, x_3)$  be a scalar and derive  $\mathbf{E}$  as

$$\mathbf{E}(x_1, x_2, x_3) = -\nabla\phi(x_1, x_2, x_3) = -\frac{\partial\phi}{\partial x_1}\mathbf{e}_1 - \frac{\partial\phi}{\partial x_2}\mathbf{e}_2 - \frac{\partial\phi}{\partial x_3}\mathbf{e}_3.$$

Is  $\mathbf{E}$  a vector? Components  $E'_i$  in a new basis are given by

$$E'_i = -\frac{\partial \phi'}{\partial x'_i} = -\frac{\partial \phi}{\partial x_j} \frac{\partial x_j}{\partial x'_i} = L_{ij} E_j,$$

i.e. they satisfy the transformation condition for the 1<sup>st</sup> order tensors. Thus,  $\mathbf{E}$  is a vector.

## 2.4 2<sup>nd</sup>- and higher-order tensors.

Many physical properties of materials are described using the language of tensors. For example, *deformation*, *dielectric* and *magnetic* permittivities, *magnetoelectric* effect, and *conductivity* are described using 2<sup>nd</sup> order tensors.

**Example.** Spin Hamiltonian used to model electron paramagnetic resonance (EPR) spectra for a system of  $N_{atm}$  atoms with nuclear spins  $\mathbf{I}_k$ :

$$H = \mu_B \mathbf{B} \mathbf{g} \mathbf{S} + \sum_{k=1}^{N_{atm}} \mathbf{S} \mathbf{A}_k \mathbf{I}_k,$$

where  $\mathbf{g}$  and  $\mathbf{A}$  are 2<sup>nd</sup> order tensors.  $\mathbf{A}_k$  is the hyperfine interaction tensor for atom  $k$ ; it is usually decomposed into isotropic and anisotropic parts:

$$\mathbf{A} = a_{iso} \mathbf{I} + \mathbf{T}.$$

These properties are related to the atomistic structure of materials, e.g., the conductivity tensor of crystals with cubic symmetry is isotropic. In this section we describe basic operations with tensors.

Quantities  $T_{ij}$  are components of a **2<sup>nd</sup>-order tensor** if they transform according to

$$T'_{ij} = L_{ik} L_{jl} T_{kl}$$

upon rotation of the coordinate system. Then, components of the tensor  $T_{ij}$  in the old basis are expressed via components  $T'_{kl}$  in the new basis as

$$T_{ij} = L_{ki} L_{lj} T'_{kl}$$

In general, components of the order  $N$  tensor should transform as

$$T'_{i_1 i_2 \dots i_N} = L_{i_1 \alpha_1} L_{i_2 \alpha_2} \dots L_{i_N \alpha_N} T_{\alpha_1 \alpha_2 \dots \alpha_N}$$

and

$$T_{i_1 i_2 \dots i_N} = L_{\alpha_1 i_1} L_{\alpha_2 i_2} \dots L_{\alpha_N i_N} T'_{\alpha_1 \alpha_2 \dots \alpha_N}.$$

$N$ th order Cartesian tensor has  $3^N$  components. Components of the 2nd order tensors are convenient to represent using matrices with elements  $T_{ij}$ , where  $i$  refers to the number of a row and  $j$  refers to the number of a column.

**Outer product.** The *outer product of vectors  $\mathbf{a}$  and  $\mathbf{b}$*  is defined as

$$A_{ij} = a_i b_j$$

and is denoted as

$$\mathbf{A} = \mathbf{a} \otimes \mathbf{b}.$$

(Note the difference from  $\mathbf{A} = \mathbf{a} \times \mathbf{b}$ .) Consider transformation of the outer product components upon rotation of the coordinate system:

$$A'_{ij} = a'_i b'_j = L_{ik} a_k L_{jl} b_l = L_{ik} L_{jl} a_k b_l = L_{ik} L_{jl} A_{kl}.$$

Thus, components of the outer products of two vectors transform in the same way as components of a 2nd order tensor (use notations  $\mathbf{T}$  and  $T_{ij}$  from now on). Since  $\mathbf{a} = a_i \mathbf{e}_i$  and  $\mathbf{b} = b_i \mathbf{e}_i$ , tensor formed by the  $\otimes$  of  $\mathbf{a}$  and  $\mathbf{b}$  can be written as

$$\mathbf{T} = a_i b_j \mathbf{e}_i \otimes \mathbf{e}_j = T_{ij} \mathbf{e}_i \otimes \mathbf{e}_j = T'_{ij} \mathbf{e}'_i \otimes \mathbf{e}'_j.$$

Note that while components of the tensor  $\mathbf{T}$  depend on the coordinate system, it is *the same* tensor in both coordinate systems.

The outer product operation can be applied to arbitrary tensors of the orders of  $N$  ( $\mathbf{A}$ ) and  $M$  ( $\mathbf{B}$ ); the resulting tensor has the order of  $N + M$ :

$$\mathbf{T} = \mathbf{A} \otimes \mathbf{B}.$$

Components of the outer product tensor are

$$T_{i_1 i_2 \dots i_N j_1 j_2 \dots j_M} = A_{i_1 i_2 \dots i_N} B_{j_1 j_2 \dots j_M}.$$

**Contraction.** *Contraction* of a tensor assumes i) equating two subscripts and ii) summing over all possible values of these subscripts. In the case of the 2nd order tensor, contraction of  $\mathbf{T}$  gives the sum of its diagonal elements

$$T_{ii} = \text{Tr}(T),$$

which gives a zero-order tensor. In general, contraction of a tensor of order  $N$  i) produces another tensor and ii) its order is  $N - 2$ . To show this we need to investigate transformation of the entity formed by contraction. (In the anticipation that it is a tensor, we call it  $\mathbf{T}$ ). For the order  $N$  tensor

$$T'_{i_1 i_2 \dots i_N} = L_{i_1 j_1} L_{i_2 j_2} \dots L_{i_N j_N} T_{j_1 j_2 \dots j_N}.$$

For the contracted tensor (use orthogonality of  $L$ ):

$$\begin{aligned} T'_{i_1 \dots i_p \dots i_p \dots i_N} &= L_{i_1 j_1} \dots L_{i_p j_p} \dots L_{i_p j_q} \dots L_{i_N j_N} T_{j_1 \dots j_p \dots j_q \dots j_N} \\ &= L_{i_1 j_1} \dots \delta_{j_p j_q} \dots L_{i_N j_N} T_{j_1 \dots j_p \dots j_q \dots j_N} \\ &= (L_{i_1 j_1} \dots L_{i_{p-1} j_{p-1}}) (L_{i_p+1 j_p+1} \dots L_{i_{q-1} j_{q-1}}) (L_{i_q+1 j_q+1} \dots L_{i_N j_N}) T_{j_1 \dots j_q \dots j_{q-1} \dots j_N} \end{aligned}$$

The contraction operation is not defined for vectors. However, one can first generate a 2nd order tensor as the outer product of two vectors:

$$T_{ij} = a_i b_j$$

and then apply the contraction operation, which gives a scalar product of the vectors

$$a_i b_i.$$

**Inner product.** Operations of multiplication and contraction can be combined in order to produce new tensors. For example, if  $\mathbf{A}$  is a 3rd order tensor and  $\mathbf{B}$  is a 4th order tensor, then new tensors

$$\begin{aligned} C_{ijmnt} &= A_{ijk} B_{kmnt} \\ C_{kln} &= A_{ijk} B_{linj} \\ C_m &= A_{ijk} B_{kmji} \end{aligned}$$

of the 5th, 3rd, and 1st order can be constructed. This process is called *inner multiplication* and the resulting tensors are called *inner products*. To prove that the inner products are, indeed, tensors, consider transformations of their components. For example,

$$C_{kn} = A_{ki} B_{ni}$$

in rotated coordinate system:

$$\begin{aligned} C'_{kn} &= A'_{ki} B'_{ni} \\ &= (L_{kp} L_{iq} A_{pq})(L_{nr} L_{is} B_{rs}) \\ &= L_{kp} L_{nr} (L_{iq} L_{is}) A_{pq} B_{rs} \\ &= L_{kp} L_{nr} (\delta_{qs}) A_{pq} B_{rs} \\ &= L_{kp} L_{nr} A_{pq} B_{rq} \\ &= L_{kp} L_{nr} C_{pr}. \end{aligned}$$

Hence,  $\mathbf{C}$  is a tensor.

**Gradient of a vector.** If  $\mathbf{v}$  is a vector, then quantities

$$T_{ij} = \frac{\partial v_i}{\partial x_j}$$

form components of a 2<sup>nd</sup> order tensor. To prove it, consider these quantities in a rotated coordinate system:

$$T'_{ij} = \frac{\partial}{\partial x'_j} v'_i = \frac{\partial}{\partial x_l} (L_{ik} v_k) \frac{\partial x_l}{\partial x'_j} = L_{ik} \frac{\partial v_k}{\partial x_l} L_{jl} = L_{ik} L_{jl} T_{kl}.$$

Tensor  $\mathbf{T} = \nabla \mathbf{v}$  can be considered as a *gradient of a vector*.

---

**Problem solving class.** Demonstrate that matrix  $T$  represents a 2<sup>nd</sup> order tensor.

$$T = \begin{pmatrix} x_2^2 & -x_1 x_2 \\ -x_1 x_2 & x_1^2 \end{pmatrix}$$


---

**Summation of tensors.** If  $A_{i_1 i_2 \dots i_N}$  and  $B_{j_1 j_2 \dots j_N}$  are components of two tensors of *the same order* and in *the same coordinate system*, then their sum and difference are defined as

$$S_{k_1 k_2 \dots k_N} = A_{k_1 k_2 \dots k_N} + B_{k_1 k_2 \dots k_N}$$

and

$$D_{k_1 k_2 \dots k_N} = A_{k_1 k_2 \dots k_N} - B_{k_1 k_2 \dots k_N}.$$

To prove that  $S_{k_1 k_2 \dots k_N}$  are components of a tensor, show that they transform as

$$S'_{k_1 k_2 \dots k_N} = L_{k_1 n_1} L_{k_2 n_2} \dots L_{k_N n_N} S_{n_1 n_2 \dots n_N}$$

upon rotation of the coordinate system.

**Symmetric tensors.** A 2<sup>nd</sup> order tensor is called *symmetric tensor* if its components are related as

$$T_{ij} = T_{ji}$$

for all values of  $i$  and  $j$ . In the case of an  $N^{th}$  order tensor, if

$$T_{i_1 \dots i_n \dots i_m \dots i_N} = T_{i_1 \dots i_m \dots i_n \dots i_N}$$

this tensor is said to be symmetric with respect to  $n^{th}$  and  $m^{th}$  subscripts.  
Examples: *stress* and *strain* tensors.

**Stress tensor** – force  $\mathbf{F}$  acting on a small surface element  $\mathbf{S}$ :

$$\sigma = \begin{bmatrix} \sigma_{11} & \sigma_{12} & \sigma_{13} \\ \sigma_{21} & \sigma_{22} & \sigma_{23} \\ \sigma_{31} & \sigma_{32} & \sigma_{33} \end{bmatrix} = \begin{bmatrix} \sigma_{xx} & \sigma_{xy} & \sigma_{xz} \\ \sigma_{yx} & \sigma_{yy} & \sigma_{yz} \\ \sigma_{zx} & \sigma_{zy} & \sigma_{zz} \end{bmatrix} = \begin{bmatrix} \sigma_x & \tau_{xy} & \tau_{xz} \\ \tau_{yx} & \sigma_y & \tau_{yz} \\ \tau_{zx} & \tau_{zy} & \sigma_z \end{bmatrix},$$

where

$$\tau_{\alpha\beta} = \tau_{\beta\alpha}.$$

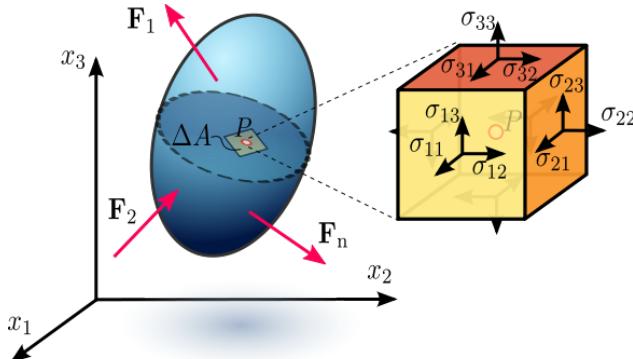


Figure 2.4: Stress in a loaded deformable body (Wiki)

**Maxwell stress tensor:**

$$\sigma_{ij} = \epsilon_0 E_i E_j + \frac{1}{\mu_0} B_i B_j - \frac{1}{2} \left( \epsilon_0 E^2 + \frac{1}{\mu_0} B^2 \right) \delta_{ij}.$$

**Antisymmetric tensors.** If

$$T_{i_1 \dots i_n \dots i_m \dots i_N} = -T_{i_1 \dots i_m \dots i_n \dots i_N},$$

the tensor is said to be *antisymmetric*. Examples: *Levi-Civita tensor* (see below), *electromagnetic tensor*.

**Electromagnetic tensor:**

$$F_{\mu\nu} = \begin{bmatrix} 0 & E_x/c & E_y/c & E_z/c \\ -E_x/c & 0 & -B_z & B_y \\ -E_y/c & B_z & 0 & -B_x \\ -E_z/c & -B_y & B_x & 0 \end{bmatrix},$$

where

$$\mathbf{E} = -\frac{\partial \mathbf{A}}{\partial t} - \nabla \phi \quad \mathbf{B} = \nabla \times \mathbf{A}$$

and  $\mathbf{A}$  and  $\phi$  are the vector and scalar potentials, respectively.

**Decomposition into a symmetric and antisymmetric parts.** An arbitrary tensor can be written as a sum of a symmetric and antisymmetric tensors. For the  $2^{nd}$  order tensors:

$$T_{ij} = \frac{1}{2} (T_{ij} + T_{ji}) + \frac{1}{2} (T_{ij} - T_{ji}) = S_{ij} + A_{ij},$$

where  $S_{ij}$  is symmetric and  $A_{ij}$  is antisymmetric. For an  $N^{th}$  order tensor we can define a symmetric tensor

$$S_{i_1 \dots i_n \dots i_m \dots i_N} = \frac{1}{2} (T_{i_1 \dots i_n \dots i_m \dots i_N} + T_{i_1 \dots i_m \dots i_n \dots i_N})$$

and an asymmetric tensor

$$A_{i_1 \dots i_n \dots i_m \dots i_N} = \frac{1}{2} (T_{i_1 \dots i_n \dots i_m \dots i_N} - T_{i_1 \dots i_m \dots i_n \dots i_N}).$$

Then

$$T_{i_1 \dots i_N} = S_{i_1 \dots i_N} + A_{i_1 \dots i_N}.$$

## 2.5 Tensors $\delta_{ij}$ and $\epsilon_{ijk}$ .

**Permutation symbol and permutation tensor.** The permutation symbol is a three-index object defined as

$$\epsilon_{ijk} = \begin{cases} 0 & \text{if } i = j, \text{ or } i = k, \text{ or } j = k \\ +1 & \text{if } i, j, k \in (1, 2, 3), (2, 3, 1), (3, 1, 2) \\ -1 & \text{if } i, j, k \in (1, 3, 2), (3, 2, 1), (2, 1, 3) \end{cases} .$$

It is also called *Levi-Civita symbol*, *Levi-Civita density*, *alternating tensor*, and *signature*. Notations  $\varepsilon_{ijk}$  and  $e_{ijk}$  are also used in literature.

The permutation symbol satisfies the following relations:

$$\begin{aligned} \delta_{ij}\epsilon_{ijk} &= 0 \\ \epsilon_{ipq}\epsilon_{jpq} &= 2\delta_{ij} \\ \epsilon_{ijk}\epsilon_{ijk} &= 6 \\ \epsilon_{ijk}\epsilon_{pqr} &= \delta_{ip}\delta_{jq} - \delta_{iq}\delta_{jp} \end{aligned}$$

and, in general,

$$\epsilon_{ijk}\epsilon_{pqr} = \begin{vmatrix} \delta_{ip} & \delta_{iq} & \delta_{ir} \\ \delta_{jp} & \delta_{jq} & \delta_{jr} \\ \delta_{kp} & \delta_{kq} & \delta_{kr} \end{vmatrix} .$$

**Prove that  $\delta_{ij}$  and  $\epsilon_{ijk}$  are tensors** Even if neither  $\delta_{ij}$  nor  $\epsilon_{ijk}$  depend on coordinates, we can formally consider transformation of their components with respect to rotation of the coordinate system. Note that  $\delta_{ij}$  has two subscripts and  $\epsilon_{ijk}$  - three subscripts. Hence, in the new coordinate system

$$\delta'_{ij} = L_{ik}L_{jl}\delta_{kl}.$$

Using the properties of  $\delta_{ij}$  and orthogonality of the transformation matrix  $L$ , obtain

$$\delta'_{ij} = L_{ik}L_{jl}\delta_{kl} = L_{ik}L_{jk} = \delta_{ij}.$$

Similarly, transformation of  $\epsilon_{ijk}$  is given by

$$\epsilon'_{ijk} = L_{il}L_{jm}L_{kn}\epsilon_{lmn}.$$

First notice that  $\epsilon_{ijk}$  can be used in order to calculate determinants of  $3 \times 3$  matrices:

$$\det(A)\epsilon_{ijk} = A_{il}A_{jm}A_{kn}\epsilon_{lmn}.$$

(Prove this, for  $i=1, j=2, k=3$  by performing the summation.) Hence, for the transformation matrix  $L$ :

$$\det(L)\epsilon_{ijk} = L_{il}L_{jm}L_{kn}\epsilon_{lmn} = \epsilon'_{ijk}.$$

Using the orthogonality of  $L$  ( $\det(L)=1$ ),

$$\epsilon'_{ijk} = \epsilon_{ijk},$$

i.e. the properties of  $\epsilon_{ijk}$  do not change under orthogonal transformation and the subscripts change as they should for the 3rd order tensor.

**4<sup>th</sup> order alternating tensor  $e_{ijkl}$**  The permutation symbol can be viewed as a tensor. Components of the rank 4 permutation tensor are

$$\epsilon_{ijkl} = \begin{cases} +1 & \text{if } i, j, k, l \text{ is an even permutation of 1,2,3,4} \\ -1 & \text{if } i, j, k, l \text{ is an odd permutation of 1,2,3,4} \\ 0 & \text{for all other combinations of } i, j, k, l \end{cases}.$$

This definition is straightforward to extend to the case of  $N$  dimensions.

**Applications of  $\epsilon_{ijk}$**  Tensor  $\epsilon_{ijk}$  simplifies complex expressions.

**Example 1.** Vector product of  $\mathbf{a}$  and  $\mathbf{b}$  can be written as

$$\mathbf{c} = \mathbf{a} \times \mathbf{b} = \begin{vmatrix} \mathbf{e}_1 & \mathbf{e}_2 & \mathbf{e}_3 \\ a_1 & a_2 & a_3 \\ b_1 & b_2 & b_3 \end{vmatrix} = \begin{vmatrix} C_{11} & C_{12} & C_{13} \\ C_{21} & C_{22} & C_{23} \\ C_{31} & C_{32} & C_{33} \end{vmatrix}.$$

Since

$$\det(A)\epsilon_{ijk} = A_{il}A_{jm}A_{kn}\epsilon_{lmn},$$

$$\mathbf{c}\epsilon_{ijk} = C_{il}C_{jm}C_{kn}\epsilon_{lmn}.$$

Setting  $i=1, j=2, k=3$  gives ( $\epsilon_{123}=1$ )

$$\mathbf{c} = C_{1l}C_{2m}C_{3n}\epsilon_{lmn}.$$

Since  $C_{1l} = \mathbf{e}_l$ ,  $C_{2m} = a_m$ , and  $C_{3n} = b_n$ , we obtain

$$\mathbf{c} = \mathbf{e}_l a_m b_n \epsilon_{lmn},$$

and  $l^{th}$  component of  $\mathbf{c}$  is

$$c_l = \epsilon_{lmn} a_m b_n.$$

**Example 2.** In the case of a double vector product

$$\mathbf{d} = [\mathbf{a} \times (\mathbf{b} \times \mathbf{c})],$$

the  $i^{th}$  component of  $\mathbf{d}$  is

$$d_i = \epsilon_{ijk} a_j (\mathbf{b} \times \mathbf{c})_k$$

and the  $k^{th}$  component of  $\mathbf{b} \times \mathbf{c}$  is

$$(\mathbf{b} \times \mathbf{c})_k = \epsilon_{klm} b_l c_m.$$

Hence

$$d_i = \epsilon_{ijk} \epsilon_{klm} a_j b_l c_m.$$

Using the fact that

$$\epsilon_{ijk} \epsilon_{klm} = \delta_{il} \delta_{jm} - \delta_{im} \delta_{jl},$$

find that

$$\begin{aligned} d_i &= (\delta_{il} \delta_{jm} - \delta_{im} \delta_{jl}) a_j b_l c_m \\ &= \delta_{il} a_m b_l c_m - \delta_{im} a_l b_l c_m \\ &= (a_m c_m) b_i - (a_l b_l) c_i, \end{aligned}$$

or, in the vector form,

$$\mathbf{d} = \mathbf{a} \times (\mathbf{b} \times \mathbf{c}) = (\mathbf{a} \cdot \mathbf{c}) \mathbf{b} - (\mathbf{a} \cdot \mathbf{b}) \mathbf{c}.$$

**Example.** Double cross product is used in solving geometrical problems. It is also used as an order parameter in complex dipolar structures in magnets and ferroelectrics [S. Prosandeev and L. Bellaiche, Phys. Rev. B, **77** 060101(R) (2008).]

**Exercise.** Find an explicit expression for the  $i^{th}$  component of vector

$$\nabla \times (\nabla \times \mathbf{a})$$

using the properties of the tensor  $\epsilon_{ijk}$ .

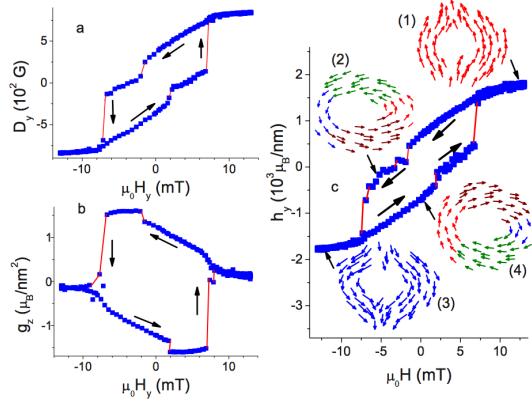


Figure 2.5: Predicted hysteresis loops in asymmetric ferromagnetic ring. From S. Prosandeev and L. Bellaiche, Phys. Rev. B, **77** 060101(R) (2008).

**Isotropic tensor.** A tensor, components of which are the same in all rotated coordinate systems is called an **isotropic tensor**. In general,  $T_{ij}$  are components of an isotropic tensor if for any element  $T_{ij} = f_{ij}(x_1, x_2, x_3, \dots)$ , there is a similar dependence for the elements  $T'_{ij}$  in all rotated coordinate systems:  $T'_{ij} = f_{ij}(x'_1, x'_2, x'_3, \dots)$ .

All rank-0 tensors (scalars) are isotropic, but no rank-1 tensors (vectors) are. Clearly tensors  $\delta_{ij}$  and  $\epsilon_{ijk}$  are isotropic. Moreover, they are unique isotropic tensors of the 2nd and 3rd orders respectively.

## 2.6 The quotient theorem.

The *quotient theorem* states that if

$$A_{i_1 \dots \alpha \dots i_N} B_{j_1 \dots \alpha \dots j_M} = C_{i_1 i_2 \dots i_N j_1 j_2 \dots j_M}$$

in all coordinate systems rotated with respect to each other and  $\mathbf{B}$  is an arbitrary order  $M$  tensor and  $\mathbf{C}$  is an order  $N+M-2$  tensor, then quantities

$$A_{i_1 i_2 \dots i_N}$$

are components of a tensor of the order  $N$ .

We will prove the quotient law for a particular case of  $N = M = 2$ . Assume that

$$A_{jk}B_{ik} = C_{ji},$$

holds for all rotated coordinate systems and for *any* 2<sup>nd</sup> order tensor  $\mathbf{B}$ ;  $\mathbf{C}$  is also a 2<sup>nd</sup> order tensor. First, consider

$$A_{jk}B_{ik}$$

in a new coordinate system:

$$\begin{aligned} A'_{jk}B'_{ik} &= C'_{ji} \\ &= L_{jp}L_{iq}C_{pq} \\ &= L_{jp}L_{iq}A_{pr}B_{qr} \\ &= L_{jp}L_{iq}A_{pr}L_{uq}L_{vr}B'_{uv} \\ &= L_{jp}(L_{iq}L_{uq})L_{vr}A_{pr}B'_{uv} \\ &= L_{jp}(\delta_{iu})L_{vr}A_{pr}B'_{uv} \\ &= L_{jp}L_{vr}A_{pr}B'_{iv} \end{aligned}$$

Compare the left and the right sides

$$A'_{jk}B'_{ik} - L_{jp}L_{vr}A_{pr}B'_{iv} = 0$$

and note that subscripts  $k$  and  $v$  are dummy subscripts. Hence, the above equality can be rewritten as

$$(A'_{jk} - L_{jp}L_{kr}A_{pr})B'_{ik} = 0.$$

Since we assumed that  $\mathbf{B}$  is arbitrary, then

$$A'_{jk} - L_{jp}L_{kr}A_{pr} = 0,$$

which means that components  $A_{pr}$  transform as components of a tensor:

$$A'_{jk} = L_{jp}L_{kr}A_{pr}.$$

**Exercise.** Show that if

$$A_{ik}B_k = C_i,$$

holds for any vector  $\mathbf{B}$  and for a vector  $\mathbf{C}$ , then  $\mathbf{A}$  is a 2<sup>nd</sup> order tensor.

## 2.7 Physical applications of tensors.

**Tensor or inertia.** Consider a collection of interconnected points  $\alpha$  with masses  $m^\alpha$  (neglect masses of the connectors). The orbital momentum of this system is defined as

$$\mathbf{L} = \sum_{\alpha} (\mathbf{r}^\alpha \times \mathbf{p}^\alpha) = \sum_{\alpha} m^\alpha (\mathbf{r}^\alpha \times (\boldsymbol{\omega} \times \mathbf{r}^\alpha)).$$

For continuous bodies, substitute the summation over  $\alpha$  with integration over  $dm$ .

Find the explicit expression for the  $i^{th}$  component of  $\mathbf{L}$ :

$$\begin{aligned} L_i &= \sum_{\alpha} m^\alpha [\epsilon_{ijk} x_j^\alpha (\boldsymbol{\omega} \times \mathbf{r}^\alpha)_k] = \sum_{\alpha} m^\alpha [\epsilon_{ijk} \epsilon_{klm} x_j^\alpha \omega_l x_m^\alpha] \\ &= \sum_{\alpha} m^\alpha [(\delta_{il} \delta_{jm} - \delta_{im} \delta_{jl}) x_j^\alpha x_m^\alpha] \omega_l \\ &= \sum_{\alpha} m^\alpha [\delta_{il} \delta_{jm} x_j^\alpha x_m^\alpha - (\delta_{im} x_m^\alpha)(\delta_{jl} x_j^\alpha)] \omega_l \\ &= \sum_{\alpha} m^\alpha [\delta_{il} x_j^\alpha x_j^\alpha - x_i^\alpha x_l^\alpha] \omega_l = I_{il} \omega_l = I_{li} \omega_l, \end{aligned}$$

where elements  $I_{ij}$  are called components of the tensor of inertia. Since  $\mathbf{L}$  and  $\boldsymbol{\omega}$  are vectors,  $I_{ij}$  are components of a true 2nd order tensor. (Why?) By construction it is a symmetric tensor.

**Kinetic energy of a rotating system** For a fixed rotation axis:

$$T = \int \frac{v^2}{2} dm = \int \frac{(\omega r)^2}{2} dm = \frac{1}{2} \omega^2 \int r^2 dm = \frac{1}{2} I \omega^2$$

In a general case

$$\begin{aligned}
T &= \frac{1}{2} \int \frac{d\mathbf{r}}{dt} \cdot \frac{d\mathbf{r}}{dt} dm \\
&= \frac{1}{2} \int (\boldsymbol{\omega} \times \mathbf{r}) \cdot (\boldsymbol{\omega} \times \mathbf{r}) dm \\
&= \frac{1}{2} \int (\boldsymbol{\omega} \times \mathbf{r})_i (\boldsymbol{\omega} \times \mathbf{r})_i dm \\
&= \frac{1}{2} \int (\epsilon_{ijk} \omega_j x_k) (\epsilon_{imn} \omega_m x_n) dm \\
&= \frac{1}{2} \int (\delta_{jm} \delta_{kn} - \delta_{jn} \delta_{km}) x_k x_n \omega_j \omega_m dm \\
&= \frac{1}{2} [\int (\delta_{jm} x_k x_k - x_j x_m) dm] \omega_j \omega_m = \frac{1}{2} I_{jm} \omega_j \omega_m.
\end{aligned}$$

**Strain tensor.** Consider a small element of an elastic body, which is subjected to deformation (see Fig. 2.4). Let us define deformation-induced displacement of a point as

$$\mathbf{u} = \mathbf{r}' - \mathbf{r}.$$

Here  $\mathbf{r} = (x_1, x_2, x_3)$  are coordinates of a point before deformation,  $\mathbf{r}' = (x'_1, x'_2, x'_3)$  are coordinates of the same point after the deformation and  $\mathbf{u}$  is *deformation vector*. Note that coordinates  $x'_i$  are functions of the coordinates  $x_k$ .

The distance between two points is changing upon deformation. Let

$$d\ell = \sqrt{dx_1^2 + dx_2^2 + dx_3^2} \quad \text{and} \quad d\ell' = \sqrt{(dx'_1)^2 + (dx'_2)^2 + (dx'_3)^2}$$

be the distance between two infinitely close points before and after deformation, respectively. Then,

$$(d\ell)^2 = (dx_1)^2 + (dx_2)^2 + (dx_3)^2 = dx_i dx_i$$

and

$$\begin{aligned}
(d\ell')^2 &= (dx'_1)^2 + (dx'_2)^2 + (dx'_3)^2 \\
&= dx'_i dx'_i \\
&= (dx_i + du_i)(dx_i + du_i) \\
&= dx_i dx_i + 2dx_i du_i + du_i du_i \\
&= (d\ell)^2 + 2dx_i du_i + du_i du_i.
\end{aligned}$$

Since components of the deformation vector  $u_i$  are functions of  $x_k$ , we have

$$du_i = \frac{\partial u_i}{\partial x_k} dx_k.$$

Thus,

$$(d\ell')^2 = (d\ell)^2 + 2 \frac{\partial u_i}{\partial x_k} dx_i dx_k + \frac{\partial u_i}{\partial x_k} \frac{\partial u_i}{\partial x_n} dx_k dx_n,$$

which can also be written as

$$(d\ell')^2 = (d\ell)^2 + \frac{\partial u_i}{\partial x_k} dx_i dx_k + \frac{\partial u_k}{\partial x_i} dx_i dx_k + \frac{\partial u_m}{\partial x_i} \frac{\partial u_m}{\partial x_k} dx_i dx_k$$

or

$$(d\ell')^2 = (d\ell)^2 + 2u_{ik} dx_i dx_k,$$

where  $u_{ik}$  is *deformation* or *strain* tensor:

$$u_{ik} = \frac{1}{2} \left( \frac{\partial u_i}{\partial x_k} + \frac{\partial u_k}{\partial x_i} + \frac{\partial u_m}{\partial x_i} \frac{\partial u_m}{\partial x_k} \right) \approx \frac{1}{2} \left( \frac{\partial u_i}{\partial x_k} + \frac{\partial u_k}{\partial x_i} \right).$$

**Stress tensor.** Stress is defined as average force per unit area of a surface within a deformable body:

$$\sigma = \frac{F}{S}.$$

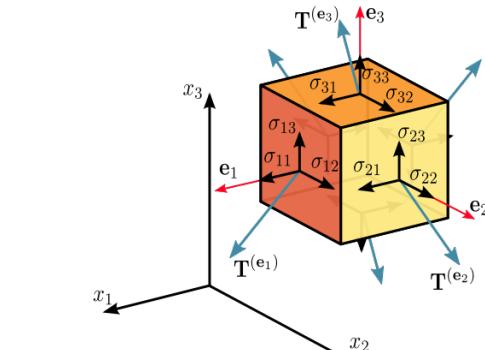


Figure 2.6: Components of the stress tensor.

Consider a small volume shown in Fig. 2.6. The  $i^{th}$  component of the total force acting on this volume is given by

$$\int F_i dV,$$

where  $F_i$  is the  $i^{th}$  components of the force  $\mathbf{F}$  acting on a unit of volume  $dV$ . This volume integral can be converted to a surface integral if  $F_i$  has a form of  $\partial\sigma_{ik}/\partial x_k$ . In addition,  $\sigma$  has to be a tensor: if  $\sigma_{ik}$  are components of a tensor, then  $\partial\sigma_{ik}/\partial x_k$  are components of a vector. Then,

$$\int F_i dV = \int \frac{\partial\sigma_{ik}}{\partial x_k} dV = \oint \sigma_{ik} dS_k$$

and  $\sigma_{ik}$  has the dimension of strain. *Here we used the divergence theorem (see Chapter 6):*

$$\int_V (\nabla \cdot \mathbf{a}) dV = \int_S \mathbf{a} \cdot d\mathbf{S},$$

where the surface  $S$  encloses the volume  $V$ .

The moment acting on a “small” volume  $dV$  is

$$m_{ik} = (F_i x_k - F_k x_i) dV.$$

Thus, the total moment acting on a body is

$$M_{ik} = \int (F_i x_k - F_k x_i) dV = \int \left( \frac{\partial\sigma_{im}}{\partial x_m} x_k - \frac{\partial\sigma_{km}}{\partial x_m} x_i \right) dV,$$

which can be re-written as

$$M_{ik} = \int \frac{\partial(\sigma_{im} x_k - \sigma_{km} x_i)}{\partial x_m} dV - \int \left( \sigma_{im} \frac{\partial x_k}{\partial x_m} - \sigma_{km} \frac{\partial x_i}{\partial x_m} \right) dV.$$

Rewrite the first term as a surface integral and use  $\partial x_k/\partial x_m = \delta_{km}$  and  $\partial x_i/\partial x_m = \delta_{im}$  in the second term:

$$M_{ik} = \oint (\sigma_{im} x_k - \sigma_{km} x_i) dS_m + \int (\sigma_{ki} - \sigma_{ik}) dV.$$

For a body in equilibrium, the momentum should not contain the contribution due to the integral over the volume. (Why?) The integral over volume in this equation vanishes if

$$\sigma_{ik} = \sigma_{ki},$$

i.e., the stress tensor is symmetric.

For a *homogeneously compressed* body, pressure  $p$  is applied to every point of its surface and the force applied to a surface element  $d\mathbf{S}$  is  $\mathbf{F} = -p d\mathbf{S}$ , i.e., components of the force are  $F_i = -p dS_i$ .

At the same time, component of the force are equal to  $F_i = \sigma_{ik} dS_k$ . Thus, the stress tensor in this case is

$$\sigma_{ik} = -p\delta_{ik}.$$

**Elastic constants.** Forces applied to a body induce its deformation. Hence, the stress and the strain tensors should be related. This relation is given by

$$\sigma_{ij} = c_{ijkl} u_{kl}.$$

The 4<sup>th</sup> order tensor  $c_{ijkl}$  is called the *stiffness tensor* or *elastic tensor* and its components are *elastic constants*. Tensor  $c_{ijkl}$  has 81 components ( $3 \times 3 \times 3 \times 3$ ). However, since the stress tensor is symmetric, there are only 21 independent components. This number can be reduced further in materials which possess crystal symmetry.

# Chapter 3

## Linear ordinary differential equations

### 3.1 Examples of physical problems.

**Newtonian mechanics.** Motion of a point mass  $m$  subjected to an external force  $\mathbf{F}$ :

$$\frac{d^2\mathbf{r}}{dt^2} = \mathbf{a} = \frac{1}{m}\mathbf{F}.$$

**Quantum mechanics.** Schrodinger equation:

$$i\frac{\partial}{\partial t}\Psi = \hat{H}\Psi \quad (i = \sqrt{-1}).$$

**Electrical circuits.**  $R$ ,  $C$ , and  $L$  are parameters of the circuit in Fig. 3.1.

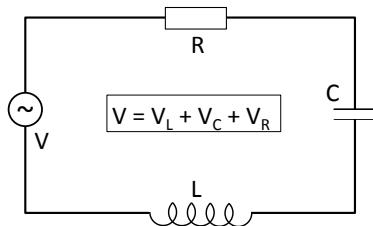


Figure 3.1: An electric circuit.

The charge on the capacitor [ $q(t)$ ] is a function of time  $t$ . To find the dependence of the current  $I$  on time, find the total voltage drop along the circuit

$$V(t) = L \frac{dI(t)}{dt} + RI(t) + \frac{q(t)}{C}.$$

Since  $I(t) = dq(t)/dt$ , after differentiating with respect to  $t$  obtain

$$L \frac{d^2I(t)}{dt^2} + R \frac{dI(t)}{dt} + \frac{I(t)}{C} = \frac{dV(t)}{dt}.$$

In general, coefficients may also depend on a variable:

$$A(x) \frac{d^2y(x)}{dx^2} + B(x) \frac{dy(x)}{dx} + C(x)y(x) = D(x).$$

## 3.2 Definitions.

**Ordinary differential equations.** An ordinary differential equation (ODE) is a relation between a function of one variable  $u(x)$ , the variable  $x$ , and the function's first and higher derivatives with respect to the variable  $x$ :

$$\frac{du}{dx}, \quad \frac{d^2u}{dx^2}, \dots$$

For example,

$$\frac{d^2y(x)}{dt^2} = \frac{1}{m}f(x).$$

**Partial differential equation.** (PDE): a relation between a function of several variables  $u(x_1, x_2, \dots, x_N)$ , variables  $x_1, x_2, \dots, x_N$ , and the function's first and higher derivatives with respect to these variables:

$$\frac{\partial u}{\partial x_k}, \quad \frac{\partial^2 u}{\partial x_k \partial x_n}, \dots$$

**Linear ordinary differential equation** is a relation, which has the form

$$a_0(x)y(x) + a_1(x)y'(x) + a_2(x)y''(x) + a_3(x)y'''(x) + \dots = b(x).$$

This definition valid to *any* order of the DE. Note that coefficients  $a_k$  ( $k=0,1,\dots$ ) and  $b$  may or may not be functions of  $x$ .

$$\begin{array}{ll} y' + 5 = -6y & \text{(linear)} \\ yy' + 5 = -6y & \text{(not linear)} \\ y'^2 + 5 = 6xy & \text{(not linear)} \\ y' + 5 = -\sin(6y) & \text{(not linear)} \end{array}$$

### 3.3 Linear first-order ODE.

The purpose of this section is to obtain general solution of the equation

$$y'(x) + P(x)y(x) = Q(x).$$

For simplicity, we will write  $y$ ,  $P$ , and  $Q$  instead of  $y(x)$ ,  $P(x)$ , and  $Q(x)$ .

**Homogeneous 1st order ODE.** First, consider the case of  $Q(x) = 0$ :

$$y' + Py = 0 \quad \text{or} \quad \frac{dy}{dx} = -Py$$

This equation is separable:

$$\frac{dy}{y} = -Pdx$$

and its solution can be obtained by integrating both parts:

$$\ln(y) = - \int Pdx + C,$$

where  $C$  is a constant. Thus,  $y$  can be written as

$$y(x) = e^{(- \int P(x)dx + C)} = e^C e^{- \int P(x)dx} = Ae^{- \int P(x)dx},$$

where  $A$  is a constant:  $A=e^C$ . It is convenient to introduce function  $S(x)$ :

$$S(x) = \int P(x) dx, \quad \text{and} \quad \frac{dS(x)}{dx} = P(x).$$

Then,

$$y(x) = Ae^{-S(x)} \quad \text{and} \quad y(x)e^{S(x)} = A.$$

By differentiating the left and right parts of the latter equation we obtain

$$\frac{d}{dx} (ye^S) = y'e^S + ye^S \frac{dS}{dx} = y'e^S + ye^S P = e^S (y' + Py) = 0$$

for  $y$  which satisfies the homogeneous equation.

**Inhomogeneous 1st order ODE.** For the inhomogeneous equation

$$\frac{d}{dx}(ye^S) = e^S(y' + Py) = e^S Q.$$

Integration of both parts with respect to  $x$  gives

$$y(x)e^{S(x)} = \int Q(x)e^{S(x)}dx + C.$$

Thus, general solution of the linear 1st order DE is

$$y(x) = e^{-S(x)} \left( \int Q(x)e^{S(x)}dx + C \right) \quad \text{where} \quad S(x) = \int P(x)dx.$$

**Example.** Find the solution of

$$y' + y = e^x.$$

In our notations,  $P(x) = 1$  and  $Q(x) = e^x$ . First, consider the homogeneous equation and find  $S(x)$ :

$$S(x) = \int P(x)dx = x \quad \text{and} \quad y(x) = Ae^{-x}.$$

For the inhomogeneous equation

$$y(x) = e^{-x} \left( \int e^x e^x dx + C \right) = e^{-x} \left( \frac{1}{2}e^{2x} + C \right) = \frac{1}{2}e^x + Ce^{-x}$$

### 3.4 Linear 2<sup>nd</sup>-order homogeneous equations.

Consider homogeneous equations with *constant* coefficients

$$a_2 \frac{d^2y}{dx^2} + a_1 \frac{dy}{dx} + a_0 = 0.$$

Let  $D$  denote the differential operation

$$D = \frac{d}{dx}.$$

Then, the above ODE can be rewritten as

$$(a_2 D^2 + a_1 D + a_0)y = a_2(D - \lambda_1)(D - \lambda_2)y = 0,$$

where  $\lambda_1$  and  $\lambda_2$  are roots of the *characteristic* equation

$$\lambda^2 + \frac{a_1}{a_2}\lambda + \frac{a_0}{a_2} = 0$$

with respect to  $\lambda$ . Note that solutions of the 1st order ODEs

$$(D - \lambda_1)y = 0 \quad \text{and} \quad (D - \lambda_2)y = 0$$

are also solutions of the 2nd order DE. We now know that solutions of these 1st order ODEs are

$$y_1 = c_1 e^{\lambda_1 x} \quad \text{and} \quad y_2 = c_2 e^{\lambda_2 x},$$

where  $c_1$  and  $c_2$  are constants. The manifold of their linear combinations form the general solution of the 2nd order ODE:

$$y(x) = c_1 e^{\lambda_1 x} + c_2 e^{\lambda_2 x}.$$

**Roots of the characteristic equation.** To solve a 2nd order ODE, we first have to find roots of the corresponding characteristic equation. This equation is quadratic and, therefore, may have three types of solutions:

- 1) two different real roots  $\lambda_1 \neq \lambda_2$ ;
- 2) two identical real roots  $\lambda_1 = \lambda_2$ ;
- 3) complex conjugated roots:  $\lambda_{1,2} = a \pm ib$ .

The case of  $\lambda_1 \neq \lambda_2$  has been considered above.

**Case  $\lambda_1 = \lambda_2$ .** In this case the differential equation can be written as

$$a_2(D - \lambda)(D - \lambda)y = 0.$$

One solution of this equation, according to what we discussed above, is

$$y(x) = A e^{\lambda x}.$$

To find the second solution, we let

$$u(x) = (D - \lambda)y(x).$$

Then  $(D - \lambda)(D - \lambda)y = 0$  can be rewritten as

$$(D - \lambda)u(x) = 0.$$

From this equation we obtain

$$u(x) = Be^{\lambda x},$$

where  $B$  is an arbitrary constant. Substituting this form of  $u(x)$  into  $u = (D - \lambda)y$  gives

$$Be^{\lambda x} = (D - \lambda)y = y' - \lambda y.$$

This is the 1st order ODE considered above with  $P(x) = -\lambda$  and  $Q(x) = Be^{\lambda x}$ . General solution of this equation is given by

$$ye^{\int P dx} = \int Q e^{\int P dx} dx + C,$$

which, in our case, is

$$ye^{-\lambda x} = B \int e^{\lambda x} e^{-\lambda x} dx + C = Bx + C.$$

Thus,

$$y(x) = (Bx + C)e^{\lambda x},$$

where  $B$  and  $C$  are arbitrary constants.

**Case  $\lambda_{1,2} = a \pm ib$ .** Similarly to the case of  $\lambda_1 = \lambda_2$ , the DE solution is

$$y(x) = c_1 e^{\lambda_1 x} + c_2 e^{\lambda_2 x}.$$

However, since  $\lambda_1$  and  $\lambda_2$  are related, this solution can be written in other forms, which might be more convenient. For example,

$$y(x) = Ae^{(a+ib)x} + Be^{(a-ib)x} = e^{ax}(Ae^{ibx} + Be^{-ibx}).$$

Since  $e^{\pm i\phi} = \cos(\phi) \pm i \sin(\phi)$ ,

$$Ae^{ibx} + Be^{-ibx} = (A+B)\cos(bx) + i(A-B)\sin(bx) = C_1 \cos(bx) + C_2 \sin(bx),$$

where  $C_1$  and  $C_2$  are new arbitrary constants. Furthermore, using the trigonometric formula

$$\sin(\alpha + \beta) = \sin \alpha \cos \beta + \cos \alpha \sin \beta,$$

we can rewrite  $C_1 \cos(bx) + C_2 \sin(bx)$  as

$$\sqrt{C_1^2 + C_2^2} \left( \frac{C_1}{\sqrt{C_1^2 + C_2^2}} \cos(bx) + \frac{C_2}{\sqrt{C_1^2 + C_2^2}} \sin(bx) \right)$$

or

$$\sqrt{C_1^2 + C_2^2} (\sin \gamma \cos(bx) + \cos \gamma \sin(bx)) = C \sin(bx + \gamma).$$

Hence,  $y(x)$  can be simplified to

$$y(x) = e^{ax} C \sin(bx + \gamma).$$

Thus, the two arbitrary constants can appear as  $A$  and  $B$ , as  $C_1$  and  $C_2$ , and as  $C$  and  $\gamma$ .

### 3.5 Laplace transform.

Finding solutions of a differential equations can be made easier if the equation is converted to an algebraic form.

Laplace transform is an integral transformation defined as

$$L[f(x)] = \int_0^\infty f(x)e^{-px} dx = F(p). \quad (3.1)$$

- By definition,  $L[f]$  does not depend on the behaviour of  $f(x)$  for  $x < 0$ . For certainty, let us set  $f(x)=0$  for  $x < 0$ .
- Note that function  $F(p)$  might be undefined for some values of  $p$ .
- Laplace transform is a linear operation:

$$L[c_1f(x) + c_2g(x)] = c_1L[f(x)] + c_2L[g(x)].$$

- It is straightforward to find the Laplace transform  $F(p)$  of any given function  $f(x)$ . To find the function  $g(x)$  given its Laplace transform  $G(p)$ , refer to a table of Laplace transforms.

**Examples.** i) for  $f(x)=a$  (constant):

$$F(p) = \int_0^\infty ae^{-px}dx = \left[ -\frac{a}{p}e^{-px} \right]_0^\infty = \frac{a}{p} \quad Re(p) > 0$$

ii) for  $f(x)=e^{-ax}$ :

$$F(p) = \int_0^\infty e^{-ax}e^{-px}dx = \frac{1}{a+p} \quad Re(a+p) > 0$$

iii) for  $f(x)=\cos(ax)$ :

$$F(p) = \int_0^\infty \cos(ax)e^{-px}dx = \frac{p}{a^2 + p^2} \quad Re(p) > |Im(a)|$$

**Laplace transform of derivatives.** Consider Laplace transforms of  $f'(x)$  and  $f''(x)$ .

$$L[f'] = \int_0^\infty f'(x)e^{-px}dx = [e^{-px}f(x)]_0^\infty + p \int_0^\infty f(x)e^{-px}dx = -f(0) + pL[f]$$

Similarly,

$$L[f''] = \int_0^\infty f''(x)e^{-px}dx = p^2L[f] - pf(0) - f'(0).$$

**Solving ODE using the Laplace transform.** Applying the Laplace transform method is convenient if:

- the variable  $x$  is defined in the interval  $[0, \infty)$  (e.g., coordinate of a point in a semi-infinite metal rod or time) and
- the values of the function  $f(x)$  and its derivatives are zero for  $x=0$ .

Consider a differential equation

$$f''(x) + 4f'(x) + 4f(x) = x^2e^{-2x}$$

with initial conditions  $f(0) = 0$  and  $f'(0) = 0$ . Laplace transform of this equation gives

$$p^2L[f] - pf(0) - f'(0) + 4pL[f] - 4f(0) + 4L[f] = L[x^2e^{-2x}].$$

Taking into account the initial conditions, we obtain

$$p^2 L[f] + 4pL[f] + 4L[f] = (p^2 + 4p + 4)L[f] = (p+2)^2 L[f] = L[x^2 e^{-2x}].$$

The Laplace transform in the right hand side is easy to calculate:

$$L[x^2 e^{-2x}] = \frac{2}{(p+2)^3}.$$

Thus, the transformed DE becomes

$$(p+2)^2 L[f] = \frac{2}{(p+2)^3},$$

i.e.,

$$L[f] = \frac{2}{(p+2)^5}.$$

Now, let us inspect a table of Laplace transforms (any relevant Maths textbook would have it) and find there a transform that looks similar to what we obtained. The most similar form is:

$$L[f] = \frac{n!}{(p-a)^{n+1}}, \quad \text{where} \quad f(x) = x^n e^{ax}$$

and the transform is valid for  $p > a$ .

In our case,

$$L[f] = \frac{2}{(p+2)^5} = \frac{1}{12} \cdot \frac{4!}{(p-(-2))^{4+1}}.$$

Thus,  $n = 4$  and  $a = -2$ . Since we requested (see above) that  $p > 0$ , the condition  $p > a$  is satisfied and, therefore, the solution of the ODE is

$$f(x) = \frac{1}{12} x^4 e^{-2x}.$$

## 3.6 Wronskian.

General solution of an inhomogeneous equation

$$a_n(x)y^{(n)} + a_{n-1}(x)y^{(n-1)} + \dots + a_2(x)y'' + a_1(x)y' + a_0(x)y = f(x)$$

has the form of

$$y(x) = y_c(x) + y_p(x).$$

Here  $y_p(x)$  is a *particular solution* of the inhomogeneous equation and  $y_c(x)$ , called *complementary function* is a linear combination of  $n$  *linearly independent* functions

$$y_c(x) = c_1 y_1(x) + c_2 y_2(x) + \dots + c_n y_n(x),$$

where each  $y_k(x)$  is a solution of the *homogeneous* equation

$$a_n(x)y^{(n)} + a_{n-1}(x)y^{(n-1)} + \dots + a_2(x)y'' + a_1(x)y' + a_0(x)y = 0.$$

Suppose we have solved the homogeneous equation. How can we check that the obtained solutions  $y_k(x)$  are linearly independent?

**Linear independence of functions.** A set of functions  $y_k(x)$  ( $k=1,\dots,n$ ) is *linearly dependent* if there are coefficients  $c_i$  (not all of them zeros), such that equality

$$c_1 y_1(x) + c_2 y_2(x) + \dots + c_n y_n(x) = 0.$$

Otherwise, these functions are linearly independent.

To develop a more practically useful method, let us differentiate the above equation  $n-1$  times and obtain a system of  $n$  linear equations:

$$\begin{array}{rcl} c_1 y_1(x) + c_2 y_2(x) + \dots + c_n y_n(x) & = & 0 \\ c_1 y'_1(x) + c_2 y'_2(x) + \dots + c_n y'_n(x) & = & 0 \\ \dots & \dots & \dots \\ c_1 y_1^{(n-1)}(x) + c_2 y_2^{(n-1)}(x) + \dots + c_n y_n^{(n-1)}(x) & = & 0 \end{array}$$

Determinant of a matrix, constructed from coefficients in front of  $c_k$  is called *Wronskian*:

$$W(y_1, y_2, \dots, y_n)(x) = \begin{vmatrix} y_1(x) & y_2(x) & \dots & y_n(x) \\ y'_1(x) & y'_2(x) & \dots & y'_n(x) \\ \dots & \dots & \dots & \dots \\ y_1^{(n-1)}(x) & y_2^{(n-1)}(x) & \dots & y_n^{(n-1)}(x) \end{vmatrix}$$

Note that  $W(y_1, y_2, \dots, y_n)(x)$  is a function of  $x$  and, therefore, should be referred to a range of definition of  $x$ .

From linear algebra we know that if  $W(y_1, y_2, \dots, y_n)(x) \neq 0$ , then the only solution of this system of equations is  $c_1 = c_2 = \dots = c_n = 0$ , i.e. functions  $y_i(x)$  are linearly independent. Conversely, if  $W(y_1, y_2, \dots, y_n)(x) = 0$ , then functions  $y_i(x)$  are linearly dependent.

**Example.** Let us consider the case of  $n=2$  and take

$$y_1(x) = f(x) \quad \text{and} \quad y_2(x) = g(x).$$

**A)** Assume that functions  $f(x)$  and  $g(x)$  are linearly dependent. By definition, this means that it is possible to find such a combination of non-zero coefficients  $c_1$  and  $c_2$  that

$$c_1 f(x) + c_2 g(x) = 0.$$

Demonstrate that in this case Wronskian  $W(f, g)(x)$  is zero. Indeed, if the above equation is differentiated with respect to  $x$ , we obtain

$$c_1 f'(x) + c_2 g'(x) = 0.$$

Then  $W(f, g)(x)$  is

$$\begin{vmatrix} f & g \\ f' & g' \end{vmatrix} = \frac{1}{c_1} \begin{vmatrix} c_1 f & g \\ c_1 f' & g' \end{vmatrix} = \frac{1}{c_1} \begin{vmatrix} c_1 f + c_2 g & g \\ c_1 f' + c_2 g' & g' \end{vmatrix} = \frac{1}{c_1} \begin{vmatrix} 0 & g \\ 0 & g' \end{vmatrix} = 0,$$

where we used the properties of determinants and the fact that  $c_1 f + c_2 g = 0$  and  $c_1 f' + c_2 g' = 0$ . Similar considerations apply for the Wronskian of  $n$  functions.

Alternatively, calculate the Wronskian explicitly:

$$W(f, g)(x) = \begin{vmatrix} f(x) & g(x) \\ f'(x) & g'(x) \end{vmatrix} = f(x)g'(x) - f'(x)g(x)$$

From  $c_1 f + c_2 g = 0$  and  $c_1 f' + c_2 g' = 0$  we find that

$$f = -\frac{c_2 g}{c_1} \quad \text{and} \quad f' = -\frac{c_2 g'}{c_1}.$$

Hence,

$$W(f, g)(x) = f g' - f' g = -\frac{c_2 g}{c_1} g' + \frac{c_2 g'}{c_1} g = 0.$$

**B)** Conversely, prove that if  $W(f, g) \neq 0$ , then  $f(x)$  and  $g(x)$  are linearly independent. Consider a system of linear equations with respect to coefficients  $c_1$  and  $c_2$ :

$$\begin{aligned} c_1 f(x) + c_2 g(x) &= 0 \\ c_1 f'(x) + c_2 g'(x) &= 0 \end{aligned}$$

or, in the matrix form,

$$\mathbf{A}\mathbf{c} = \mathbf{b},$$

where  $\mathbf{b} = 0$  and

$$\mathbf{A} = \begin{pmatrix} f(x) & g(x) \\ f'(x) & g'(x) \end{pmatrix}$$

Since  $\det(\mathbf{A}) = W(f, g) \neq 0$ , we can find  $\mathbf{A}^{-1}$  and, therefore, find  $\mathbf{c}$

$$\mathbf{c} = \mathbf{A}^{-1}\mathbf{b}.$$

However, since  $\mathbf{b} = 0$ ,  $\mathbf{c}$  is also zero. Thus, functions  $f(x)$  and  $g(x)$  are linearly independent. The same considerations apply for any value of  $n$ .

### 3.7 Variation of parameters.

Let us solve the ODE

$$a_n(x)y^{(n)} + a_{n-1}(x)y^{(n-1)} + \dots + a_2(x)y'' + a_1(x)y' + a_0(x)y = f(x), \quad (3.2)$$

where coefficients  $a_i(x)$  may or may not be functions of  $x$ . First, assume that the complementary solution of the equation

$$a_n(x)y^{(n)} + a_{n-1}y^{(n-1)} + \dots + a_2(x)y'' + a_1(x)y' + a_0(x)y = 0$$

is known and is represented in the form

$$y_c(x) = c_1 y_1(x) + c_2 y_2(x) + \dots + c_n y_n(x),$$

where  $c_i$  are numbers and  $y_i(x)$  are known linearly independent functions.

We will consider a particular solution of the inhomogeneous equation in the form

$$y_p(x) = k_1(x)y_1(x) + k_2(x)y_2(x) + \dots + k_n(x)y_n(x),$$

where coefficients  $k_i(x)$  are, in general, functions of  $x$ . These functions can be determined if we can impose  $n$  non-equivalent conditions on them. The ODE itself gives one of these conditions. How to choose the others?

**Example: n=2.** Consider the equation

$$a_2(x)y'' + a_1(x)y' + a_0(x)y = f(x). \quad (3.3)$$

and assume that the solutions of the corresponding homogeneous equation – functions  $y_1(x)$  and  $y_2(x)$  – are known. Then,

$$y_c(x) = c_1y_1(x) + c_2y_2(x)$$

is a complementary function.

Consider a particular solution in the form

$$y_p(x) = k_1(x)y_1(x) + k_2(x)y_2(x)$$

Substitute  $y_p(x)$  into the original equation (3.3):

$$f(x) = a_0(k_1y_1 + k_2y_2) + a_1\frac{d}{dx}(k_1y_1 + k_2y_2) + a_2\frac{d^2}{dx^2}(k_1y_1 + k_2y_2).$$

$$\begin{aligned} f(x) &= a_0(k_1y_1 + k_2y_2) \\ &+ a_1(k'_1y_1 + k'_2y_2) + a_1(k_1y'_1 + k_2y'_2) \\ &+ a_2\frac{d}{dx}(k'_1y_1 + k'_2y_2) + a_2(k'_1y'_1 + k'_2y'_2) + a_2(k_1y''_1 + k_2y''_2). \end{aligned}$$

If we impose conditions

$$k'_1y_1 + k'_2y_2 = 0 \quad \text{and} \quad f(x) = a_2(k'_1y'_1 + k'_2y'_2), \quad (3.4)$$

this equation becomes

$$0 = a_0(k_1y_1 + k_2y_2) + a_1(k_1y'_1 + k_2y'_2) + a_2(k_1y''_1 + k_2y''_2).$$

After regrouping this gives

$$0 = k_1(a_0y_1 + a_1y'_1 + a_2y''_1) + k_2(a_0y_2 + a_1y'_2 + a_2y''_2),$$

which is satisfied because  $y_1(x)$  and  $y_2(x)$  are components of the complementary function. Hence, if coefficients  $k_1(x)$  and  $k_2(x)$  are chosen according to conditions in Eqs. (3.4), then function

$$y_p(x) = k_1(x)y_1(x) + k_2(x)y_2(x)$$

is, indeed, a particular solution of equation (3.3).

**Can we extend this method to the higher order ODEs?** If the particular solution of  $n^{th}$  order equation is ( $k_i$  and  $y_i$  are functions of  $x$ )

$$y_p = k_1 y_1 + k_2 y_2 + \dots + k_n y_n,$$

then its first derivative is

$$y'_p = k_1 y'_1 + k_2 y'_2 + \dots + k_n y'_n + (k'_1 y_1 + k'_2 y_2 + \dots + k'_n y_n).$$

By analogy with the case of  $n=2$  [see the first condition in Eqs.(3.4)], request that

$$(\dots) = k'_1 y_1 + k'_2 y_2 + \dots + k'_n y_n = 0.$$

Then, the second derivative of  $y_p$  is

$$y''_p = k_1 y''_1 + k_2 y''_2 + \dots + k_n y''_n + (k'_1 y'_1 + k'_2 y'_2 + \dots + k'_n y'_n).$$

Again, request that

$$(\dots) = k'_1 y'_1 + k'_2 y'_2 + \dots + k'_n y'_n = 0.$$

Carry out this procedure  $n-1$  times and obtain  $n-1$  conditions with respect to the functions  $k_i(x)$ :

$$\sum_{i=1}^n k'_i(x) y_i^{(0)}(x) = 0 \quad \sum_{i=1}^n k'_i(x) y_i^{(1)}(x) = 0 \quad \dots \quad \sum_{i=1}^n k'_i(x) y_i^{(n-2)}(x) = 0.$$

Finally, calculate  $n^{th}$  derivative of  $y_p$ :

$$y_p^{(n)} = k_1 y_1^{(n)} + k_2 y_2^{(n)} + \dots + k_n y_n^{(n)} + (k'_1 y_1^{(n-1)} + k'_2 y_2^{(n-1)} + \dots + k'_n y_n^{(n-1)}).$$

In order to obtain the  $n^{th}$  condition, substitute  $y_p$ ,  $y'_p$ ,  $y''_p$ , ...,  $y^{(n)}$  into Eq. (3.2). This gives

$$\sum_{m=0}^n a_m y_p^{(m)} = \sum_{m=0}^n a_m \left( \sum_{i=1}^n k_i y_i^{(m)} \right) + a_n \left( k'_1 y_1^{(n-1)} + \dots + k'_n y_n^{(n-1)} \right) = f(x).$$

Since both sums a finite, we can rearrange the order of summation in the first term:

$$\sum_{i=1}^n k_i \left( \sum_{m=0}^n a_m y_i^{(m)} \right) + a_n \left( k'_1 y_1^{(n-1)} + k'_2 y_2^{(n-1)} + \dots + k'_n y_n^{(n-1)} \right) = f(x).$$

The first term vanishes for any  $k_i(x)$  because functions  $y_i(x)$  are solutions of the homogeneous equation. Hence, the  $n^{th}$  condition is

$$a_n \left( k'_1 y_1^{(n-1)} + k'_2 y_2^{(n-1)} + \dots + k'_n y_n^{(n-1)} \right) = f(x),$$

which is equivalent to the  $2^{nd}$  condition for the case of  $n=2$  considered above:

$$a_2(k'_1 y'_1 + k'_2 y'_2) = f(x).$$

**Existence of  $k_i(x)$ .** The  $n$  conditions with respect to functions  $k_i(x)$  ( $i=1,2,\dots,n$ ) are equivalent to a system of  $n$  linear equations with respect to their first derivatives  $k'_i(x)$ .

$$\begin{pmatrix} y_1(x) & y_2(x) & \dots & y_{n-1}(x) & y_n(x) \\ y'_1(x) & y'_2(x) & \dots & y'_{n-1}(x) & y'_n(x) \\ \dots & \dots & \dots & \dots & \dots \\ y_1^{(n-2)}(x) & y_2^{(n-2)}(x) & \dots & y_{n-1}^{(n-2)}(x) & y_n^{(n-2)}(x) \\ y_1^{(n-1)}(x) & y_2^{(n-1)}(x) & \dots & y_{n-1}^{(n-1)}(x) & y_n^{(n-1)}(x) \end{pmatrix} \begin{pmatrix} k'_1(x) \\ k'_2(x) \\ \dots \\ k'_{n-1}(x) \\ k'_n(x) \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ \dots \\ 0 \\ f(x)/a_n(x) \end{pmatrix}$$

This system of equations can be solved if determinant

$$\begin{vmatrix} y_1(x) & y_2(x) & \dots & y_{n-1}(x) & y_n(x) \\ y'_1(x) & y'_2(x) & \dots & y'_{n-1}(x) & y'_n(x) \\ \dots & \dots & \dots & \dots & \dots \\ y_1^{(n-2)}(x) & y_2^{(n-2)}(x) & \dots & y_{n-1}^{(n-2)}(x) & y_n^{(n-2)}(x) \\ y_1^{(n-1)}(x) & y_2^{(n-1)}(x) & \dots & y_{n-1}^{(n-1)}(x) & y_n^{(n-1)}(x) \end{vmatrix} = W(y_1, y_2, \dots, y_n)(x) \neq 0.$$

Since functions  $y_i(x)$  are independent solutions of the homogeneous ODE, the Wronskian  $W(y_1, y_2, \dots, y_n)(x) \neq 0$  at least at some points  $x$ . Hence, it is always possible to find functions  $k'_i(x)$  by solving this system of equations and, therefore, it is possible to find functions  $k_i(x)$  by integrating  $k'_i(x)$ .

Note that integration of  $k'_i(x)$  gives rise to an arbitrary constant for each  $i$ . We can write  $k_i(x)$  as

$$k_i(x) = \tilde{k}_i(x) + d_i \quad (i=1,2,\dots,n),$$

where  $d_i$  are arbitrary constants and functions  $\tilde{k}_i(x)$  contain no terms independent on  $x$ . Hence, the full solution of the Equation (3.2) is

$$y(x) = y_c(x) + y_p(x) = \sum_{i=1}^n c_i y_i(x) + \sum_{i=1}^n (\tilde{k}_i(x) + d_i) y_i(x) = \sum_{i=1}^n (\tilde{k}_i(x) + d_i + c_i) y_i(x),$$

which is equivalent to

$$y(x) = y_c(x) + y_p(x) = \sum_{i=1}^n (\tilde{k}_i(x) + C_i)y_i(x),$$

where  $C_i$  are a new set of arbitrary constants.

**Example.** Find general solution of the inhomogeneous equation

$$\frac{d^2y}{dx^2} + y = x.$$

General solution of the corresponding homogeneous equation is

$$y_c(x) = c_1 y_1(x) + c_2 y_2(x) = c_1 \sin x + c_2 \cos x.$$

Consider a particular solution in the form of

$$y_p(x) = k_1(x) \sin x + k_2(x) \cos x,$$

subject to the conditions

$$k'_1(x)y_1(x) + k'_2y_2(x) = k'_1(x) \sin x + k'_2 \cos x = 0$$

and

$$k'_1(x)y'_1(x) + k'_2y'_2(x) = k'_1(x) \sin x - k'_2 \cos x = x.$$

From the 1st condition:

$$k'_1 = -k'_2 \frac{\cos x}{\sin x}.$$

Hence, the 2nd condition gives

$$-k'_2 \left( \cos x \frac{\cos x}{\sin x} + \sin x \right) = -k'_2 \frac{\cos^2 x + \sin^2 x}{\sin x} = -k'_2 \frac{1}{\sin x} = x.$$

From here:

$$k'_2 = -x \sin x \quad \text{and} \quad k'_1 = x \cos x.$$

Integrate  $k'_1$  and  $k'_2$  by parts:

$$k_1(x) = \int x \cos x dx = x \sin x - \int \sin x dx = x \sin x + \cos x + d_1$$

$$k_2(x) = - \int x \sin x dx = x \cos x - \int \cos x dx = x \cos x - \sin x + d_2.$$

Thus,

$$\begin{aligned} y(x) &= (c_1 + x \sin x + \cos x + d_1) \sin x + (c_2 + x \cos x - \sin x + d_2) \cos x \\ &= (a_1 \sin x + a_2 \cos x) + x \sin^2 x + \cos x \sin x + x \cos^2 x - \sin x \cos x \\ &= (a_1 \sin x + a_2 \cos x) + x, \end{aligned}$$

where  $c_1$ ,  $c_2$ ,  $d_1$ , and  $d_2$  are arbitrary constants and we set  $a_1 = c_1 + d_1$  and  $a_2 = c_2 + d_2$ .

### 3.8 The Dirac delta function.

**Definition.** Let us introduce a function  $\delta(x)$  with properties

$$\delta(x - a) = \begin{cases} 0 & \text{if } x \neq a \\ \infty & \text{if } x = a \end{cases}$$

where constant  $a$  is finite and

$$\int_{-\infty}^{\infty} \delta(x) dx = 1.$$

This function is also called *impulse function* because it can be used to represent external perturbation: finite in magnitude and infinitely short in duration.

The  $\delta$ -function belongs to a class of *generalised functions*, i.e., its properties are determined by the properties of integrals with *probe functions*  $f(x)$ :

$$\int_{\infty}^{+\infty} f(x) \delta(x - a) dx,$$

where:

1. function  $f(x)$  is defined on a required interval of  $x$ , e.g.,  $x \in (-\infty, +\infty)$ ;
2.  $f(x)$  and all of its derivatives are continuous and finite functions of  $x$ ;
3.  $f(x) = 0$  for all values of  $x$  outside of some finite interval  $[x_1, x_2]$ .

**Properties of the  $\delta$ -function.** It follows from the definition that a product of  $\delta(x - a)$  and any finite function is zero everywhere except  $x = a$ . Hence

$$\int_{-\infty}^{\infty} f(x) \delta(x - x_0) dx = f(x_0) \int_{-\infty}^{\infty} \delta(x - x_0) dx = f(x_0).$$

To find  $\delta(-x)$ , we have to consider integral

$$\int_{-\infty}^{\infty} f(x) \delta(-x) dx.$$

After substituting  $x = -t$  and  $dx = -dt$ , we have

$$\int_{-\infty}^{\infty} f(x) \delta(-x) dx = \int_{+\infty}^{-\infty} f(-t) \delta(t) (-dt) = \int_{-\infty}^{\infty} f(-t) \delta(t) dt = f(0) = \int_{-\infty}^{\infty} f(t) \delta(t) dt.$$

Compare the left and right hand sides of this equation:

$$\int_{-\infty}^{\infty} f(x)\delta(-x)dx = \int_{-\infty}^{\infty} f(t)\delta(t)dt$$

for any probe function  $f(x)$ . Hence,

$$\delta(-x) = \delta(x).$$

Similarly, to calculate  $\delta(ax)$  we need to consider integral

$$\int_{-\infty}^{\infty} f(x)\delta(ax)dx.$$

Substitute  $ax = t$ , then  $dx = dt/a$

$$\int_{-\infty}^{\infty} f(x)\delta(ax)dx = \int_{-\infty}^{\infty} f(t/a)\delta(t)\frac{dt}{a} = \frac{1}{a}f(0/a) = \frac{1}{a}f(0) = \frac{1}{a} \int_{-\infty}^{\infty} f(s)\delta(s)ds$$

Hence

$$\delta(ax) = \frac{1}{a}\delta(x).$$

It follows that for negative  $b$ :

$$\delta(bx) = \delta(-|b|x) = \delta(|b|x) = \frac{1}{|b|}\delta(x).$$

Thus, by combining  $\delta(-x) = \delta(x)$  and  $\delta(ax) = (1/a)\delta(x)$ , obtain

$$\delta(ax) = \frac{1}{|a|}\delta(x) \quad \text{for any real } a.$$

**Laplace transform of the  $\delta$ -function.** Evaluate  $L[\delta(x - a)]$ :

$$L[\delta(x - a)] = \int_0^{\infty} \delta(x - a)e^{-px}dx = e^{-pa} \quad (\text{for } a > 0)$$

**Derivatives of the  $\delta$  function.** To attach meaning to  $\delta'(x - a)$ , consider

$$\int_{-\infty}^{\infty} f(x)\delta'(x - a)dx = f(x)\delta(x - a)|_{-\infty}^{+\infty} - \int_{-\infty}^{\infty} f'(x)\delta(x - a)dx = -f'(a).$$

The term  $f(x)\delta(x - a)|_{-\infty}^{+\infty} = 0$  because probe functions  $f(x) = 0$  for all  $x$  outside of some finite interval  $[x_1, x_2]$ .

Similarly, we can find the  $n^{th}$  derivative of the  $\delta(x - a)$  function by calculating  $\int_{-\infty}^{\infty} f(x)\delta^{(n)}(x - a)dx$ . Integrating it by parts  $n$  times gives

$$\int_{-\infty}^{\infty} f(x)\delta^{(n)}(x - a)dx = (-1)^n \int_{-\infty}^{\infty} f^{(n)}(x)\delta(x - a)dx = (-1)^n f^{(n)}(a).$$

**Other generalised functions.** Consider the following examples:

1)  $x\delta(x)$ :

$$\int_{-\infty}^{\infty} f(x)[x\delta(x)]dx = \int_{-\infty}^{\infty} [f(x)x]\delta(x)dx = 0 \cdot f(0) = 0$$

2)  $x\delta'(x)$ :

$$\int_{-\infty}^{\infty} f(x)[x\delta'(x)]dx = xf(x)\delta(x)|_{-\infty}^{\infty} - \int_{\infty}^{\infty} [f(x) + xf'(x)]\delta(x)dx = -f(0)$$

3)  $x^2\delta''(x)$ :

$$\begin{aligned} \int_{-\infty}^{\infty} f(x)[x^2\delta''(x)]dx &= x^2f(x)\delta''(x)|_{-\infty}^{\infty} - \int_{\infty}^{\infty} [2xf(x) + x^2f'(x)]\delta'(x)dx \\ &= -[2xf(x) + x^2f'(x)]\delta(x)|_{-\infty}^{\infty} + \\ &\quad \int_{\infty}^{\infty} [2f(x) + 2xf'(x) + 2xf''(x) + x^2f''(x)]\delta(x)dx \\ &= 2f(0) \end{aligned}$$

Thus,

$$x\delta(x) = 0, \quad x\delta'(x) = -\delta(x), \quad x^2\delta''(x) = 2\delta(x).$$

**Gaussian distribution.** The normal distribution, also known as Gaussian distribution, is given by

$$g(x, a, \sigma) = \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{(x-a)^2}{2\sigma^2}}.$$

In the limit of infinitely small  $\sigma$  ( $\sigma \rightarrow 0$ ) function  $g(x, a, \sigma)$  behaves similarly to the  $\delta(x - a)$  in that

$$\lim_{\sigma \rightarrow 0} \int_{-\infty}^{+\infty} f(x)g(x, a, \sigma)dx = f(a)$$

Yet, we will not equate  $\delta(x - a)$  and

$$\lim_{\sigma \rightarrow 0} g(x, a, \sigma)$$

because  $\delta(x - a)$  is a generalised function defined via its integral with other functions

$$\int f(x)\delta(x - a)dx,$$

while  $g(x, a, \sigma)$  is a function in the usual sense.

### 3.9 Green's functions.

We can represent the left-hand-side of an ODE

$$a_n(x)y^{(n)} + a_{n-1}(x)y^{(n-1)} + \dots + a_2(x)y'' + a_1(x)y' + a_0(x)y = f(x) \quad (3.5)$$

in the form

$$\mathcal{L}(x)y(x) = f(x),$$

where the operator  $\mathcal{L}(x)$  is

$$\mathcal{L}(x) = a_n(x)\frac{d^n}{dx^n} + a_{n-1}(x)\frac{d^{n-1}}{dx^{n-1}} + \dots + a_1(x)\frac{d}{dx} + a_0(x).$$

Let us suppose that there is a function  $G(x, t)$ , such that the solution of the Equation 3.5 is derived by integrating  $f(x)$  with  $G(x, t)$ :

$$y(x) = \int_a^b G(x, t)f(t)dt. \quad (3.6)$$

Note that the integral is a definite one:  $a$  and  $b$  define the interval of possible values of  $x$ :  $a \leq x \leq b$ .

**Does  $G(x, t)$  exist and, if so, how to find it?**

Let us derive a differential equation with respect to  $G(x, t)$ . Apply the operator  $\mathcal{L}(x)$  to both sides of the Equation (3.6):

$$\mathcal{L}(x)y(x) = f(x) = \int_a^b [\mathcal{L}(x)G(x, t)f(t)] dt \quad (3.7)$$

and compare this equation with

$$f(x) = \int_a^b \delta(t - x)f(t)dt. \quad (3.8)$$

The operator  $\mathcal{L}(x)$  in the RHS of Eq. (3.7) is acting of the function  $G(x, t)$  only; it does not act on  $f(t)$  because  $\mathcal{L}(x)$  depends on the variable  $x$  and  $f(t)$  depends on the variable  $t$ .

Since the left hand sides in Equations (3.7) and (3.8) are the same, we have to equate their right hand sides:

$$\int_a^b \delta(t - x)f(t)dt = \int_a^b [\mathcal{L}(x)G(x, t)f(t)] dt,$$

which means that

$$\int_a^b [\delta(t - x) - \mathcal{L}(x)G(x, t)] f(t) dt = 0.$$

This equation is valid for any  $f(t)$  if the function  $G(x, t)$  satisfies:

$$\mathcal{L}(x)G(x, t) = \delta(t - x),$$

or

$$\left( a_n(x) \frac{d^n}{dx^n} + a_{n-1}(x) \frac{d^{n-1}}{dx^{n-1}} + \dots + a_1(x) \frac{d}{dx} + a_0(x) \right) G(x, t) = \delta(t - x), \quad (3.9)$$

i.e., function  $G(x, t)$  should satisfy the same ODE as function  $y(x)$ , but with a specific right-hand-side.

**Other restrictions on  $G(x, t)$ :**

- 1) Boundary conditions. If, for example,  $y(a) = y(b) = 0$ , we can request that  $G(a, t) = G(b, t) = 0$  for *any* value of  $t$ . Clearly, equation (3.6) will be satisfied in this case.
- 2) Continuity and discontinuity of  $G(x, t)$ ,  $G'(x, t)$ , ...,  $G^{(n-1)}(x, t)$  at  $x=t$ . [Function  $\delta(t - x)$ , see Eq. (3.9), is a generalised function which turns to infinity at  $x=t$ .]

### 3.9.1 Continuity of $G(x, t)$ at $x = t$ : 2<sup>nd</sup> order ODE.

Let us consider the 2nd order equation

$$a_2(x)y''(x) + a_1(x)y'(x) + a_0(x)y(x) = f(x), \quad x \in [a, b],$$

where  $y(a) = y(b) = 0$ .

The Green's function for this equation should satisfy

$$a_2(x)G''(x, t) + a_1(x)G'(x, t) + a_0(x)G(x, t) = \delta(x - t), \quad x \in [a, b]$$

and  $G(a, t) = G(b, t) = 0$ .

Investigate the behaviour of  $G(x, t)$  near the point  $x = t$ .

Integrate both parts of the Eq. for  $G(x, t)$  with respect to  $x$  near  $x = t$ , i.e., in the interval of  $x \in [t - \epsilon, t + \epsilon]$ , where  $\epsilon$  is small. Integration of the right hand side gives

$$\int_{t-\epsilon}^{t+\epsilon} \delta(x - t) dx = 1.$$

Integration of the left hand side gives three terms:

$$\begin{aligned} I_0(t, \epsilon) &= \int_{t-\epsilon}^{t+\epsilon} a_0(x) G(x, t) dx \\ I_1(t, \epsilon) &= \int_{t-\epsilon}^{t+\epsilon} a_1(x) G'(x, t) dx = [a_1(x) G(x, t)]_{t-\epsilon}^{t+\epsilon} - \int_{t-\epsilon}^{t+\epsilon} a'_1(x) G(x, t) dx \\ I_2(t, \epsilon) &= \int_{t-\epsilon}^{t+\epsilon} a_2(x) G''(x, t) dx = [a_2(x) G'(x, t)]_{t-\epsilon}^{t+\epsilon} - \int_{t-\epsilon}^{t+\epsilon} a'_2(x) G'(x, t) dx = \\ &= [a_2(x) G'(x, t)]_{t-\epsilon}^{t+\epsilon} - [a'_2(x) G(x, t)]_{t-\epsilon}^{t+\epsilon} + \int_{t-\epsilon}^{t+\epsilon} a''_2(x) G(x, t) dx. \end{aligned}$$

Collect these terms together:

$$I_0(t, \epsilon) + I_1(t, \epsilon) + I_2(t, \epsilon) = 1.$$

After rearranging the contributions in  $I_k(t, \epsilon)$ , we obtain:

$$\int_{t-\epsilon}^{t+\epsilon} (a_0 - a'_1 + a''_2) G(x, t) dx + [(a_1 - a'_2) G(x, t)]_{t-\epsilon}^{t+\epsilon} + [a_2 G'(x, t)]_{t-\epsilon}^{t+\epsilon} = 1. \quad (3.10)$$

We assume that coefficients  $a(x)$  and their derivatives are continuous functions. Then, their linear combinations are also continuous functions. For simplicity, set:

$$p_0(x) = a_0(x) - a'_1(x) + a''_2(x), \quad p_1(x) = a_1(x) - a'_2(x), \quad p_2(x) = a_2(x).$$

Then, the equality (3.10) becomes

$$\int_{t-\epsilon}^{t+\epsilon} p_0(x) G(x, t) dx + [p_1(x) G(x, t)]_{t-\epsilon}^{t+\epsilon} + [p_2(x) G'(x, t)]_{t-\epsilon}^{t+\epsilon} = 1. \quad (3.11)$$

Let us consider the limit of the left hand side of Eq. (3.11) for  $\epsilon \rightarrow 0$ . Since  $p_k(x)$  are continuous functions, we can define  $J_k$  as

$$\begin{aligned} J_0 &= \lim_{\epsilon \rightarrow 0} \left\{ \int_{t-\epsilon}^{t+\epsilon} p_0(x) G(x, t) dx \right\} = p_0(t) \lim_{\epsilon \rightarrow 0} \left\{ \int_{t-\epsilon}^{t+\epsilon} G(x, t) dx \right\}, \\ J_1 &= \lim_{\epsilon \rightarrow 0} \left\{ [p_1(x) G(x, t)]_{t-\epsilon}^{t+\epsilon} \right\} = p_1(t) \lim_{\epsilon \rightarrow 0} \left\{ [G(x, t)]_{t-\epsilon}^{t+\epsilon} \right\} = p_1(t) \lim_{\epsilon \rightarrow 0} \{G(t + \epsilon, t) - G(t - \epsilon, t)\} \\ J_2 &= \lim_{\epsilon \rightarrow 0} \left\{ [p_2(x) G'(x, t)]_{t-\epsilon}^{t+\epsilon} \right\} = p_2(t) \lim_{\epsilon \rightarrow 0} \left\{ [G'(x, t)]_{t-\epsilon}^{t+\epsilon} \right\} = p_2(t) \lim_{\epsilon \rightarrow 0} \{G'(t + \epsilon, t) - G'(t - \epsilon, t)\}, \end{aligned}$$

where, according to the Eq. (3.11) above,  $J_0 + J_1 + J_2 = 1$ .

If we assume that  $G'(x, t)$  is continuous at  $x = t$ , i.e.,

$$\lim_{\epsilon \rightarrow 0} \{G'(t + \epsilon, t) - G'(t - \epsilon, t)\} = 0,$$

then  $G(x, t)$  is also continuous and so is  $\int G(x, t) dx$ . In other words,  $J_2 = 0$ ,  $J_1 = 0$ , and  $J_0 = 0$  and, consequently,

$$J_0 + J_1 + J_2 = 0,$$

which contradicts to the Eq. (3.11).

Alternatively, if we assume that  $G'(x, t)$  has a finite discontinuity at  $x = t$ , i.e.,

$$p_2(t) \lim_{\epsilon \rightarrow 0} \{G'(t + \epsilon, t) - G'(t - \epsilon, t)\} = 1,$$

then  $G(x, t)$  and  $\int G(x, t) dx$  are continuous functions, i.e.,  $J_2 = 1$  and  $J_1 = J_0 = 0$  and, consequently,

$$J_0 + J_1 + J_2 = 1$$

as required by the Eq (3.11).

Thus, the continuity and discontinuity conditions for  $G(x, t)$  are:

$$\lim_{\epsilon \rightarrow 0} \{G'(t + \epsilon, t) - G'(t - \epsilon, t)\} = \frac{1}{a_2(x)} \quad (3.12)$$

$$\lim_{\epsilon \rightarrow 0} \{G(t + \epsilon, t) - G(t - \epsilon, t)\} = 0. \quad (3.13)$$

### 3.9.2 Continuity of $G(x, t)$ at $x = t$ : $n^{th}$ order ODE.

Consider an infinitely small region of  $x$  in the vicinity of  $x=t$ :  $x \in [t-\epsilon, t+\epsilon]$ . Integrate both parts of Eq. (3.9) over  $x \in [t-\epsilon, t+\epsilon]$ . Integration of the right hand side gives

$$\int_{t-\epsilon}^{t+\epsilon} \delta(t-x) dx = 1$$

by the definition of the  $\delta$  function.

Before integrating the left part of Eq. (3.9), let us introduce auxiliary functions

$$I_k(g(x)) = \int_{t-\epsilon}^{t+\epsilon} g(x) \frac{d^{n+1-k}}{dx^{n+1-k}} G(x, t) dx$$

and

$$S_k(g(x)) = \left[ g(x) \frac{d^{n-k}}{dx^{n-k}} G(x, t) \right]_{t-\epsilon}^{t+\epsilon} = g(t+\epsilon)G^{(n-k)}(t+\epsilon, t) - g(t-\epsilon)G^{(n-k)}(t-\epsilon, t),$$

where  $n$  is the order of the ODE in Eq. (3.9) and  $g(x)$  is some continuous function of  $x$ . Then, integration of the first term of the left hand side (LHS) of Eq. (3.9) gives

$$I_1(a_n) = \int_{t-\epsilon}^{t+\epsilon} a_n(x) \frac{d^n}{dx^n} G(x, t) dx,$$

which, when integrated by parts, becomes

$$I_1(a_n) = \left[ a_n(x) \frac{d^{n-1}}{dx^{n-1}} G(x, t) \right]_{t-\epsilon}^{t+\epsilon} - \int_{t-\epsilon}^{t+\epsilon} a'_n(x) \frac{d^{n-1}}{dx^{n-1}} G(x, t) dx.$$

Using the auxiliary functions  $I_k(g(x))$  and  $S_k(g(x))$ , we notice that

$$I_1(a_n) = S_1(a_n) - I_2(a'_n),$$

where [apply the general definition for  $I_k(g(x))$  and  $S_k(g(x))$  ]

$$S_1(a_n) = [a_n(t + \epsilon)G^{(n-1)}(t + \epsilon, t) - a_n(t - \epsilon)G^{(n-1)}(t - \epsilon, t)]$$

and

$$I_2(a'_n) = \int_{t-\epsilon}^{t+\epsilon} a'_n(x) G^{(n-1)}(x, t) dx.$$

Similarly, integration of the second term in the LHS of Eq. (3.9) gives:

$$I_2(a_{n-1}) = \int_{t-\epsilon}^{t+\epsilon} a_{n-1}(x) \frac{d^{n-1}}{dx^{n-1}} G(x, t) dx = S_2(a_{n-1}) - I_3(a'_{n-1}),$$

where

$$S_2(a_{n-1}) = [a_{n-1}(t + \epsilon) G^{(n-2)}(t + \epsilon, t) - a_{n-1}(t - \epsilon) G^{(n-2)}(t - \epsilon, t)]$$

and

$$I_3(a'_{n-1}) = \int_{t-\epsilon}^{t+\epsilon} a'_{n-1}(x) G^{(n-2)}(x, t) dx.$$

Note that  $I_2(a'_n)$  and  $I_2(a_{n-1})$  have  $(n-1)^{th}$  derivative under the integral, i.e.

$$I_2(a'_n) - I_2(a_{n-1}) = I_2(a'_n - a_{n-1}).$$

Thus, integrating the first two terms of Eq. (3.9) gives:

$$I_1(a_n) + I_2(a_{n-1}) = S_1(a_n) - I_2(a'_n) + I_2(a_{n-1}) = S_1(a_n) + S_2(-a'_n + a_{n-1}) - I_3(-a''_n + a'_{n-1}).$$

For convenience, we can introduce functions  $p_k(a)$ , which are linear combinations of various derivatives of  $a_m(x)$ , such that

$$\begin{aligned} p_1(x) &= a_n(x) \\ p_2(x) &= -p'_1(x) + a_{n-1}(x) = -a'_n(x) + a_{n-1}(x) \\ p_3(x) &= -p'_2(x) + a_{n-2}(x) = a''_n(x) - a'_{n-1}(x) + a_{n-2}(x) \\ &\dots &&\dots \\ p_n(x) &= -p'_{n-1}(x) + a_1(x) \\ p_{n+1}(x) &= -p'_n(x) + a_0(x) \end{aligned}$$

Then,

$$I_1(a_n) + I_2(a_{n-1}) = S_1(p_1) + S_2(p_2) - I_3(p'_2).$$

Since functions  $I_k$  are linear, we can write  $-I_3(p'_2) = I_3(-p'_2)$ :

$$I_1(a_n) + I_2(a_{n-1}) = S_1(p_1) + S_2(p_2) + I_3(-p'_2).$$

We can use this relation in order to re-write the integral of Eq. (3.9) as a sum

$$I_1(a_n) + I_2(a_{n-1}) + \dots + I_{n+1}(a_0).$$

Taking into account that the integral of the right-hand side of (3.9) is 1 (see above), we have:

$$\begin{aligned}
\int_{t-\epsilon}^{t+\epsilon} \mathcal{L}G(x, t) dx &= I_1(a_n) + I_2(a_{n-1}) + \dots + I_n(a_1) + I_{n+1}(a_0) \\
&= S_1(p_1) + S_2(p_2) + \dots + S_n(p_n) + I_{n+1}(-p'_n) + I_{n+1}(a_0) \\
&= S_1(p_1) + S_2(p_2) + \dots + S_n(p_n) + I_{n+1}(-p'_n + a_0) \\
&= S_1(p_1) + S_2(p_2) + \dots + \int_{t-\epsilon}^{t+\epsilon} p_{n+1}(x) G(x, t) dx \\
&= \int_{t-\epsilon}^{t+\epsilon} \delta(x - t) dx \\
&= 1
\end{aligned} \tag{3.14}$$

Consider the limit of Eq. (3.14) for  $\epsilon \rightarrow 0$ . Since, functions  $p_k$  are derived from continuous functions  $a_m$ , they are also continuous. Therefore, for each  $S_k(p_k)$ :

$$\begin{aligned}
\lim_{\epsilon \rightarrow 0} S_k(p_k) &= \lim_{\epsilon \rightarrow 0} [p_k(t + \epsilon) G^{(n-k)}(t + \epsilon, t) - p_k(t - \epsilon) G^{(n-k)}(t - \epsilon, t)] \\
&= p_k(t) \lim_{\epsilon \rightarrow 0} [G^{(n-k)}(t + \epsilon, t) - G^{(n-k)}(t - \epsilon, t)]
\end{aligned}$$

and, if  $G^{(n-k)}(x, t)$  is continuous at  $x = t$ , then

$$\lim_{\epsilon \rightarrow 0} S_k(p_k) = 0.$$

In our case,

$$\lim_{\epsilon \rightarrow 0} \int_{t-\epsilon}^{t+\epsilon} \mathcal{L}G(x, t) dx = 1,$$

which is satisfied if the  $(n-1)^{th}$  derivative of  $G(x, t)$  in Eq. (3.14) has a finite discontinuity at  $x = t$ :

$$p_1(t) \lim_{\epsilon \rightarrow 0} [G^{(n-1)}(t + \epsilon, t) - G^{(n-1)}(t - \epsilon, t)] = 1$$

and all lower derivatives of  $G(x, t)$  are continuous:

$$\lim_{\epsilon \rightarrow 0} [G^{(n-k)}(t + \epsilon, t) - G^{(n-k)}(t - \epsilon, t)] = 0 \quad (\text{for } k=2,3,\dots,n).$$

Clearly, if  $G(x, t)$  is continuous, then  $\int p_{n+1}(x)G(x, t)dx$  is also continuous and

$$\lim_{\epsilon \rightarrow 0} \int_{t-\epsilon}^{t+\epsilon} p_{n+1}(x)G(x, t)dx = 0.$$

Thus, the single discontinuity condition and  $n-1$  continuity conditions for the function  $G(x, t)$  at  $x = t$  are:

$$\lim_{\epsilon \rightarrow 0} \left[ \frac{d^{n-1}G(x, t)}{dx^{n-1}} \right]_{t-\epsilon}^{t+\epsilon} = \frac{1}{a_n(x)} \quad (3.15)$$

and

$$\lim_{\epsilon \rightarrow 0} \left[ \frac{d^k G(x, t)}{dx^k} \right]_{t-\epsilon}^{t+\epsilon} = 0 \quad (\text{for } k=0,1,\dots,n-2). \quad (3.16)$$

Note that  $G(x, t)$  does not depend on the function  $f(x)$  but it does depend on the ODE operator  $\mathcal{L}$  and on the boundary conditions. If the ODE and/or boundary conditions are changed, the  $G(x, t)$  needs to be recalculated.

### 3.9.3 Solving differential equations using Green's function: example.

Find the general solution of the inhomogeneous equation

$$\frac{d^2y}{dx^2} + y = \left( \frac{d^2}{dx^2} + 1 \right) y = \mathcal{L}y = x,$$

where  $y(x)$  satisfies the boundary conditions  $y(0) = y(\pi/2) = 0$ .

First, consider the ODE with respect to  $G(x, t)$

$$\frac{d^2G(x, t)}{dx^2} + G(x, t) = \delta(t - x)$$

and write down solutions for the homogeneous equation for  $x < t$  and  $x > t$  (note that these solutions should be different because of the discontinuity at  $x = t$ ):

$$G(x, t) = \begin{cases} A(t) \sin x + B(t) \cos x & (x < t) \\ C(t) \sin x + D(t) \cos x & (x > t) \end{cases}$$

Use the two boundary conditions and the continuity and discontinuity conditions in order to determine  $A(t)$ ,  $B(t)$ ,  $C(t)$ ,  $D(t)$ . From the boundary conditions we have for  $x < t$

$$G(0, t) = A(t) \sin 0 + B(t) \cos 0 = A(t) \cdot 0 + B(t) \cdot 1 = B(t) = 0$$

and for  $x > t$

$$G(\pi/2, t) = C(t) \sin \pi/2 + D(t) \cos \pi/2 = C(t) \cdot 1 + D(t) \cdot 0 = C(t) = 0.$$

Hence,

$$G(x, t) = \begin{cases} A(t) \sin x & (x < t) \\ D(t) \cos x & (x > t) \end{cases}$$

Continuity condition for  $G(x, t)$  at  $x=t$ :

$$D(t) \cos t - A(t) \sin t = 0$$

Discontinuity condition for  $G'(x, t)$  at  $x=t$ :

$$-D(t) \sin t - A(t) \cos t = 1.$$

Hence,  $A(t) = -\cos t$  and  $D(t) = -\sin t$  and

$$G(x, t) = \begin{cases} -\cos t \sin x & (x < t) \\ -\sin t \cos x & (x > t) \end{cases}$$

Now use this  $G(x, t)$  to find  $y(x)$ :

$$y(x) = \int_0^{\pi/2} G(x, t) f(t) dt = \int_0^x G_{x>t}(x, t) f(t) dt + \int_x^{\pi/2} G_{x<t}(x, t) f(t) dt$$

For  $x > t$ :

$$\int_0^x G(x, t) t dt = \cos x \left[ \int_0^x t (-\sin t) dt \right] = \cos x [x \cos x - \sin x].$$

For  $x > t$ :

$$\int_x^{\pi/2} G(x, t) t dt = \sin x \left[ \int_0^x t (-\cos t) dt \right] = \sin x \left[ -\frac{\pi}{2} + x \sin x + \cos x \right].$$

Thus, a particular solution is:

$$y(x) = x - \frac{\pi}{2} \sin x.$$

Taking into account the solutions of the homogeneous equation, we can write a general solution as

$$y(x) = x - \frac{\pi}{2} \sin x + a_1 \sin x + a_2 \cos x.$$

However, since the boundary conditions demand that  $y(0) = y(\pi/2) = 0$ , the constants  $a_1$  and  $a_2$  are necessarily equal to zero. Thus, the general solution is

$$y(x) = x - \frac{\pi}{2} \sin x.$$

### 3.9.4 Boundary conditions

An  $n^{th}$  order ODE requires  $n$  boundary conditions which can be given in a variety forms. For example,  $n$ -point conditions

$$y(x_1) = y_1, \quad y(x_2) = y_2, \quad \dots, \quad y(x_n) = y_n.$$

or the one point boundary conditions:

$$y(x_0) = a, \quad y'(x_0) = b, \quad \dots, \quad y^{(n)}(x_n) = c.$$

So far, we applied homogeneous boundary conditions. For inhomogeneous ones, use substitution

$$u(x) = y(x) - h(x),$$

where  $h(x)$  is a polynomial function of the order  $n-1$  (i.e. it has  $n$  coefficients), which satisfies to the inhomogeneous boundary conditions. Then function  $u(x)$  will satisfy homogeneous boundary conditions.



# Chapter 4

## Sturm-Liouville theory

### 4.1 The Sturm-Liouville boundary problem.

The Sturm-Liouville form.

$$p(x) \frac{d^2y}{dx^2} + r(x) \frac{dy}{dx} + q(x)y + \lambda \rho(x)y = 0, \quad (4.1)$$

where

$$r(x) = \frac{dp(x)}{dx}.$$

Here,

- $x$  belongs to an interval:  $a \leq x \leq b$ .
- All functions are real.
- Functions  $p(x)$  and  $\rho(x)$  are positive.
- Function  $p(x)$  should have a continuous derivative, i.e.  $r(x)$  is continuous.

Function  $\rho(x)$  is called “weight” or “density”. The value of  $\lambda$  is not specified by the equation. Instead, it is defined via boundary conditions, which  $y(x)$  should satisfy to. For example,

$$a_1y(a) + a_2y'(a) = 0 \quad \text{and} \quad b_1y(b) + b_2y'(b) = 0 \quad (4.2)$$

When the boundary conditions are defined, the above equation becomes a SL boundary problem and  $y(x)$  and  $\lambda$  are called *eigenfunction* and *eigenvalue*, respectively.

**Other representations of the SL form.** The SL form (4.1) can be rewritten as

$$-\left[p(x)\frac{d^2}{dx^2} + \frac{dp(x)}{dx}\frac{d}{dx} + q(x)\right]y(x) = \lambda\rho(x)y(x) \quad (4.3)$$

or

$$-\left[\frac{d}{dx}\left(p(x)\frac{d}{dx}\right) + q(x)\right]y(x) = \lambda\rho(x)y(x). \quad (4.4)$$

Operator

$$\mathcal{L}(x) = -\left[\frac{d}{dx}\left(p(x)\frac{d}{dx}\right) + q(x)\right] \quad (4.5)$$

is called Sturm-Liouville operator. Using this definition, the ODE becomes

$$\mathcal{L}(x)y(x) = \lambda\rho(x)y(x), \quad (4.6)$$

i.e.  $\lambda$  and  $y(x)$  are an eigenvalue and an eigenfunction of the SL differential operator  $\mathcal{L}(x)$ .

**Conversion to the SL form.** Any equation of the form

$$a_2(x)y'' + a_1(x)y' + a_0(x)y + \lambda f(x)y = 0 \quad (4.7)$$

can be converted to the SL form:

$$\left[\frac{d}{dx}\left(p(x)\frac{d}{dx}\right) + q(x) + \lambda\rho(x)\right]y = 0.$$

Therefore, all results obtained for the SL form are valid for any Equation (4.7).

To demonstrate this equivalence, let us set

$$p(x) = F(x)a_2(x), \quad q(x) = F(x)a_0(x), \quad \rho(x) = F(x)f(x)$$

and

$$F(x) = \exp\left(\int_0^x \frac{a_1(u) - a'_2(u)}{a_2(u)}du\right).$$

Then, notice that

$$\begin{aligned} (py')' &= (Fa_2y')' \\ &= F'a_2y' + Fa'_2y' + Fa_2y'' \\ &= \left(\frac{a_1 - a'_2}{a_2}\right)Fa_2y' + Fa'_2y' + Fa_2y'' \\ &= F(a_2y'' + a_1y'). \end{aligned}$$

Thus,

$$(py')' + qy + \lambda\rho y = F(a_2y'' + a_1y' + a_0y + \lambda fy) = 0,$$

i.e. the SL form is equivalent to the original Equation (4.7).

**Example.** Consider the Hermite equation

$$y'' - 2xy' + 2vy = 0.$$

Show that in the SL form  $p(x) = e^{-x^2}$ ,  $q(x) = 0$ ,  $\rho(x) = e^{-x^2}$ , and  $\lambda = 2v$ .

## 4.2 Self-adjoint linear differential operators.

**Lagrange's identity.** Consider the integral

$$\int_a^b (\mathcal{L}[u]) \cdot v \, dx = \int_a^b [-(pu')' + qu] \cdot v \, dx = \int_a^b [-(pu')'v + quv] \, dx$$

for two functions  $u(x)$  and  $v(x)$ , which have continuous 2nd derivatives for  $a \leq x \leq b$ . Integrating the right hand side of this equation by parts gives

$$\begin{aligned} \int_a^b (\mathcal{L}[u]) v \, dx &= - \int_a^b (pu')' v \, dx + \int_a^b quv \, dx \\ &= -(pu')v|_a^b + \int_a^b u'(pv') \, dx + \int_a^b quv \, dx \\ &= -(pu')v|_a^b + puv'|_a^b - \int_a^b u(pv')' \, dx + \int_a^b quv \, dx \\ &= -p[u'v - uv']|_a^b + \int_a^b u(\mathcal{L}[v]) \, dx \end{aligned}$$

Hence,

$$\int_a^b (\mathcal{L}[u] \cdot v - u \cdot \mathcal{L}[v]) \, dx = [-p(x)(u'v - uv')]_a^b = [p(x)W(u, v)(x)]_a^b, \quad (4.8)$$

which is known as the *Lagrange identity*.

For the boundary conditions given above in Eq. (4.2)

$$\{-p(x) [u'(x)v(x) - u(x)v'(x)]\}_a^b = 0$$

and, therefore,

$$\int_a^b [(\mathcal{L}[u]) v - u (\mathcal{L}[v])] dx = 0. \quad (4.9)$$

**Exercise:** Show that Eq. (4.8) turns into Eq. (4.9) if functions  $u(x)$  and  $v(x)$  satisfy the boundary conditions given by Eq. (4.2).

**Adjoint operator.** In general, for complex functions  $u(x)$  and  $v(x)$  we can write

$$\int_a^b v^*(x) \cdot [\mathcal{L}u(x)] dx = \int_a^b [\mathcal{L}^\dagger v(x)]^* \cdot u(x) dx + F(a, b).$$

Hence, if  $\mathcal{L}$  is a linear differential operator, its *adjoint* operator can be found by integrating by parts.

We have shown by the integration by parts, that for the SL operator

$$\mathcal{L} = \mathcal{L}^\dagger,$$

i.e. the SL operator is *self-adjoint*.

If the boundary conditions or the operator are selected so as

$$\int_a^b v^*(x) \cdot [\mathcal{L}u(x)] dx = \int_a^b [\mathcal{L}^\dagger v(x)]^* \cdot u(x) dx,$$

the operator  $\mathcal{L}$  is called *Hermitian* operator.

### 4.3 Properties of eigenfunctions of Sturm-Liouville equations.

**Inner product of two functions.** The inner product of real functions  $u(x)$  and  $v(x)$  (also known as an *overlap integral* and a *scalar product*) is defined as:

$$(u, v) = \int_a^b u(x)v(x) dx.$$

For complex functions  $u(x) = u_1(x) + iu_2(x)$  and  $v(x) = v_1(x) + iv_2(x)$ , where  $u_1$ ,  $u_2$ ,  $v_1$ , and  $v_2$  are real functions of  $x$ , the inner product is defined as:

$$(u, v) = \int_a^b u(x)\bar{v}(x)dx = \int_a^b (u_1(x) + iu_2(x))(v_1(x) - iv_2(x))dx$$

Note that

$$(u, u) = \int_a^b u(x)\bar{u}(x)dx = \int_a^b (u_1(x) + iu_2(x))(u_1(x) - iu_2(x))dx = \int_a^b (u_1^2(x) + u_2^2(x))dx.$$

In these notations, the Lagrange identity (4.9) is

$$(\mathcal{L}[u], v) - (u, \mathcal{L}[v]) = 0.$$

If  $u(x)$  is an eigenfunction of  $\mathcal{L}$ , then the inner product of  $\mathcal{L}[u]$  and  $v$  is

$$(\mathcal{L}[u], v) = \int_a^b (\mathcal{L}[u]) v dx = \int_a^b \lambda \rho(x) u(x) v(x) dx.$$

**Eigenvalues of the SL problem are real.** Let us assume that we found  $\lambda$  and  $\phi$ , which satisfy the SL boundary problem

$$\mathcal{L}\phi = \lambda \rho \phi,$$

with the boundary conditions given by Eq. (4.2) and  $\lambda$  and  $\phi$  are complex:

$$\lambda = \mu + i\nu$$

$$\phi(x) = u(x) + iv(x).$$

Clearly,

$$(\mathcal{L}[\phi], \phi) = (\phi, \mathcal{L}[\phi]).$$

Since  $\phi(x)$  is an eigenfunction, this becomes

$$(\lambda \rho \phi, \phi) = (\phi, \lambda \rho \phi),$$

which is, according to the definition of the inner product:

$$\int_a^b \lambda \rho(x) \phi(x) \bar{\phi}(x) dx = \int_a^b \phi(x) \bar{\lambda} \bar{\rho}(x) \bar{\phi}(x) dx.$$

Subtracting one side of this equation from the other gives

$$(\lambda - \bar{\lambda}) \int_a^b \rho(x) \phi(x) \bar{\phi}(x) dx = (\lambda - \bar{\lambda}) \int_a^b \rho(x) (u^2(x) + v^2(x)) dx = 0.$$

Since  $\rho(x)$  is positive and  $u^2(x) + v^2(x) > 0$  unless both  $u(x)$  and  $v(x)$  are equal to zero for all  $x \in [a, b]$ , the only possibility is that

$$\lambda = \bar{\lambda}.$$

**Eigenfunctions of the SL problem are real.** Consider equation

$$\mathcal{L}\phi = \lambda \rho \phi$$

and its complex conjugation:

$$(\mathcal{L}\phi)^* = (\lambda \rho \phi)^*.$$

Since the operator  $\mathcal{L}(x)$ , function  $\rho(x)$ , and eigenvalues  $\lambda$  are all real,

$$(\mathcal{L}\phi)^* = \mathcal{L}\phi^* = \lambda^* \rho \phi^* = \lambda \rho \phi^*.$$

If  $\phi(x)$  is complex, we can put  $\phi(x) = u(x) + iv(x)$ , where  $u(x)$  and  $v(x)$  are real functions, and construct two non-trivial linear combinations of  $\phi$  and  $\phi^*$ :

$$\phi_1(x) = \phi(x) + \phi^*(x) = 2u(x) \quad \text{and} \quad \phi_2(x) = -i(\phi(x) - \phi^*(x)) = 2v(x).$$

Applying the operator  $\mathcal{L}$  to functions  $\phi_1$  and  $\phi_2$  gives

$$\mathcal{L}\phi_1 = \mathcal{L}(\phi + \phi^*) = \lambda \rho \phi + \lambda \rho \phi^* = \lambda \rho \phi_1 = \lambda \rho (2u)$$

and

$$\mathcal{L}\phi_2 = -i\mathcal{L}(\phi - \phi^*) = -i(\lambda \rho \phi - \lambda \rho \phi^*) = \lambda \rho \phi_2 = \lambda \rho (2v),$$

i.e., real functions  $\phi_1$  and  $\phi_2$  are eigenfunctions of the operator  $\mathcal{L}$  with the same eigenvalues as  $\phi$  and  $\phi^*$ . Thus, one can always choose real eigenfunctions.

**Non degenerate eigenstates.** If two eigenvalues of the SL problem differ ( $\lambda_1 \neq \lambda_2$ ), the corresponding eigenfunctions  $\phi_1$  and  $\phi_2$  obey:

$$\int_a^b \rho(x)\phi_1(x)\phi_2(x)dx = 0,$$

i.e., they are said to be orthogonal with the weight  $\rho(x)$ .

Indeed, let us consider two eigenfunctions and two corresponding eigenvalues of an SL operator  $\mathcal{L}$  with appropriate boundary conditions:

$$\mathcal{L}\phi_1 = \lambda_1\rho\phi_1 \quad \text{and} \quad \mathcal{L}\phi_2 = \lambda_2\rho\phi_2.$$

Use the Lagrange identity for  $\phi_1$  and  $\phi_2$ :

$$(\lambda_1\rho\phi_1, \phi_2) - (\phi_1, \lambda_2\rho\phi_2) = 0.$$

For real eigenfunctions this gives

$$(\lambda_1 - \lambda_2) \int_a^b \rho(x)\phi_1(x)\phi_2(x)dx = 0.$$

Thus, if  $\lambda_1 \neq \lambda_2$ , then

$$\int_a^b \rho(x)\phi_1(x)\phi_2(x)dx = 0.$$

**The case of degenerate  $\lambda_k$ .** Suppose an operator  $\mathcal{L}$  has eigenvalues

$$\lambda_1 \dots \lambda_{k-1} \lambda_k \lambda_{k+1} \lambda_{k+2} \dots \lambda_{k+n} \lambda_{k+n+1} \lambda_{k+n+2} \dots$$

and one of the eigenvalues is  $n$ -times degenerate, i.e.

$$\lambda_{k+1} = \lambda_{k+2} = \dots = \lambda_{k+n} = \lambda.$$

Then, any linear combination of the corresponding eigenfunctions

$$\phi = c_1\phi_{k+1} + c_2\phi_{k+2} + \dots + c_{n-1}\phi_{k+n-1} + c_n\phi_{k+n}$$

is also an eigenfunction of  $\mathcal{L}$  with the same eigenvalue

$$\mathcal{L}\phi = \sum_{i=1}^n c_{k+i} [\mathcal{L}\phi_{k+i}] = \sum_{i=1}^n c_{k+i} [\lambda_{k+i} \rho \phi_{k+i}] = \lambda \rho \sum_{i=1}^n c_{k+i} \phi_{k+i} = \lambda \rho \phi.$$

Thus, infinite number of eigenfunctions with the eigenvalue of  $\lambda$  can be constructed.

Since the eigenfunctions corresponding to  $\lambda_1$  and  $\lambda_2$ , where  $\lambda_1 \neq \lambda_2$  are orthogonal, linear combinations

$$\phi = c_1 \phi_{k+1} + c_2 \phi_{k+2} + \dots + c_{n-1} \phi_{k+n-1} + c_n \phi_{k+n}$$

are orthogonal to the eigenfunctions  $\phi_m$  of  $\mathcal{L}$  for all  $m \leq k$  and all  $m > k+n$  for any selection of the coefficients  $c_i$ . Is it possible to define such combinations of the coefficients  $c_i^{(j)}$  ( $1 \leq i, j \leq n$ ) that any two of the functions

$$\phi^{(i)} = \sum_{j=1}^n c_j^{(i)} \phi_{k+j}, \quad (i = 1, 2, \dots, n) \quad \text{i.e.,}$$

$$\begin{aligned} \phi^{(1)} &= c_1^{(1)} \phi_{k+1} + c_2^{(1)} \phi_{k+2} + \dots + c_{n-1}^{(1)} \phi_{k+n-1} + c_n^{(1)} \phi_{k+n} \\ \phi^{(2)} &= c_1^{(2)} \phi_{k+1} + c_2^{(2)} \phi_{k+2} + \dots + c_{n-1}^{(2)} \phi_{k+n-1} + c_n^{(2)} \phi_{k+n} \\ \dots &\dots \dots \\ \phi^{(n)} &= c_1^{(n)} \phi_{k+1} + c_2^{(n)} \phi_{k+2} + \dots + c_{n-1}^{(n)} \phi_{k+n-1} + c_n^{(n)} \phi_{k+n}, \end{aligned}$$

are also orthogonal for any  $i \neq j$ ?

**Gram-Schmidt orthogonalisation.** This is one of the methods used for orthogonalisation of linearly independent functions. We can set

$$\phi^{(1)} = \phi_{k+1}$$

and normalise it so as

$$\int_a^b \phi^{(1)}(x) \phi^{(1)}(x) \rho(x) dx = 1.$$

Then, construct  $\phi^{(2)}$  as

$$\phi^{(2)} = \phi_{k+2} - \phi^{(1)} \left( \int_a^b \phi^{(1)} \phi_{k+2} \rho dx \right).$$

To check that  $\phi^{(1)}$  and  $\phi^{(2)}$  are orthogonal, calculate

$$\int_a^b \phi^{(1)} \phi^{(2)} \rho dx = \int_a^b \phi^{(1)} \phi_{k+2} \rho dx - \left[ \int_a^b \phi^{(1)} \phi^{(1)} \rho dx \right] \left[ \int_a^b \phi^{(1)} \phi_{k+2} \rho dx \right] = 0.$$

In order to proceed further, normalise  $\phi^{(2)}$  and construct  $\phi^{(3)}$  as

$$\phi^{(3)} = \phi_{k+3} - \phi^{(1)} \left( \int_a^b \phi^{(1)} \phi_{k+3} \rho dx \right) - \phi^{(2)} \left( \int_a^b \phi^{(2)} \phi_{k+3} \rho dx \right),$$

and so on for  $\phi^{(4)}, \dots, \phi^{(n)}$ .

Thus, the eigenfunctions of the SL boundary problem are either orthogonal (for  $\lambda_i \neq \lambda_j$ ) or can be made orthogonal (for  $\lambda_i = \lambda_j$ ).

## 4.4 Basis set.

Suppose functions  $\phi_i$  ( $i = 1, 2, \dots$ ) are normalised and orthogonal to each other. These functions are called *orthonormal* and they are convenient to use as a *basis set* in order to represent (reasonably well behaved) functions as linear combinations of the type:

$$f(x) = \sum_{i=1}^{\infty} c_i \phi_i(x).$$

To find the coefficients  $c_n$ , multiply both parts by  $\phi_n^* \rho$  and integrate over  $dx$  (use the orthonormality of  $\phi_k$ ):

$$\int_a^b \phi_n^* f \rho dx = \sum_{i=1}^{\infty} c_i \left( \int_a^b \phi_n^* \phi_i \rho dx \right) = \sum_{i=1}^{\infty} c_i \delta_{ni} = c_n.$$

**Dirichlet conditions.** A “reasonably well behaved function”  $f(x)$  for  $x \in [a, b]$ , where  $a$  and  $b$  are finite, satisfies these conditions:

- 1) It must be single valued (examples).
- 2) It must be continuous except, possibly, a finite number of finite discontinuities (examples).
- 3) It must have a finite number of maxima and minima (examples).
- 4) The integral

$$\int_a^b |f(x)| dx$$

must converge (examples).

**Completeness of a basis set.** If the basis set  $\phi_i$  is such that expansion

$$f(x) = \sum_{i=1}^{\infty} c_i \phi_i(x)$$

holds for any “reasonably well behaved” function, the basis set is said to be complete.

Can we express the completeness of a basis set in a formal way? Substitute the expression for the coefficients  $c_i$ :

$$f(x) = \sum_{i=1}^{\infty} \phi_i(x) c_i = \sum_{i=1}^{\infty} \phi_i(x) \left( \int_a^b \phi_i^*(t) f(t) \rho(t) dt \right) = \int_a^b f(t) \rho(t) \left( \sum_{i=1}^{\infty} \phi_i^*(t) \phi_i(x) \right) dt.$$

Compare this expression with

$$f(x) = \int_a^b f(t) \delta(x - t) dt.$$

Hence, if the basis set is complete, we should have

$$\rho(t) \left( \sum_{i=1}^{\infty} \phi_i^*(t) \phi_i(x) \right) = \delta(x - t),$$

which is called the *completeness* or *closure* condition.

Basis sets used in practical calculations are always finite. In this case, completeness of a basis set can be expressed in terms of deviations of a function  $f(x)$  from its approximate value

$$\sum_{i=1}^N \phi_i(x) c_i = \sum_{i=1}^N \phi_i(x) \left( \int_a^b \phi_i^*(t) f(t) \rho(t) dt \right)$$

for all  $x \in [a, b]$ . (Note that the sum is up to a finite  $N$ .) As  $N$  increases, these deviations should become smaller. Hence, for a complete basis  $\phi_i$ :

$$\lim_{N \rightarrow \infty} \int_a^b \left| f(x) - \sum_{i=1}^N \phi_i(x) c_i \right|^2 \rho(x) dx = 0.$$

## 4.5. CONSTRUCTION OF GREENS FUNCTIONS AND REPRESENTATION OF THE $\delta$ -FUNCTION

This conditions also gives a criterion for estimating proximity of a finite and, in general, incomplete basis set to a complete basis set.

**Examples.** In *ab initio* materials modelling: representation of Slater exponential functions using a finite number of Gaussian-type functions; expansion of electron density over a basis set of plane-waves.

**Examples of complete basis sets.** Two of the most widely used systems include:

- 1) A set of  $\sin(nx)$  and  $\cos(nx)$ , where  $n=0,1,2,\dots$ , which form a special case of bi-orthogonal complete basis set for  $x \in [0, 2\pi]$ .
- 2) Polynomial functions  $p_n(x) = x^n$ , where  $n=0,1,2,\dots$ . Special linear combinations of  $p_n(x)$  are considered below.

## 4.5 Construction of Greens functions and representation of the $\delta$ -function.

Suppose  $\phi_n$  and  $\lambda_n$  are eigenfunctions and eigenvalues of a Hermitian operator

$$\mathcal{L}(x) = - \left[ \frac{d}{dx} \left( p(x) \frac{d}{dx} \right) + q(x) \right],$$

i.e.,

$$\mathcal{L}\phi_n(x) = \lambda_n \rho(x) \phi_n(x) \quad x \in [a, b]$$

and functions  $\phi_n(x)$  satisfy boundary conditions that make operator  $\mathcal{L}$  Hermitian. Thus, according to what we have proven above,  $\phi_n(x)$  and  $\lambda_n$  are real and functions  $\phi_n(a)$  are orthogonal, i.e.,

$$\int_a^b \phi_k(x) \phi_n(x) \rho(x) dx = 0 \quad \text{if } k \neq n.$$

Importantly,  $\phi_n(a)$  form a complete basis set.

Now, let us solve an ODE

$$\mathcal{L}y(x) = f(x).$$

A solution  $y(x)$  can be represented as an expansion over functions  $\phi_n$ :

$$y(x) = \sum_{n=1}^{\infty} c_n \phi_n(x).$$

Then, function  $f(x)$  can be written as

$$f(x) = \mathcal{L}y(x) = \mathcal{L} \left[ \sum_{n=1}^{\infty} c_n \phi_n(x) \right] = \sum_{n=1}^{\infty} c_n [\mathcal{L}\phi_n(x)] = \sum_{n=1}^{\infty} c_n \lambda_n \rho(x) \phi_n(x).$$

If  $\phi_n$  and  $\lambda_n$  are known, we can determine all coefficients  $c_n$ . For that, multiply both parts by  $\phi_k$  and integrate over  $dx$  (use the orthogonality of  $\phi_n$ ):

$$\int_a^b \phi_k(x) f(x) dx = \sum_{n=1}^{\infty} \int_a^b c_n \lambda_n \phi_k(x) \phi_n(x) \rho(x) dx = c_k \lambda_k \int_a^b \phi_k(x) \phi_k(x) \rho(x) dx.$$

If functions  $\phi_k(x)$  are normalised so as

$$\int_a^b \phi_k(x) \phi_k(x) \rho(x) dx = 1,$$

we have

$$\int_a^b \phi_k(x) f(x) dx = \sum_{n=1}^{\infty} \int_a^b c_n \lambda_n \phi_k(x) \phi_n(x) \rho(x) dx = c_k \lambda_k.$$

Hence, coefficients  $c_k$  are

$$c_k = \frac{1}{\lambda_k} \int_a^b \phi_k(x) f(x) dx.$$

Use these coefficients to write down a solution of the ODE:

$$y(x) = \sum_{n=1}^{\infty} c_n \phi_n(x) = \sum_{n=1}^{\infty} \frac{1}{\lambda_n} \phi_n(x) \left( \int_a^b \phi_n(t) f(t) dt \right).$$

We can rearrange the terms and rewrite  $y(x)$  as

$$y(x) = \int_a^b \left( \sum_{n=1}^{\infty} \frac{1}{\lambda_n} \phi_n(x) \phi_n(t) \right) f(t) dt.$$

Compare this expression with the Green's function, as we defined it earlier:

$$y(x) = \int_a^b G(x, t) f(t) dt.$$

#### 4.5. CONSTRUCTION OF GREENS FUNCTIONS AND REPRESENTATION OF THE $\delta$ -FUNCTION

From here we find that the Green's function can be expressed as

$$G(x, t) = \sum_{n=1}^{\infty} \frac{1}{\lambda_n} \phi_n(x) \phi_n(t),$$

which is called *spectral representation*.

Finally, previously we established the  $G(x, t)$  should satisfy equation

$$\mathcal{L}[G(x, t)] = \delta(x - t).$$

Let us apply  $\mathcal{L}$  to both parts of the spectral representation of  $G(x, t)$ :

$$\sum_{n=1}^{\infty} \frac{1}{\lambda_n} [\mathcal{L}\phi_n(x)] \phi_n(t) = \sum_{n=1}^{\infty} \frac{1}{\lambda_n} [\lambda_n \rho(x) \phi_n(x)] \phi_n(t) = \rho(x) \sum_{n=1}^{\infty} \phi_n(x) \phi_n(t) = \delta(x - t),$$

which is the condition for the completeness of the basis set formed by  $\phi_n(x)$ .

**Generalise this approach** to more complex equations

$$\mathcal{L}y(x) - \mu\rho(x)y(x) = f(x),$$

where  $\mathcal{L}$  is Hermitian and  $\mu$  is a constant. Similarly to what we discussed before, search for a solution  $y(x)$  in the form of  $\sum c_n \phi_n$ . To find coefficients  $c_n$ , substitute  $y(x)$  into the ODE:

$$\rho(x) \left( \sum_{n=1}^{\infty} (\lambda_n - \mu) c_n \phi_n(x) \right) = \rho(x) \left( \sum_{n=1}^{\infty} \phi_n(x) \int_a^b \phi_n(t) f(t) dt \right).$$

Multiply both parts by  $\phi_k(x)$  and integrate over  $dx$ :

$$(\lambda_k - \mu) c_k = \int_a^b \phi_k(t) f(t) dt \quad \text{i.e.} \quad c_k = \frac{1}{\lambda_k - \mu} \int_a^b \phi_k(t) f(t) dt.$$

Hence,

$$y(x) = \sum_{n=1}^{\infty} c_n \phi_n(x) = \sum_{n=1}^{\infty} \frac{\phi_n(x)}{\lambda_n - \mu} \int_a^b \phi_n(t) f(t) dt.$$

Clearly, if there is  $k$  such that  $\mu = \lambda_k$ , solution  $y(x)$  turns to infinity. In order to eliminate this singularity, we can request that

$$\int_a^b \phi_k(t) f(t) dt = 0$$

for a particular  $k$  so as the ratio

$$\frac{1}{\lambda_n - \mu} \int_a^b \phi_n(t) f(t) dt$$

is finite.

## 4.6 Examples of orthogonal polynomials.

**Legendre functions.** Legendre's differential equation

$$(1 - x^2)y'' - 2xy' + \ell(\ell + 1)y = 0 \quad (4.10)$$

is a particular case of the SL form with  $p(x) = 1 - x^2$ ,  $q(x) = 0$ ,  $\rho(x) = 1$ , and  $\lambda = \ell(\ell + 1)$ .

We can look for solutions of this equations in the form

$$y(x) = \sum_{n=0}^{\infty} a_n x^n.$$

Substituting this into the Legendre equation (4.10) gives

$$\sum_{n=0}^{\infty} [n(n-1)a_n x^{n-2} - n(n-1)a_n x^n - 2na_n x^n + \ell(\ell+1)a_n x^n] = 0,$$

from which we can obtain the recurrence equation by comparing coefficients in front of  $x^n$ :

$$(n+2)(n+1)a_{n+2} - n(n-1) - 2n - \ell(\ell+1) = 0.$$

Thus,

$$a_{n+2} = \frac{n(n+1) - \ell(\ell+1)}{(n+1)(n+2)} a_n,$$

i.e. any element  $a_k$  can be calculated if  $a_{k-2}$  is known ( $k - 2 \geq 0$ ).

Using this recurrence equation, we can generate two solutions:

**1)** Let us set  $a_0=1$  and  $a_1=0$ . Then, coefficients  $a_{2k}$  ( $2k=2,4,\dots$ ) can be calculated as:

$$a_2 = \frac{-\ell(\ell+1)}{1 \cdot 2} \quad a_4 = \frac{2(2+1) - \ell(\ell+1)}{3 \cdot 4} a_2 = \frac{1}{4!} [\ell(\ell+1) - 6]\ell(\ell+1)$$

and, therefore, the solution with *even* powers of  $x$  is

$$y_{\text{even}}(x) = 1 - \ell(\ell+1) \frac{x^2}{2!} + (\ell-2)\ell(\ell+1)(\ell+3) \frac{x^4}{4!} + \dots$$

**2)** Let us set  $a_0=0$  and  $a_1=1$ . Then, coefficients  $a_{2k+1}$  ( $2k+1=3,5,\dots$ ) are

$$a_3 = \frac{1 \cdot 2 - \ell(\ell+1)}{2 \cdot 3} \quad a_5 = \frac{3(3+1) - \ell(\ell+1)}{4 \cdot 5} a_3$$

and the corresponding solution contains only *odd* powers of  $x$ :

$$y_{\text{odd}}(x) = x - (\ell-1)(\ell+2) \frac{x^3}{3!} + (\ell-3)(\ell-1)(\ell+2)(\ell+4) \frac{x^5}{5!} + \dots$$

The general solution of the ODE is given by a linear combination of  $y_{\text{even}}(x)$  and  $y_{\text{odd}}(x)$ :

$$y(x) = c_1 y_{\text{even}}(x) + c_2 y_{\text{odd}}(x).$$

**Consider a particular case of integer  $\ell$ .** If  $\ell$  is integer, then for  $n = \ell$  we have

$$a_{\ell+2} = \frac{\ell(\ell+1) - \ell(\ell+1)}{(\ell+1)(\ell+2)} a_\ell = 0.$$

Thus, the series for  $y_{\text{even}}(x)$  becomes finite if  $\ell$  is even and the series for  $y_{\text{odd}}(x)$  becomes finite if  $\ell$  is odd:

$$y(x) = \sum_{n=0}^{\ell} a_n x^n.$$

Such functions  $y(x)$  are denoted  $P_\ell(x)$  and called Legendre polynomials. They are normalised so as

$$P_\ell(1) = 1$$

and, consequently

$$P_\ell(-1) = (-1)^\ell.$$

First two functions  $P_\ell(x)$  for even  $\ell$  are:

$$P_0(x) = 1 \quad P_2(x) = \frac{1}{2}(3x^2 - 1)$$

and for odd  $\ell$ :

$$P_1(x) = x \quad P_3(x) = \frac{1}{2}(5x^3 - 3x).$$

### Rodrigues' formula.

$$P_\ell(x) = \frac{1}{2^\ell \ell!} \frac{d^\ell}{dx^\ell} (x^2 - 1)^\ell.$$

To prove it, introduce  $u = (x^2 - 1)^\ell$ . Then

$$u' = 2\ell x(x^2 - 1)^\ell$$

and

$$(x^2 - 1)u' - 2\ell xu = 0.$$

After differentiating this  $\ell + 1$  time obtain:

$$[(x^2 - 1)u^{(\ell+2)} + 2x(\ell + 1)u^{(\ell+1)} + \ell(\ell + 1)u^{(\ell)}] - 2\ell[xu^{(\ell+1)} + (\ell + 1)u^{(\ell)}] = 0$$

or

$$(x^2 - 1)u^{(\ell+2)} + 2xu^{(\ell+1)} - \ell(\ell + 1)u^{(\ell)} = 0.$$

Hence,

$$u^{(\ell)}(x) = cP_\ell(x).$$

**Orthogonality of  $P_\ell(x)$ .** Polynomials  $P_k(x)$  and  $P_n(x)$  are orthogonal on the interval  $x \in [-1, 1]$  if  $k \neq n$ . To prove it consider

$$[(1 - x^2)P'_k]' + k(k + 1)P_k = 0,$$

multiply it by  $P_n$  and integrate by parts.

**Chebyshev functions.** These functions are the solutions of

$$(1 - x^2)y'' - xy' + \mu^2 y = 0.$$

Solutions for integer  $\nu$  are called Chebyshev polynomials given by

$$T_n(x) = \frac{(-1)^n \sqrt{\pi} (1 - x^2)^{1/2}}{2^n (n - 1/2)!} \frac{d^n}{dx^n} (1 - x^2)^{n-1/2}$$

and

$$U_n(x) = \frac{(-1)^n \sqrt{\pi} (n + 1)}{2^{n+1} (n + 1/2)! (1 - x^2)^{1/2}} \frac{d^n}{dx^n} (1 - x^2)^{n+1/2},$$

where

$$\left(\frac{1}{2}\right)! = \frac{1}{2} \sqrt{\pi}.$$

## Problem solving session: Sturm-Liouville theory.

**1.** Use the properties of Legendre polynomials.

(a) Find the solution of

$$(1-x^2)y'' - 2xy' + by = f(x)$$

for  $-1 \leq x \leq 1$  and finite at  $x = 0$

(b) Find the explicit solution for  $b=14$  and  $f(x) = 5x^3$ . Verify by direct substitution.

**2.** Find an eigenfunction expansion for the solution with boundary conditions  $y(0) = y(\pi) = 0$  of the inhomogeneous equation

$$y'' + ky = f(x),$$

where  $k$  is a constant and

$$f(x) = x, \quad \text{for } 0 \leq x \leq \frac{\pi}{2}$$

and

$$f(x) = \pi - x, \quad \text{for } \frac{\pi}{2} \leq x \leq \pi.$$

**3.** Consider a set of functions  $\{f(x)\}$  of a real variable  $x$  defined for  $-\infty < x < \infty$  and approaching zero value at least as quickly as  $1/x$  as  $x \rightarrow \pm\infty$ . Determine whether each of the following linear operators is Hermitian when acting upon  $\{f(x)\}$  (assume that the weight function is equal to 1 for all values of  $x$ ):

$$\frac{d}{dx} + x \quad -i\frac{d}{dx} + x^2 \quad ix\frac{d}{dx} \quad i\frac{d^3}{dx^3}$$

An operator  $\mathcal{L}$  is Hermitian *over the given range* if

$$\int_{-\infty}^{+\infty} f^*(x) [\mathcal{L}g(x)] dx = \left\{ \int_{-\infty}^{+\infty} g^*(x) [\mathcal{L}f(x)] dx \right\}^*.$$

# Chapter 5

## Numerical methods

### 5.1 Tridiagonal matrices.

In many physical systems only the interaction between “nearest neighbours” is important (see examples of quasi-one-dimensional systems).

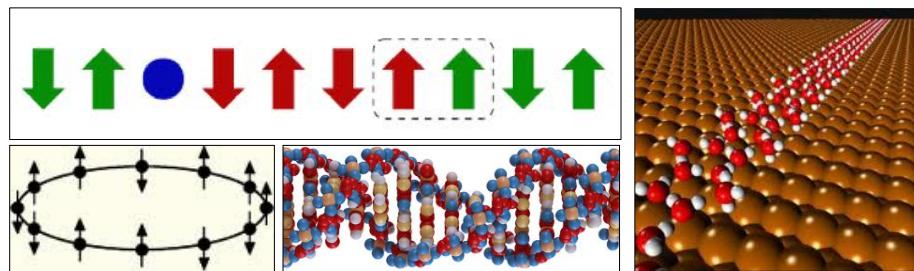


Figure 5.1: Examples of (quasi-)one-dimensional systems.

Properties of these system may be described using systems of linear algebraic equations with sparse matrices, i.e. matrices, in which only small number of elements differ from zero. In this case, straightforward diagonalisation method may not be convenient nor practical.

(a)

$$\begin{bmatrix} \neq 0 & & & \\ & \neq 0 & & \\ & & \neq 0 & \\ & & & \neq 0 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ \vdots \\ y_n \end{bmatrix}$$

(b)

$$\begin{bmatrix} & & & & & 0 \\ & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ 0 & & & & & \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ \vdots \\ y_n \end{bmatrix}$$

Figure 5.2: Examples of algebraic systems with a sparse matrix (a) and an  $N$ -diagonal matrix (b).

We will consider a special case of a sparse matrix - a tridiagonal matrix.

$$\begin{pmatrix} b_1 & c_1 & 0 & 0 & \dots & 0 & 0 & 0 \\ a_2 & b_2 & c_2 & 0 & \dots & 0 & 0 & 0 \\ 0 & a_3 & b_3 & c_3 & \dots & 0 & 0 & 0 \\ \dots & \dots \\ 0 & 0 & 0 & 0 & \dots & a_{n-1} & b_{n-1} & c_{n-1} \\ 0 & 0 & 0 & 0 & \dots & 0 & a_n & b_n \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \\ x_{n-1} \\ x_n \end{pmatrix} = \begin{pmatrix} y_1 \\ y_2 \\ y_3 \\ \vdots \\ y_{n-1} \\ y_n \end{pmatrix}.$$

This matrix corresponds to a system of equations

$$a_i x_{i-1} + b_i x_i + c_i x_{i+1} = y_i \quad (5.1)$$

with  $i = 1, 2, \dots, n$  and  $a_1 = c_n = 0$ . To solve these equations we assume that there is a set of numbers  $\delta_k$  and  $\lambda_k$ , such that  $x_i$  and  $x_{i+1}$  are related as

$$x_{i-1} = \delta_{i-1} x_i + \lambda_{i-1}. \quad (5.2)$$

Use the Eq. (5.2) to eliminate  $x_{i-1}$  from Eq. (5.1):

$$a_i(\delta_{i-1} x_i + \lambda_{i-1}) + b_i x_i + c_i x_{i+1} = y_i$$

$$a_i \delta_{i-1} x_i + a_i \lambda_{i-1} + b_i x_i + c_i x_{i+1} = y_i$$

$$(a_i \delta_{i-1} + b_i) x_i + c_i x_{i+1} = y_i - a_i \lambda_{i-1}$$

Hence,  $x_i$  can be represented in the form equivalent to that for  $x_{i-1}$  [see Eq. (5.2)]:

$$x_i = -\frac{c_i}{a_i \delta_{i-1} + b_i} x_{i+1} + \frac{y_i - a_i \lambda_{i-1}}{a_i \delta_{i-1} + b_i} = \delta_i x_{i+1} + \lambda_i. \quad (5.3)$$

Eq. (5.3) allows us to write *recursive* expressions for  $\delta_i$  and  $\lambda_i$  in terms of  $\delta_{i-1}$ ,  $\lambda_{i-1}$  and known coefficients  $a_i$ ,  $b_i$ , and  $c_i$ :

$$\delta_i = -\frac{c_i}{a_i \delta_{i-1} + b_i}, \quad \lambda_i = \frac{y_i - a_i \lambda_{i-1}}{a_i \delta_{i-1} + b_i}. \quad (5.4)$$

Since  $a_1 = 0$ ,

$$\delta_1 = -\frac{c_1}{b_1}, \quad \lambda_1 = \frac{y_1}{b_1}.$$

Thus, all numbers  $\delta_i$  and  $\lambda_i$  can be calculated using these recursive equations. To find  $x_i$ , note that  $\delta_n = 0$  because  $c_n = 0$ . Therefore,

$$x_n = \lambda_n = \frac{y_n - a_n \lambda_{n-1}}{a_n \delta_{n-1} + b_n}.$$

Once  $x_n$  is known, all other  $x_i$  can be found recursively.

Thus, all  $x_i$  can be determined using a two-step procedure:

1. Find all values of  $\delta_i$  and  $\lambda_i$ : recursion from  $i=1$  to  $i=n$ .
2. Find all values of  $x_k$ : recursion from  $k=n$  to  $k=1$ .

For this method to work, two conditions have to be satisfied. The procedure is called **correctly defined** if

$$a_i \delta_{i-1} + b_i \neq 0$$

for any  $i$  and **stable** if  $|\delta_i| < 1$ . Both of these conditions are satisfied if the matrix is **diagonal-dominant**, i.e.

$$|b_i| > |a_i| + |c_i| \quad (i = 1, 2, \dots, n),$$

assuming that  $a_i \neq 0$  and  $c_i \neq 0$  for  $i = 2, 3, \dots, n - 1$ . To prove this, notice that

$$|b_1| > |c_1| \geq 0$$

and

$$|\delta_1| = \left| -\frac{c_1}{b_1} \right| < 1.$$

Assume that for  $i - 1$

$$a_i \delta_{i-1} + b_i \neq 0 \quad \text{and} \quad |\delta_{i-1}| < 1$$

and use the mathematical induction method to show this for  $i$ . Indeed,

$$|b_i + a_i \delta_{i-1}| \geq |b_i| - |a_i \delta_{i-1}| > |a_i| + |c_i| - |a_i| |\delta_{i-1}| = |c_i| + |a_i|(1 - |\delta_{i-1}|) > |c_i| > 0$$

and

$$|\delta_i| = \left| -\frac{c_i}{b_i + a_i \delta_{i-1}} \right| = \frac{|c_i|}{|b_i + a_i \delta_{i-1}|} < \frac{|c_i|}{|c_i|} = 1.$$

## 5.2 Euler method and its modifications.

In this section we will learn several methods for calculating a shape of a curve  $y(x)$ , which

1. satisfies a given differential equation and
2. passes through a point  $(x_0, y_0)$ , where  $y_0 = y(x_0)$ .

### 5.2.1 Definitions

**Explicit methods.** This is a group of methods, in which a function  $y(x)$  can be represented as

$$y(x + \Delta x) = F[y(x)],$$

where  $F[\dots]$  is a *recipe* for generating  $y(x + \Delta x)$  from known  $y(x)$ . These methods may be sensitive to the value of  $\Delta x$  and may lead to inaccuracies and numerical instabilities if  $\Delta x$  is too large.

**Implicit methods.** In this group of methods a function  $y(x)$  satisfies

$$P[y(x), y(x + \Delta x)] = 0,$$

where  $P[\dots]$  is a problem (an equation), which needs to be *solved* in order to find  $y(x + \Delta x)$ , assuming that  $y(x)$  is known. These methods require more effort than the explicit method – solving an equation is more difficult than applying a recipe. On the other hand, they can be less sensitive to the value of  $\Delta x$ .

**Stiff equations.** This term refers to differential equations for which numerical solutions are unstable unless  $\Delta x$  is very small. For example, if the value of  $|k|$  in the equation

$$\frac{dy}{dx} = ky(x) + f(x)$$

is large, then relatively small uncertainty in the value of  $y(x)$  may result in a large uncertainty in the value of  $y'(x)$ , which, in turn, results in a large uncertainty in the value of  $y(x + \Delta x)$ .

### 5.2.2 Euler method.

**Forward Euler method (explicit).** Consider equation:

$$y'(x) = f[x, y(x)]$$

with the initial condition

$$y(x_0) = y_0.$$

According to the Taylor series for  $y(x)$ :

$$y(x + \Delta x) = y(x) + y'(x)\Delta x + \frac{1}{2!}y''(x)(\Delta x)^2 + \frac{1}{3!}y'''(x)(\Delta x)^3 + \dots,$$

one can approximate  $y(x + \Delta x)$  as

$$y(x + \Delta x) \approx y(x) + f[x, y(x)]\Delta x,$$

if  $\Delta x$  is sufficiently small.

**Discretisation.** Introduce the grid of  $x$ :  $x_{i+1} = x_i + \Delta x$ ,  $y_i = y(x_i)$ . Then,

$$y_{i+1} = y_i + f[x_i, y_i]\Delta x.$$

Thus, construct  $y(x)$  as a set of values  $y_k$ , where each  $y_{i+1}$  is an explicit function of  $y_i$ .

**Backward Euler method (implicit).** Approximate the  $y'(x)$  as:

$$y'(x) \approx \frac{y(x) - y(x - \Delta x)}{\Delta x}$$

and use it to express  $y(x)$  via  $y(x - \Delta x)$  and  $y'(x)$ :

$$y(x) \approx y(x - \Delta x) + y'(x)\Delta x = y(x - \Delta x) + f[x, y(x)]\Delta x.$$

Thus,

$$y_i = y_{i-1} + f[x_i, y_i]\Delta x.$$

This equation needs to be solved with respect to  $y_i$ . Complexity of this equation depends on the function  $f[x, y(x)]$  and its solution may require using numerical methods.

**Example.** Consider equation

$$y'(x) = -y^2(x),$$

where  $y \in [0, a]$ ,  $a > 0$  and  $y(x_0) = y_0 > 0$ , and using the *forward* Euler method to solve it. Notice that in our notations  $f[x, y(x)] = -y^2$ . Therefore,

$$y_{i+1} = y_i - y_i^2 \Delta x,$$

which is a recipe for calculating  $y_{i+1}$  using known  $y_i$  and given  $\Delta x$ .

In the case of the *backward* method, obtain:

$$y_i = y_{i-1} - y_i^2 \Delta x.$$

This is not a recipe yet. To solve this equation with respect to  $y_i$ , rearrange the terms to the standard form of the quadratic equation with respect to  $y_i$ :

$$y_i^2 \Delta x + y_i - y_{i-1} = 0.$$

Solutions of this equation are:

$$y_i = \frac{-1 \pm \sqrt{1 + 4\Delta x y_{i-1}}}{2\Delta x}.$$

The proper solution is chosen on the basis of the initial conditions. In this particular example we set  $y_0 > 0$ , which can be obtained only if

$$y_i = \frac{-1 + \sqrt{1 + 4\Delta x y_{i-1}}}{2\Delta x}.$$

**Accuracy.** According to the Euler method,

$$y(x_0 + \Delta x) = y(x_0) + f[x_0, y(x_0)]\Delta x.$$

Since  $y'(x) = f[x, y(x)]$

$$y(x_0 + \Delta x) = y(x_0) + y'(x_0)\Delta x.$$

Compare this with the Taylor series; the difference is

$$\frac{1}{2!}y''(x_0)(\Delta x)^2 + \frac{1}{3!}y'''(x_0)(\Delta x)^3 + \dots = \frac{1}{2!}y''(x_0)(\Delta x)^2 + O((\Delta x)^3),$$

i.e., the largest contribution to the error is proportional to  $(\Delta x)^2$  per step for small  $\Delta x$ . For an interval of  $[x_1, x_2]$ , the number of such steps is

$$\frac{x_2 - x_1}{\Delta x}.$$

We assume that  $y(x)$  and  $y'(x)$  are continuous functions and that derivative of  $y'(x)$  exist for any  $x \in [x_1, x_2]$ . Then,  $y''(x)$  is finite at the interval  $[x_1, x_2]$  and we can define a constant  $C$  as

$$C = \max[y''(x_i)] \quad \text{for} \quad x_i \in [x_1, x_2].$$

Then, the total error is proportional to

$$\frac{1}{2!}C(\Delta x)^2 \times \frac{x_2 - x_1}{\Delta x} \sim \Delta x.$$

Therefore, the Euler method is said to be the first order method.

**Milne's method.** Use central differences, as opposed to forward differences:

$$y'(x) = \frac{y(x + \Delta x) - y(x - \Delta x)}{2\Delta x}$$

Then, for  $y'(x) = f[x, y(x)]$ , the explicit form is

$$y_{i+1} = y_{i-1} + f[x_i, y_i](2\Delta x).$$

This method requires knowledge of two initial values:  $y_0$  and  $y_1$  at the points  $x_0$  and  $x_0 + \Delta x$ , respectively.

**Euler-Cromer algorithm.** Let us consider a system of equations with respect to functions the  $y(x)$  and  $z(x)$  with corresponding initial conditions.

$$\begin{aligned}\frac{dy(x)}{dx} &= F(x, z(x)) & y(x_0) &= y_0 \\ \frac{dz(x)}{dx} &= G(x, y(x)) & z(x_0) &= z_0.\end{aligned}$$

$$\frac{dy(x)}{dx} = F(x, z(x)) \quad \text{and} \quad \frac{dz(x)}{dx} = G(x, y(x))$$

with respect to functions  $y(x)$  and  $z(x)$ , which satisfy initial conditions:

$$y(x_0) = y_0 \quad \text{and} \quad z(x_0) = z_0.$$

This system of equations can be written as

$$y_{i+1} = y_i + F(x_i, z_i)\Delta x \quad z_{i+1} = z_i + G(x_i, y_{i+1})\Delta x,$$

where  $y_{i+1}$  depends on  $z_i$  and  $z_{i+1}$  depends on  $y_{i+1}$ .

Alternatively, we can write it as

$$z_{i+1} = z_i + G(x_i, y_i)\Delta x \quad y_{i+1} = y_i + F(x_i, z_{i+1})\Delta x,$$

where  $z_{i+1}$  depends on  $y_i$  and  $y_{i+1}$  depends on  $z_{i+1}$ .

### 5.2.3 Adams method.

The forward difference estimate

$$y_{i+1} = y_i + f[x_i, y_i]\Delta x$$

is accurate if the function  $y(x)$  is sufficiently close to being linear for  $x \in [x_i, x_{i+1}]$  [see Fig. 5.3(a)]. Let us, instead, approximate  $y(x)$  using a quadratic function  $a_2x^2 + a_1x + a_0$  for  $x \in [x_{i-1}, x_{i+1}]$ , as shown in Fig. 5.3(b). In other words, we use a *more complex function* defined for a *wider interval* of  $x$ .

If  $y(x)$  is nearly *quadratic*, then  $y'(x)$  can be well approximated by a *linear* function in this range. Let us select this linear function in the form:

$$y'(x) = f[x, y(x)] \approx a + b(x - x_i), \quad x \in [x_i - \Delta x, x_i + \Delta x].$$

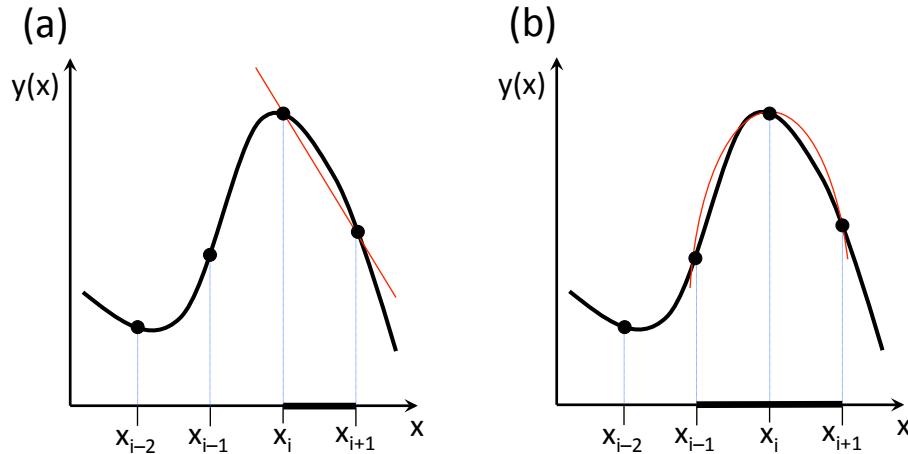


Figure 5.3: Adams method: instead of approximating function  $y(x)$  with a linear function for  $x \in [x_i, x_{i+1}]$  (a), it is approximated using a quadratic function for  $x \in [x_{i-1}, x_{i+1}]$  (b).

Calculate the derivatives of  $y'(x)$  at the points  $i$  (use  $x_i$  and  $y_i$ ) and  $i - 1$  (use  $x_{i-1}$  and  $y_{i-1}$ ):

$$f[x_i, y_i] = f_i \approx a + b(x_i - x_i) = a$$

$$f[x_{i-1}, y_{i-1}] = f_{i-1} \approx a + b(x_{i-1} - x_i) = a - b\Delta x.$$

From here we can find the coefficients  $a$  and  $b$ :

$$a = f_i \quad \text{and} \quad b = \frac{f_i - f_{i-1}}{\Delta x}.$$

Thus, for  $y'(x)$  in the interval of  $x \in [x_i - \Delta x, x_i + \Delta x]$ , we can write

$$y'(x) = f_i + \frac{f_i - f_{i-1}}{\Delta x}(x - x_i).$$

To find the difference between  $y_{i+1}$  and  $y_i$ , integrate the  $y'(x)$ :

$$y_{i+1} - y_i \approx$$

$$\int_{x_i}^{x_i+\Delta x} \left[ f_i + \frac{f_i - f_{i-1}}{\Delta x}(x - x_i) \right] dx = \left[ f_i x - \frac{f_i - f_{i-1}}{\Delta x} x_i x + \frac{f_i - f_{i-1}}{2\Delta x} x^2 \right]_{x_i}^{x_i+\Delta x}.$$

Hence,

$$y_{i+1} = y_i + f_i \Delta x + \frac{\Delta x}{2} (f_i - f_{i-1}),$$

which is a more accurate expression for  $y_{i+1}$  than that given by the Euler method. The corrective term can be written as

$$\frac{\Delta x}{2} (f_i - f_{i-1}) = \frac{(\Delta x)^2}{2} \times \frac{f_i - f_{i-1}}{\Delta x} = \frac{1}{2} (\Delta x)^2 y''_{i-1/2},$$

i.e., it is a second-order correction to the first-order formula.

**Prediction-correction method.** Accuracy of the numerical solutions can be improved by applying *retrospective corrections*. Suppose  $y_{i+1}$  has been evaluated using

$$y_{i+1} = y_i + f_i \Delta x.$$

Then  $f_{i+1}$  can be evaluated as  $f[x_{i+1}, y_{i+1}]$ . Since

$$\frac{f_i + f_{i+1}}{2}$$

is a better approximation of  $y'$  within  $[x_i, x_{i+1}]$  than either  $f_i$  or  $f_{i+1}$ , the value of  $y_{i+1}$  can be improved if it is recalculated as

$$y_{i+1} = y_i + \frac{f_i + f_{i+1}}{2} \Delta x.$$

This procedure can be repeated in order to find a better approximation of  $y'$ .

### 5.3 Runge-Kutta method.

Here we continue to work on solving equations

$$\frac{dy(x)}{dx} = f[x, y(x)].$$

and setup a different procedure of obtaining approximation for  $y_{i+1}$  by starting from  $y_i$ .

The essence of the Runge-Kutta: construct accurate Taylor series for  $y(x_i + \Delta x)$  by calculating **first derivatives at special points, as opposed to higher-order derivatives**. The accuracy can be made to the order of  $(\Delta x)^n$ , where  $n$  is however large, at the cost of larger amount of computations.

**Case n=2.** The Taylor expansion of  $y(x)$  is

$$y(x + \Delta x) = y(x) + (\Delta x)y'(x) + \frac{(\Delta x)^2}{2}y''(x)$$

$$y_{i+1} = y_i + (\Delta x)f_i + \frac{(\Delta x)^2}{2} \left( \frac{df}{dx} \right)_{x_i} = y_i + (\Delta x)f_i + \frac{(\Delta x)^2}{2} \left( \frac{\partial f}{\partial x} + f \frac{\partial f}{\partial y} \right)_{x_i}$$

Assume that this can be approximated by

$$y_{i+1} = y_i + \alpha_1 \Delta x f(x_i, y_i) + \alpha_2 \Delta x f(x_i + \beta_1 \Delta x, y_i + \beta_2 \Delta x f(x_i, y_i))$$

and choose appropriate coefficients  $\alpha_1$ ,  $\alpha_2$ ,  $\beta_1$ , and  $\beta_2$ . Expand  $f$  in the last term in the Taylor series

$$f(x_i + \beta_1 \Delta x, y_i + \beta_2 \Delta x f_i) = f(x_i, y_i) + \beta_1 \Delta x \frac{\partial f_i}{\partial x} + \beta_2 \Delta x f_i \frac{\partial f_i}{\partial y} + O((\Delta x)^2),$$

substitute it in the previous equation to obtain

$$y_{i+1} = y_i + \alpha_1 \Delta x f(x_i, y_i) + \alpha_2 \Delta x \left[ f(x_i, y_i) + \beta_1 \Delta x \frac{\partial f_i}{\partial x} + \beta_2 \Delta x f_i \frac{\partial f_i}{\partial y} + O((\Delta x)^2) \right],$$

neglect the terms  $\sim O((\Delta x)^3)$ , and regroup. Thus, obtain to the second order of  $\Delta x$

$$y_{i+1} = y_i + (\alpha_1 + \alpha_2) \Delta x f(x_i, y_i) + \alpha_2 (\Delta x)^2 \left( \beta_1 \frac{\partial f_i}{\partial x} + \beta_2 f_i \frac{\partial f_i}{\partial y} \right).$$

Compare this expression with the Taylor expansion of  $y(x)$  at  $x + \Delta x$  (above). From this comparison we can find conditions for the coefficients:

$$\alpha_1 + \alpha_2 = 1 \quad \alpha_2 \beta_1 = \alpha_2 \beta_2 = \frac{1}{2}.$$

One can set  $\alpha_1=0.5$  giving  $\alpha_2=0.5$  and  $\beta_1=\beta_2=1$ . With this choice of the parameters  $\alpha_1$ ,  $\alpha_2$ ,  $\beta_1$ , and  $\beta_2$ , the original expression for  $y_{i+1}$  becomes

$$y_{i+1} = y_i + \frac{1}{2}\Delta x f(x_i, y_i) + \frac{1}{2}\Delta x f(x_i + 1\Delta x, y_i + 1\Delta x f(x_i, y_i))$$

Thus, a step-by-step procedure for finding  $y_{i+1}$  is:

1. evaluate

$$a_1 = \Delta x f(x_i, y_i)$$

2. evaluate

$$a_2 = \Delta x f(x_i + \Delta x, y_i + a_1)$$

3. use  $a_1$  and  $a_2$  to find  $y_{i+1}$  according to

$$y_{i+1} = y_i + \frac{a_1 + a_2}{2}.$$

**Case  $n=3$  (without derivation).** The formula for calculating  $y_{i+1}$  is

$$y_{i+1} = y_i + \frac{1}{6}(b_1 + 4b_2 + b_3),$$

where values  $b_1$ ,  $b_2$ , and  $b_3$  have to be pre-calculated according to

1.  $b_1 = \Delta x f(x_i, y_i)$ ,
2.  $b_2 = \Delta x f(x_i + \frac{1}{2}\Delta x, y_i + \frac{1}{2}b_1)$ ,
3.  $b_3 = \Delta x f(x_i + \Delta x, y_i + 2b_2 - b_1)$ .

**Case of the  $N^{\text{th}}$  order.** To construct the  $N^{\text{th}}$  order Runge-Kutta method, apply the following procedure.

1. For each grid point  $i$  calculate quantities

$$c_1^i = f(x_i, y_i)$$

and

$$c_p^i = f \left( x_i + \alpha_p \Delta x, y_i + \Delta x \left( \sum_{v=1}^{p-1} \beta_{pv} c_v^i \right) \right) \quad (\text{for } p=2, \dots, N)$$

2. Then use these quantities to calculate  $y_{i+1}$ :

$$y_{i+1} = y_i + \Delta x \left( \sum_{p=1}^N \gamma_p c_p^i \right),$$

where parameters  $\alpha_p$ ,  $\beta_{pv}$ , and  $\gamma_p$  are chosen so as the value of  $y_{i+1}$ , calculated above, coincides with the value of  $y(x_{i+1})$ , obtained using the Taylor expansion, to within  $O((\Delta x)^N)$ .



# Chapter 6

## Integral transforms

We have already introduced the Laplace integral transform and used it in order to solve ordinary differential equations. In this chapter we will use Laplace and Fourier integral transforms in order to solve partial differential equations (PDE). The strategy of the integral transform method is to reduce the number of variables in a PDE and to convert it to a simpler PDE or to an ordinary differential equation.

### 6.1 Laplace transform.

Laplace transform (see Eq. 3.1) is a natural method of choice if the problem concerns with a process, in which at least one of the variables can have values from zero to infinity. We will demonstrate application of integral transforms to solving PDE using particular examples.

**Example.** Consider a semi-infinite tube filled initially with pure water and brought in contact with a salt solution maintained at a fixed concentration. Find the total amount of salt diffused into the tube by the time  $t$  if the diffusion constant is  $k$ .

The semi-infinite tube is an one-dimensional system. Therefore, concentration of salt in the tube  $u$  can be described using two variables only:  $x$  – the distance from the salt container and  $t$  – duration of the contact. Hence,  $u = u(x, t)$ .

The diffusion process is described by the equation

$$k \frac{\partial^2 u(x, t)}{\partial x^2} = \frac{\partial u(x, t)}{\partial t}$$

and the following conditions:

- $u(0, t) = u_0$ , i.e., the concentration of the salt solution “at the source” is the same at all times.
- $u(x, 0) = 0$ , i.e., the tube contained pure water prior to be brought in contact with the salt reservoir at  $t = 0$ .
- $u(\infty, t) = 0$ , i.e., salt will never rich the far end of the semi-infinite tube.
- $u(x, t)$  is finite for all  $x$  and all  $t$ .

Our strategy is to convert this PBE into an ODE by eliminating the dependence on one of the variables.

Taking the Laplace transform from both with respect to  $t$  gives

$$\int_0^\infty k \frac{\partial^2 u}{\partial x^2} e^{-st} dt = \int_0^\infty \frac{\partial u}{\partial t} e^{-st} dt. \quad (6.1)$$

Swap the order of the  $\partial^2/\partial x^2$  and  $\int \dots dt$  operations. This gives

$$k \frac{\partial^2}{\partial x^2} \left( \int_0^\infty u(x, t) e^{-st} dt \right) = k \frac{\partial^2}{\partial x^2} U(x, s) = \int_0^\infty \frac{\partial u}{\partial t} e^{-st} dt,$$

where  $U(x, s)$  is the Laplace transform of  $u(x, t)$ . Integrate the RHS by parts, as we have done it in the past:

$$\int_0^\infty \frac{\partial u}{\partial t} e^{-st} dt = u(x, t) e^{-st} \Big|_0^\infty + s \int_0^\infty u(x, t) e^{-st} dt = s U(x, s) - u(x, 0).$$

Taking into account the boundary condition  $u(x, 0) = 0$ , Eq. (6.1) becomes

$$k \frac{\partial^2}{\partial x^2} U(x, s) = s U(x, s), \quad (6.2)$$

which is an ordinary differential equation with respect to  $U(x, s)$ . Solutions of this equation is given by

$$U(x, s) = A(s) \exp\left(\sqrt{\frac{s}{k}}x\right) + B(s) \exp\left(-\sqrt{\frac{s}{k}}x\right), \quad (6.3)$$

where  $A(s)$  and  $B(s)$  are, in general, functions of  $s$ . Only one of the terms in Eq. (6.3) is physically meaningful in the context of this problem. Indeed, assuming that  $u(\infty, t) = 0$ , i.e. salt never reaches the far end of the semi-infinite tube, we have

$$U(x, s) = B(s) \exp\left(-\sqrt{\frac{s}{k}}x\right).$$

Function  $B(s)$  can be determined from the boundary conditions by calculating the Laplace transform of  $u(0, t) = u_0$ :

$$U(0, s) = \int_0^\infty u_0 e^{-st} dt = u_0 \int_0^\infty e^{-st} dt = \frac{u_0}{s}.$$

Hence,

$$U(x, s) = \frac{u_0}{s} \exp\left(-\sqrt{\frac{s}{k}}x\right).$$

At this point we need to examine a table of Laplace transforms and choose an appropriate function  $u(x, t)$ :

$$u(x, t) = u_0 \left[ 1 - \operatorname{erf}\left(\frac{x}{\sqrt{4kt}}\right) \right],$$

where

$$\operatorname{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-p^2} dp.$$

Then, to find the total amount of salt diffused into the tube, we need to calculate

$$w(t) = \int_0^\infty u(x, t) dx.$$

However, the problem requires us to find  $w(t)$  only, i.e. there is no need to

find  $u(x, t)$  explicitly.

In order to find  $w(t)$ , we can consider the Laplace transform of  $w(t)$ :

$$W(s) = \int_0^\infty w(t)e^{-st} dt = \int_0^\infty \left( \int_0^\infty u(x, t) dx \right) e^{-st} dt = \int_0^\infty \left( \int_0^\infty u(x, t)e^{-st} dt \right) dx.$$

The inner integral is the Laplace transform of  $u(x, t)$  defined earlier. Thus,

$$W(s) = \int_0^\infty \left( \int_0^\infty u(x, t)e^{-st} dt \right) dx = \int_0^\infty U(x, s) dx.$$

Since we have already found  $U(x, s)$ , the latter integral can be evaluated:

$$W(s) = u_0 k^{1/2} s^{-3/2}.$$

Again, function  $w(t)$  can be found by inspection of the Laplace transforms table

$$w(t) = 2 \left( \frac{k}{\pi} \right)^{1/2} u_0 t^{1/2}.$$

**Exercise.** A semi-infinite metal bar has initial temperature  $T=0$  K everywhere along the bar. At the time  $t \geq 0$  one end of this bar is brought into contact with a constant temperature heat reservoir with  $T=100$  K. Find the temperature distribution along the bar after time  $t$ .

## 6.2 Inverse Laplace transform.

Consider a 2nd-order ODE

$$Ay''(t) + By'(t) + Cy(t) = f(t),$$

where the boundary conditions imposed on the function  $y$  are  $y(0) = y'(0) = 0$ ,  $t \geq 0$ , and  $A, B, C$  are constant coefficients.

Laplace transform of this equation gives

$$Ap^2Y(p) + BpY(p) + CY(p) = F(p),$$

where  $Y(p)$  is the Laplace transform of  $y(t)$  and  $F(p)$  is the transform of  $f(t)$ . From here we find

$$Y(p) = \frac{1}{Ap^2 + Bp + C} F(p) = \frac{1}{A(p+a)(p+b)} F(p),$$

where  $a$  and  $b$  are some constants.

We already know the inverse Laplace transform of  $F(p)$  (it is given to us as  $f(t)$ ) and we can always find the inverse transform of

$$\frac{1}{A(p+a)(p+b)}$$

by inspecting the table of Laplace transforms. Can we find the inverse transform of  $Y(p)$ ?

More generally, assume that inverse Laplace transforms of  $H(p)$  and  $G(p)$  are known functions  $h(t)$  and  $g(t)$ , respectively. How to find the inverse Laplace transform of  $H(p)G(p)$ ?

### 6.2.1 Convolution.

Consider the product  $H(p)G(p)$ , where  $H(p)$  and  $G(p)$  are Laplace transforms of  $h(t)$  and  $g(t)$ , respectively.

$$H(p)G(p) = \int_0^\infty h(s)e^{-ps} ds \int_0^\infty g(t)e^{-pt} dt = \int_0^\infty \int_0^\infty h(s)g(t)e^{-p(s+t)} ds dt.$$

Introduce new variable  $r = s+t$  for any fixed  $t$ . Then,  $s = r - t$  and  $ds = dr$ . To define the limits of integration with respect to  $dr$ , we notice that  $r = t$  if  $s = 0$  and  $r = \infty$  if  $s = \infty$ . Therefore,

$$H(p)G(p) = \int_0^\infty \left[ \int_t^\infty h(r-t)g(t)e^{-pr} dr \right] dt. \quad (6.4)$$

Diagram in Fig. 6.1(a) shows schematically the order of integration in Eq. (6.4): each horizontal line corresponds to the inner integration from  $r = t$  to  $r = \infty$ ; all lines together cover one half of the first quadrangle, which corresponds to the outer integral for  $0 \leq t < \infty$ .

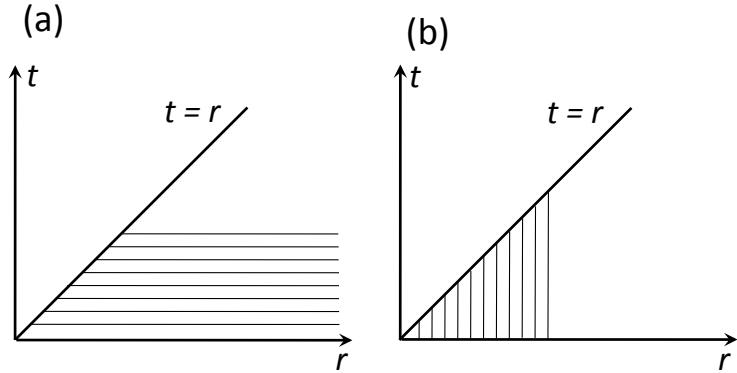


Figure 6.1: Integration in  $r - t$  plane. (a) inner integral (over  $r$ ):  $t \leq r < \infty$ , outer integral (over  $t$ ):  $0 \leq t < \infty$ ; (b) inner integral (over  $t$ ):  $0 \leq t < r$ , outer integral (over  $r$ )  $0 \leq r < \infty$ .

We can change the order of integration with respect to  $t$  and  $r$  in Eq. (6.4), as illustrated in Fig. 6.1(b), so as

$$H(p)G(p) = \int_0^\infty \left[ \int_0^r h(r-t)g(t) dt \right] e^{-pr} dr. \quad (6.5)$$

The inner integral in Eq. (6.5)

$$\int_0^r g(r-t)h(t) dt = g * h$$

is called the *convolution* of functions  $g(x)$  and  $h(x)$ . (Do not confuse symbol “ $*$ ” indicating the convolution operation with that indicating the multiplication operation.)

Thus, Equation (6.5) can be written as

$$H(p)G(p) = \int_0^\infty [h * g] e^{-pr} dr, \quad (6.6)$$

i.e., *Laplace transform of a convolution of functions  $h(x)$  and  $g(x)$  equals the product of the Laplace transforms of these functions*. In other words,  $g * h$  is the inverse Laplace transform of  $H(p)G(p)$ .

**Exercise.** Demonstrate that convolution has the property

$$g * h = h * g.$$

**Example.** Find solution of equation

$$y'' + 3y' + 2y = e^{-t} \quad \text{for } y(0) = y'(0) = 0$$

using the convolution method.

After Laplace transform:

$$p^2Y(p) + 3pY(p) + 2Y(p) = L(e^{-t}),$$

which gives

$$Y(p) = \frac{1}{p^2 + 3p + 2} L(e^{-t}) = \frac{1}{(p+1)(p+2)} L(e^{-t}).$$

Inverse Laplace transform of

$$\frac{1}{(p+a)(p+b)}$$

is

$$\frac{e^{-at} - e^{-bt}}{b-a} = \quad (\text{for } a=1 \text{ and } b=2) \quad = e^{-t} - e^{-2t}$$

Therefore,

$$Y(p) = L(e^{-t} - e^{-2t})L(e^{-t}).$$

To find  $y(t)$  we need to calculate the convolution of  $e^{-t} - e^{-2t}$  and  $e^{-t}$ :

$$\begin{aligned} y(t) &= \int_0^t g(\tau)h(t-\tau) d\tau = \int_0^t (e^{-\tau} - e^{-2\tau})e^{-(t-\tau)} d\tau = e^{-t} \left( \int_0^t d\tau - \int_0^t e^{-\tau} d\tau \right) = \\ &= e^{-t} [t + e^{-\tau}]_0^t = te^{-t} + e^{-2t} - e^{-t}. \end{aligned}$$

## 6.3 Fourier transform.

### 6.3.1 Convolution theorem.

Let us consider two functions  $f(x)$  and  $g(x)$ . Their Fourier transforms can be defined as

$$F(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} f(x)e^{-ikx} dx$$

and

$$G(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} g(x)e^{-ikx} dx,$$

respectively. **Note** that other definitions of the Fourier transform may use a different factor in front of the integral.

Is it possible to give meaning to the product  $F(k)G(k)$ ?

Rewrite  $F(k)G(k)$  as

$$F(k)G(k) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} f(s)e^{-iks} ds \int_{-\infty}^{+\infty} g(t)e^{-ikt} dt,$$

which is

$$F(k)G(k) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} f(s)g(t)e^{-ik(s+t)} ds dt. \quad (6.7)$$

For any fixed  $t$  we can introduce a new variable  $p = s + t$ , Then,  $s = p - t$  and  $ds = dp$ . Rewrite the integral in Eq. (6.7) in terms of variables  $p$  and  $t$ . Note that the integration limits remain unchanged:

$$F(k)G(k) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} f(p-t)g(t)e^{-ikp} dp dt. \quad (6.8)$$

Change the order of integration with respect to  $dt$  and  $dp$  and multiply both parts of Eq. (6.8) by  $\sqrt{2\pi}$ :

$$\sqrt{2\pi}F(k)G(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \left[ \int_{-\infty}^{+\infty} f(p-t)g(t) dt \right] e^{-ikp} dp. \quad (6.9)$$

The integral in square parenthesis is called convolution (note that the integration limits are different from those defined for the case of the Laplace

transform):

$$\int_{-\infty}^{+\infty} f(p-t)g(t) dt. \quad (6.10)$$

Thus, Eq. (6.9) states that *the product of the Fourier transforms of functions  $f(x)$  and  $g(x)$  is proportional to the Fourier transform of a convolution of these functions*. This statement is called *convolution theorem*.

**Exercise.** Demonstrate that

$$\int_{-\infty}^{+\infty} f(p-t)g(t) dt. = \int_{-\infty}^{+\infty} f(t)g(p-t) dt.$$

### 6.3.2 Temperature distribution in an infinite bar.

An infinite metal bar has the initial temperature distribution along the bar  $f(x)$ . Find the temperature distribution after time  $t$ .

Let  $u(x, t)$  be the temperature at a point  $x$  along the bar at the time  $t$ . Assume that the far ends of the bar remain cold, i.e.

$$u(\pm\infty, t) = \partial u(x, t)/\partial x|_{(x=\pm\infty)} = 0.$$

The temperature along the bar is described by the heat flow equation

$$\kappa \frac{\partial^2 u}{\partial x^2} = \frac{\partial u}{\partial t}. \quad (6.11)$$

Natural boundary conditions for this problem are:

- The far ends of the bar remain cold:  $u(x, t) \rightarrow 0$  for  $x \rightarrow \pm\infty$
- The temperature does not change at the ends of the bar:  $\partial u(x, t)/\partial x \rightarrow 0$  for  $x \rightarrow \pm\infty$

Apply the Fourier transform to both parts of the equation:

$$\kappa \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \frac{\partial^2 u}{\partial x^2} e^{-ikx} dx = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \frac{\partial u}{\partial t} e^{-ikx} dx.$$

The LHS can be integrated by parts:

$$\int_{-\infty}^{\infty} \frac{\partial^2 u}{\partial x^2} e^{-ikx} dx = -k^2 \int_{-\infty}^{\infty} u(x, t) e^{-ikx} dx,$$

while in the RHS the  $\partial/\partial t$  can be moved outside of the integration. Thus, the PDE 6.11 is transformed into

$$-k^2 \kappa \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} u(x, t) e^{-ikx} dx = \frac{\partial}{\partial t} \left[ \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} u(x, t) e^{-ikx} dx \right]. \quad (6.12)$$

If we define the Fourier transform of  $u(x, t)$  as

$$U(k, t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} u(x, t) e^{-ikx} dx,$$

PDE 6.12 can be simplified further:

$$-k^2 \kappa U(k, t) = \frac{\partial U(k, t)}{\partial t}.$$

The latter equation has a solution of the form

$$U(k, t) = U(k, 0) e^{-k^2 \kappa t}.$$

Function  $U(k, 0)$  is defined from the initial condition at the time  $t = 0$ :

$$U(k, 0) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} u(x, 0) e^{-ikx} dx = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x) e^{-ikx} dx = F(k),$$

i.e.  $U(k, 0)$  is given by the Fourier transform of the function  $f(x)$ .

Thus,

$$\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} u(x, t) e^{-ikx} dx = U(k, t) = F(k) e^{-k^2 \kappa t} = \sqrt{2\pi} F(k) G(k, t),$$

where we introduced function  $G(k, t)$  defined as

$$G(k, t) = \frac{1}{\sqrt{2\pi}} e^{-k^2 \kappa t}.$$

Function  $G(k, t)$  can be considered as a Fourier transform of some function  $g(x, t)$ . Since  $U(k, t)$  is represented as a product of two Fourier transforms, we can apply convolution theorem, proven above (see Eq. 6.9), to find  $u(x, t)$ :

$$u(x, t) = \int_{-\infty}^{\infty} g(x - s, t) f(s) ds. \quad (6.13)$$

In other words, the problem will be solved if we find function  $g(x, t)$  explicitly.

Function  $g(x, t)$  can be found by *inverse* Fourier transform of  $G(k, t)$ :

$$g(x, t) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-k^2 \kappa t} e^{ikx} dk.$$

To take this integral, first complete the square:

$$g(x, t) = \frac{1}{2\pi} \exp\left(\frac{-x^2}{4\kappa t}\right) \int_{-\infty}^{\infty} \exp\left[-\kappa t \left(k - \frac{ix}{2\kappa t}\right)^2\right] dk$$

and change variables:

$$s = k - \frac{ix}{2\kappa t}$$

to obtain

$$g(x, t) = \frac{1}{2\pi} \exp\left(\frac{-x^2}{4\kappa t}\right) \int_{-\infty}^{\infty} e^{-\kappa ts^2} ds$$

and use the fact that

$$\int_{-\infty}^{\infty} e^{-as^2} ds = \sqrt{\frac{\pi}{a}}.$$

Thus,

$$g(x, t) = \frac{1}{2\pi} e^{\frac{-x^2}{4\kappa t}} \sqrt{\frac{\pi}{\kappa t}} = \frac{1}{\sqrt{4\pi\kappa t}} e^{\frac{-x^2}{4\kappa t}}.$$

Finally, the temperature distribution at the time  $t$  can be calculated, according to Eq. 6.13, using function  $g(x, t)$  and the initial temperature distribution  $f(x)$ .



# Chapter 7

## Linear partial differential equations

### 7.1 Important PDE.

Consider a function  $u = u(x_1, x_2, \dots, x_n)$ , which depends on  $n$  variables  $x_1, x_2, \dots, x_n$ . In physical problems, these variables are usually spatial coordinates, e.g.,  $x, y, z$ , and time  $t$ . Depending on the problem at hands, it can be convenient to consider function  $u$  in Cartesian, polar, or spherical coordinate systems:

$$\begin{aligned} u &= u(x, y, z, t) && \text{in Cartesian coordinates} \\ u &= u(r, \phi, z, t) && \text{in polar coordinates} \\ u &= u(r, \phi, \theta, t) && \text{in spherical coordinates.} \end{aligned}$$

**The wave equation.**

$$\nabla^2 u = \frac{1}{v^2} \frac{\partial^2 u}{\partial t^2},$$

where

$$\nabla^2 u = \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) u = \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \frac{\partial^2 u}{\partial z^2}$$

and  $v$  is the wave velocity. In one-dimensional case, the wave equation is

$$\frac{\partial^2 u(x, t)}{\partial x^2} = \frac{1}{v^2} \frac{\partial^2 u(x, t)}{\partial t^2}.$$

**The diffusion equation.**

$$k\nabla^2 u = \frac{\partial u}{\partial t}.$$

This equation is also used to describe heat flow.

**Laplace's equation.**

$$\nabla^2 u = 0.$$

**Poisson's equation.**

$$\nabla^2 u = \rho(\mathbf{r}).$$

**Schrödinger's equation.**

$$-\frac{\hbar^2}{2m}\nabla^2 u + V(\mathbf{r})u = i\hbar\frac{\partial u}{\partial t}.$$

## 7.2 Linear 1<sup>st</sup> order PDE.

General form of the linear first order partial differential equation with respect to function  $u(x, y)$  of two variables  $x$  and  $y$ :

$$A(x, y) \frac{\partial u}{\partial x} + B(x, y) \frac{\partial u}{\partial y} + C(x, y)u = R(x, y), \quad (7.1)$$

where  $A(x, y)$ ,  $B(x, y)$ ,  $C(x, y)$ , and  $R(x, y)$  are functions of  $x$  and  $y$ .

Importantly, there could be many solutions due to

1. integrating constants and
2. existence of independent solutions.

**Case of  $C(x, y) = R(x, y) = 0$ .** If  $C = R = 0$ , Eq. (7.1) becomes

$$A(x, y) \frac{\partial u}{\partial x} + B(x, y) \frac{\partial u}{\partial y} = 0. \quad (7.2)$$

Consider solutions of this equation in the form of

$$u(x, y) = f(p),$$

where  $p$  is a parameter formed by some *fixed* combination of  $x$  and  $y$ . Note that  $p$  is a function of  $x$  and  $y$ :  $p(x, y)$ .

Use the chain rule of differentiation to obtain  $\partial u / \partial x$  and  $\partial u / \partial y$ :

$$\frac{\partial u(x, y)}{\partial x} = \frac{df(p)}{dp} \frac{\partial p}{\partial x} \quad \text{and} \quad \frac{\partial u(x, y)}{\partial y} = \frac{df(p)}{dp} \frac{\partial p}{\partial y}.$$

Substitute these into Eq. 7.2 and obtain:

$$\left[ A(x, y) \frac{\partial p}{\partial x} + B(x, y) \frac{\partial p}{\partial y} \right] \frac{df(p)}{dp} = 0. \quad (7.3)$$

This equation is satisfied if

$$\frac{df(p)}{dp} = 0,$$

which means that function  $f(p)$  is a constant, i.e. it has no dependence on  $p$  and, therefore, has no dependence on  $x$  and  $y$ . Alternatively, Eq. (7.3) is satisfied if

$$A(x, y) \frac{\partial p}{\partial x} + B(x, y) \frac{\partial p}{\partial y} = 0. \quad (7.4)$$

Notice that this equation is similar to Eq. (7.2), in which  $u$  is replaced with  $p$ .

On the other hand, for  $p$  to remain a constant combination of  $x$  and  $y$ , we should have

$$dp = \frac{\partial p}{\partial x}dx + \frac{\partial p}{\partial y}dy = 0. \quad (7.5)$$

Note that this equation is identical to Eq. (7.4) if we set

$$dx = \frac{A(x, y)}{B(x, y)}dy.$$

Hence, instead of solving Eqs. (7.4) and (7.5), we can integrate equation

$$\frac{dx}{A(x, y)} = \frac{dy}{B(x, y)}$$

in order to find  $p$ .

**Example.** Consider

$$x^3 \frac{\partial u}{\partial x} + 3y^2 \frac{\partial u}{\partial y} = 0. \quad (7.6)$$

In this case we have  $A(x, y) = x^3$  and  $B(x, y) = 3y^2$ . Following the previous discussion, this equation is converted to

$$\frac{dx}{x^3} = \frac{dy}{3y^2}.$$

After integration

$$-\frac{1}{2x^2} = -\frac{1}{3y} + C$$

or

$$\frac{1}{2x^2} = \frac{1}{3y} + C.$$

Associate the constant  $C$  with the fixed combination of  $x$  and  $y$  and denote it as  $p$ :

$$C = \frac{1}{2x^2} - \frac{1}{3y} = \frac{3y - 2x^2}{6x^2y} = p$$

Hence, the general solution of Eq. (7.6) is an *arbitrary* function of the argument  $(3y - 2x^2)/6x^2y$ :

$$u(x, y) = f\left(\frac{3y - 2x^2}{6x^2y}\right).$$

To find particular solutions, we have to introduce the boundary conditions. For example, if we demand that  $u(x, y) = 0$  at the point (2,2), i.e., at the point where  $x=2$  and  $y=2$ . Then, a possible particular solution is

$$u(x, y) = \frac{3y - 2x^2}{6x^2y} + \frac{1}{24}.$$

**Case of  $R(x, y) = 0$ .** If  $R = 0$ , Equation (7.1) becomes

$$A(x, y) \frac{\partial u}{\partial x} + B(x, y) \frac{\partial u}{\partial y} + C(x, y)u = 0. \quad (7.7)$$

Apply the same logic as above but consider a solution in the form

$$u(x, y) = h(x, y)f(p).$$

In this case,

$$\begin{aligned} \frac{\partial u}{\partial x} &= \frac{\partial h(x, y)}{\partial x}f(p) + h(x, y)\frac{df(p)}{dp}\frac{\partial p}{\partial x} \\ \frac{\partial u}{\partial y} &= \frac{\partial h(x, y)}{\partial y}f(p) + h(x, y)\frac{df(p)}{dp}\frac{\partial p}{\partial y} \end{aligned}$$

Substitute these derivatives into PDE (7.7):

$$\left[ A(x, y) \left( \frac{\partial h}{\partial x}f(p) + h\frac{df(p)}{dp}\frac{\partial p}{\partial x} \right) + B(x, y) \left( \frac{\partial h}{\partial y}f(p) + h\frac{df(p)}{dp}\frac{\partial p}{\partial y} \right) + C(x, y)hf(p) \right] = 0.$$

After rearranging the terms:

$$\left[ A(x, y)\frac{\partial h}{\partial x} + B(x, y)\frac{\partial h}{\partial y} + C(x, y)h \right] f(p) + \left[ A(x, y)\frac{\partial p}{\partial x} + B(x, y)\frac{\partial p}{\partial y} \right] h\frac{df(p)}{dp} = 0. \quad (7.8)$$

The first term turns to zero if function  $h(x, y)$  is any, however simple, solution of the original PDE given by Eq. (7.7). Let us assume that we have found such a function  $h(x, y)$ . Then, only the second term is remaining:

$$\left[ A(x, y)\frac{\partial p}{\partial x} + B(x, y)\frac{\partial p}{\partial y} \right] h\frac{df(p)}{dp} = 0.$$

Non-trivial solutions of this equation can be found by solving

$$A(x, y) \frac{\partial p}{\partial x} + B(x, y) \frac{\partial p}{\partial y} = 0.$$

In other words, the problem reduced to the previously considered case of  $C(x, y)=R(x, y)=0$  given by Eq. (7.2).

**Example.** Consider equation

$$x \frac{\partial u}{\partial x} + 2 \frac{\partial u}{\partial y} - 2u = 0. \quad (7.9)$$

Here  $A(x, y) = x$ ,  $B(x, y) = 2$ ,  $C(x, y) = -2$ . First, integrate

$$\frac{dx}{x} = \frac{dy}{2},$$

which gives

$$\ln x = \frac{1}{2}y + C.$$

From here we obtain

$$x = c \exp(y/2),$$

where  $c$  is a constant, which can be associated with the parameter  $p$ :

$$p = xe^{-y/2}.$$

Therefore, a general solution of Equation (7.9) is given by

$$u(x, y) = h(x, y)f(xe^{-y/2}),$$

where  $f$  is an arbitrary function.

It remains to find an expression for  $h(x, y)$ . In the simplest case we can consider  $h(x, y)$  being a function of  $x$  only. Therefore, the corresponding equation with respect to  $h(x)$

$$A(x, y) \frac{\partial h}{\partial x} + B(x, y) \frac{\partial h}{\partial y} + C(x, y)h = 0 \quad (7.10)$$

is simplified to

$$x \frac{\partial h}{\partial x} - 2h = 0$$

and its particular solution is  $h(x) = x^2$ .

Alternatively, we can consider function  $h(x, y)$  as a function of  $y$  only. According to Eq. (7.10), the corresponding equation with respect to  $h(y)$  is

$$2 \frac{\partial h}{\partial y} - 2h = 0,$$

which has a particular solution  $h(y) = e^y$ .

Hence, the corresponding two sets of general solutions are

$$u_1(x, y) = x^2 f(xe^{-y/2}) \quad \text{and} \quad u_2(x, y) = e^y g(xe^{-y/2}),$$

where  $f$  and  $g$  are arbitrary functions of  $xe^{-y/2}$ .

Superposition

$$u(x, y) = u_1(x, y) + u_2(x, y)$$

is also a solution of the PDE (7.9).

### Homogeneity.

- *Homogeneous partial differential equation:* if  $u(x, y)$  is a solution of a PDE, then  $v(x, y) = c \cdot u(x, y)$ , where  $c$  is an arbitrary constant, is also a solution of the same PDE;
- *Homogeneous boundary conditions:* if  $u(x, y)$  satisfies the boundary conditions, then  $v(x, y) = c \cdot u(x, y)$ , where  $c$  is an arbitrary constant, also satisfies the same boundary conditions.

**Solutions of non-homogeneous equations.** Given the equation

$$A(x, y) \frac{\partial u}{\partial x} + B(x, y) \frac{\partial u}{\partial y} + C(x, y)u(x, y) = R(x, y)$$

and the boundary condition, for example,  $u(0, y) = g(y)$ , a general solution of this equation can be written as

$$u(x, y) = v(x, y) + w(x, y),$$

where  $v(x, y)$  is any solution of the non-homogeneous equation and  $w(x, y)$  is a general solution of the homogeneous equation.

### 7.3 Linear 2<sup>nd</sup> order PDE.

**Classification.** General form of the 2nd order PDE is given by

$$A(x, y) \frac{\partial^2 u}{\partial x^2} + B(x, y) \frac{\partial^2 u}{\partial x \partial y} + C(x, y) \frac{\partial^2 u}{\partial y^2} + D(x, y) \frac{\partial u}{\partial x} + E(x, y) \frac{\partial u}{\partial y} + F(x, y)u = R(x, y) \quad (7.11)$$

We will work with a specific form of Eq. (7.11):

$$A \frac{\partial^2 u}{\partial x^2} + B \frac{\partial^2 u}{\partial x \partial y} + C \frac{\partial^2 u}{\partial y^2} = 0, \quad (7.12)$$

where  $A$ ,  $B$ , and  $C$  are constants. These equations are split into three groups according to the relations between coefficients  $A$ ,  $B$ , and  $C$ :

- $B^2 > 4AC$  – *hyperbolic* equations; they describe propagating oscillations (waves);
- $B^2 = 4AC$  – *parabolic* equations; they describe transport processes, such as heat conduction and diffusion;
- $B^2 < 4AC$  – *elliptic* equations describe stationary systems, such as steady electric fields and temperature distributions.

**Solving 2<sup>nd</sup> order PDE.** Similarly to the case of the 1st order PDE, consider solutions in the form  $u(x, y) = f(p)$ . To find a suitable form of the parameter  $p$ , inspect partial derivatives of  $u(x, y)$  with respect to  $x$  and  $y$ .

First derivatives are

$$\frac{\partial u}{\partial x} = \frac{df(p)}{dp} \frac{\partial p}{\partial x} \quad \text{and} \quad \frac{\partial u}{\partial y} = \frac{df(p)}{dp} \frac{\partial p}{\partial y}.$$

Then, 2nd derivatives are

$$\begin{aligned} \frac{\partial^2 u}{\partial x^2} &= \frac{\partial}{\partial x} \left( \frac{df(p)}{dp} \frac{\partial p}{\partial x} \right) = \frac{d^2 f(p)}{dp^2} \frac{\partial p}{\partial x} \frac{\partial p}{\partial x} + \frac{df(p)}{dp} \frac{\partial^2 p}{\partial x^2} \\ \frac{\partial^2 u}{\partial y^2} &= \frac{\partial}{\partial y} \left( \frac{df(p)}{dp} \frac{\partial p}{\partial y} \right) = \frac{d^2 f(p)}{dp^2} \frac{\partial p}{\partial y} \frac{\partial p}{\partial y} + \frac{df(p)}{dp} \frac{\partial^2 p}{\partial y^2} \end{aligned}$$

$$\frac{\partial^2 u}{\partial y \partial x} = \frac{\partial}{\partial y} \left( \frac{df(p)}{dp} \frac{\partial p}{\partial x} \right) = \frac{d^2 f(p)}{dp^2} \frac{\partial p}{\partial y} \frac{\partial p}{\partial x} + \frac{df(p)}{dp} \frac{\partial^2 p}{\partial y \partial x}.$$

If we request that

$$\frac{\partial p}{\partial x} = \text{Constant} \quad \text{and} \quad \frac{\partial p}{\partial y} = \text{Constant},$$

all second derivatives will have the same common factor of

$$\frac{d^2 f(p)}{dp^2},$$

which simplifies solving Equation (7.12).

It follows from the conditions  $\partial p / \partial x = \text{Constant}$  and  $\partial p / \partial y = \text{Constant}$  that parameter  $p$  is a linear function of  $x$  and  $y$  simultaneously. Therefore, we choose it in the form

$$p = ax + by,$$

where  $a$  and  $b$  are some constants. Thus, we can search for solutions of Eq. (7.12) in the form

$$u(x, y) = f(ax + by).$$

Then, calculate derivatives

$$\frac{\partial^2 u}{\partial x^2} \quad \frac{\partial^2 u}{\partial x \partial y} \quad \frac{\partial^2 u}{\partial y^2}$$

(see above) for this particular form of the parameter  $p$  and substitute them in the original Equation (7.12). After the substitution obtain

$$(Aa^2 + Bab + Cb^2) \frac{d^2 f(p)}{dp^2} = 0. \quad (7.13)$$

Eq. (7.13) is satisfied if either

$$\frac{d^2 f(p)}{dp^2} = 0 \quad \text{or} \quad Aa^2 + Bab + Cb^2 = 0.$$

The condition  $d^2f(p)/dp^2 = 0$  means that  $f(p)$  is a linear function of  $p$ . Indeed, integrating this equation gives,

$$\frac{df(p)}{dp} = k \quad \text{and} \quad f(p) = kp + m,$$

where  $k$  and  $m$  are some constants.

Using the expression for  $p = ax + by$ , we obtain a solution

$$u(x, y) = f(p) = kp + m = k(ax + by) + m = \alpha x + \beta y + \gamma,$$

where  $\alpha = ka$ ,  $\beta = kb$ , and  $\gamma = m$ . Importantly, this form of  $u(x, y)$  has only zero second derivatives. Thus, it is a trivial solution of Eq. (7.12) because any linear function of  $x$  and  $y$  is a solution of this equation.

Non-trivial solutions of Eq. (7.12) can be obtained by solving

$$Aa^2 + Bab + Cb^2 = 0.$$

This expression can be considered as a quadratic equation with respect to  $\lambda = b/a$ :

$$C\left(\frac{b}{a}\right)^2 + B\left(\frac{b}{a}\right) + A = 0.$$

Solving it gives

$$\left(\frac{b}{a}\right)_{1,2} = \lambda_{1,2} = \frac{-B \pm \sqrt{B^2 - 4AC}}{2C}.$$

Hence, parameter  $p$  may have two values:

$$p_1 = a(x + \lambda_1 y) \quad \text{and} \quad p_2 = a(x + \lambda_2 y).$$

The prefactor  $a$  can be omitted without the loss of generality and we can write

$$p_1 = x + \lambda_1 y \quad \text{and} \quad p_2 = x + \lambda_2 y.$$

Consequently, the solution  $u(x, y)$  becomes a superposition of two solutions:

$$u(x, y) = f(x + \lambda_1 y) + g(x + \lambda_2 y),$$

where  $f$  and  $g$  are arbitrary functions.

**Note** that we used the discriminant

$$D = B^2 - 4AC$$

of the quadratic equation

$$C\lambda^2 + B\lambda + A = 0.$$

The classification of the 2nd order PDE we have introduced above, corresponds to the different values of this discriminant:

1. If  $B^2 > 4AC$ , the discriminant is positive and  $\lambda_1$  and  $\lambda_2$  are real; such equations are called *hyperbolic*.
2. If  $B^2 < 4AC$ , the discriminant is negative, i.e.  $\lambda_1$  and  $\lambda_2$  are complex; such equations are called *elliptic*.
3. If  $B^2 = 4AC$ , the discriminant is zero and  $\lambda_1 = \lambda_2$ ; such equations are called *parabolic*.

**Example.** Compare the two equations:

$$\frac{\partial^2 v}{\partial x^2} - \frac{1}{c^2} \frac{\partial^2 v}{\partial t^2} = 0 \quad \text{1-dimensional wave equation}$$

and

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = 0 \quad \text{2-dimensional Laplace equation.}$$

For the wave equations we have

$$1 - \frac{\lambda^2}{c^2} = 0,$$

which has two real roots  $\lambda_1 = c$  and  $\lambda_2 = -c$ . Hence, the solution is

$$u(x, t) = f(x + ct) + g(x - ct).$$

For the Laplace equation:

$$1 + \lambda^2 = 0,$$

which has two imaginary roots  $\lambda_1 = i$  and  $\lambda_2 = -i$ . Hence, its solution is

$$u(x, y) = f(x + iy) + g(x - iy).$$

**Parabolic equation.** Let us consider a special case of  $B = 4AC$ . Then  $\lambda_1 = \lambda_2$  and only one solution

$$u(x, y) = f\left(x - \frac{B}{2C}y\right)$$

exists. Similarly to the case of the 1st order PDE, we can try to find the second solution of the 2nd order PDE in the form

$$u(x, y) = h(x, y)g\left(x - \frac{B}{2C}y\right),$$

where  $g$  is an arbitrary function and equation for  $h(x, y)$  can be obtained using the following considerations.

Calculate the first derivatives of  $u(x, y)$ :

$$\frac{\partial u}{\partial x} = \frac{\partial h}{\partial x}g(p) + h\frac{dg(p)}{dp}\frac{\partial p}{\partial x} = \frac{\partial h}{\partial x}g(p) + h\frac{dg(p)}{dp}$$

$$\frac{\partial u}{\partial y} = \frac{\partial h}{\partial y}g(p) + h\frac{dg(p)}{dp}\frac{\partial p}{\partial y} = \frac{\partial h}{\partial y}g(p) - h\frac{dg(p)}{dp}\frac{B}{2C}$$

and the second derivatives of  $u(x, y)$ :

$$\frac{\partial^2 u}{\partial x^2} = \frac{\partial^2 h}{\partial x^2}g(p) + 2\frac{\partial h}{\partial x}\frac{dg(p)}{dp} + h\frac{d^2 g(p)}{dp^2}$$

$$\frac{\partial^2 u}{\partial x \partial y} = \frac{\partial^2 h}{\partial x \partial y}g(p) + \frac{\partial h}{\partial y}\frac{dg(p)}{dp} - \frac{\partial h}{\partial x}\frac{dg(p)}{dp}\frac{B}{2C} - h\frac{d^2 g(p)}{dp^2}\frac{B}{2C}$$

$$\frac{\partial^2 u}{\partial y^2} = \frac{\partial^2 h}{\partial y^2}g(p) - 2\frac{\partial h}{\partial y}\frac{dg(p)}{dp}\frac{B}{2C} + h\frac{d^2 g(p)}{dp^2}\frac{B^2}{4C^2}$$

and substitute them in Eq. (7.12). The contributions proportional to  $dg(p)/dp$  and  $d^2g(p)/dp^2$  turn to zero exactly because  $B^2 = 4AC$ :

$$\begin{aligned} \left(2A\frac{\partial h}{\partial x} - B\frac{\partial h}{\partial x}\frac{B}{2C}\right)\frac{\partial h}{\partial x} \cdot \frac{dg}{dp} + \left(B\frac{\partial h}{\partial y} - 2C\frac{\partial h}{\partial y}\frac{B}{2C}\right)\frac{\partial h}{\partial y} \cdot \frac{dg}{dp} &= 0 \\ \left(A - \frac{B^2}{2C} + C\frac{B^2}{4C^2}\right)h\frac{d^2g(p)}{dp^2} &= 0. \end{aligned}$$

Therefore, the equation with respect to  $h(x, y)$  is:

$$\left(A\frac{\partial^2 h}{\partial x^2} + B\frac{\partial^2 h}{\partial x \partial y} + C\frac{\partial^2 h}{\partial y^2}\right)g = 0. \quad (7.14)$$

We can use the simplest possible  $h(x, y)$ , which satisfies this equation, e.g.  $h(x, y) = x$ . Hence, the general solution of the original PDE (Eq. 7.12) is

$$u(x, y) = f\left(x - \frac{B}{2C}y\right) + xg\left(x - \frac{B}{2C}y\right). \quad (7.15)$$

**Exercise.** In the example above, function  $h(x, y) = y$  also satisfies Eq. 7.14. What would be the general solution of Eq. 7.12 in this case? Demonstrate that it is equivalent to the solution given by Eq. 7.15. *Hint:* express  $x$  via  $p$  and  $y$ .

## 7.4 Poisson's equation

**Green's functions in 3-dimensional space.** Let us consider a linear PDE

$$\mathcal{L}u(\mathbf{r}) = \rho(\mathbf{r}),$$

where  $\mathcal{L}$  is a linear PDE operator. Similarly to the case of ODEs, assume that we can find the solution  $u(\mathbf{r})$  with a help of Green's function  $G(\mathbf{r}, \mathbf{r}_0)$ :

$$u(\mathbf{r}) = \int G(\mathbf{r}, \mathbf{r}_0)\rho(\mathbf{r}_0)d^3\mathbf{r}_0. \quad (7.16)$$

(Here and below  $d^3\mathbf{r}$  indicates integration over a volume in the space of coordinates  $\mathbf{r}$ . Similarly,  $d^2\mathbf{r}$  indicates integration over a surface.) Substitute this function  $u(\mathbf{r})$  into the original PDE and observe that  $G(\mathbf{r}, \mathbf{r}_0)$  should satisfy to

$$\mathcal{L}G(\mathbf{r}, \mathbf{r}_0) = \delta(\mathbf{r} - \mathbf{r}_0),$$

where  $\mathbf{r}_0$  is within the “volume of interest”  $V$ .

Alternatively,  $G(\mathbf{r}, \mathbf{r}_0)$  can be obtained as

$$G(\mathbf{r}, \mathbf{r}_0) = \sum_{n=1}^{\infty} \frac{1}{\lambda_n} u_n(\mathbf{r}) u_n^*(\mathbf{r}_0),$$

where  $u_n(\mathbf{r})$  and  $\lambda_n$  ( $n = 1, 2, 3, \dots$ ) are eigenfunctions and eigenvalues of the PDE operator  $\mathcal{L}$ :

$$\mathcal{L}u_n(\mathbf{r}) = \lambda_n u_n(\mathbf{r}).$$

**Divergence theorem.** Integral form of divergence is

$$\nabla \cdot \mathbf{a} = \lim_{V \rightarrow 0} \left( \frac{1}{V} \int_S \mathbf{a} \cdot d\mathbf{S} \right)$$

Here and below  $dS$  is a small element of the surface  $S$  and  $d\mathbf{S}$  is a vector of the magnitude  $dS$  oriented perpendicular to the surface element  $dS$ .

For a sufficiently small but finite volume  $v$  enclosed by a surface  $s$  we can write

$$(\nabla \cdot \mathbf{a})v \approx \int_s \mathbf{a} \cdot d\mathbf{s}.$$

If a volume  $V$  is split into such sufficiently small volumes  $v$ , then summing over all  $v$  gives

$$\int_V (\nabla \cdot \mathbf{a})dV = \int_S \mathbf{a} \cdot d\mathbf{S},$$

where  $S$  encloses the volume  $V$ .

**Green's identity.** If  $f(\mathbf{r})$  and  $g(\mathbf{r})$  are continuous differentiable *scalar* functions defined in a volume  $V$  enclosed by a surface  $S$ , then one can construct vectors

$$f(\mathbf{r}) \nabla g(\mathbf{r}) \quad \text{and} \quad g(\mathbf{r}) \nabla f(\mathbf{r}).$$

Applying the divergence theorem to the first vector gives

$$\int_S (f \nabla g) \cdot d\mathbf{S} = \int_V \nabla \cdot (f \nabla g) dV = \int_V [f \nabla^2 g + (\nabla f) \cdot (\nabla g)] dV.$$

A similar expression for vector  $g(\mathbf{r}) \nabla f(\mathbf{r})$  is

$$\int_S (g \nabla f) \cdot d\mathbf{S} = \int_V \nabla \cdot (g \nabla f) dV = \int_V [g \nabla^2 f + (\nabla g) \cdot (\nabla f)] dV.$$

By subtracting the two last equations from each other, we obtain

$$\int_S [(f \nabla g) - (g \nabla f)] \cdot d\mathbf{S} = \int_V [f \nabla^2 g - g \nabla^2 f] dV. \quad (7.17)$$

This equality is called Green's second theorem. Note that the terms in the square parenthesis on the left are vectors and on the right – scalars.

**Poisson's equation.** Consider equation

$$\nabla^2 u(\mathbf{r}) = \rho(\mathbf{r}).$$

To find the solution of it, use Green's second theorem

$$\int_V (f \nabla^2 g - g \nabla^2 f) dV = \int_S (f \nabla g - g \nabla f) \cdot d\mathbf{S} = \int_S (f \nabla g - g \nabla f) \cdot \mathbf{n} dS,$$

where  $\mathbf{n}$  is a vector of the length 1 oriented perpendicular to the surface element  $dS$ .

Let us use  $f = u(\mathbf{r})$  and  $g = G(\mathbf{r}, \mathbf{r}_0)$ . Then, according to Eq. 7.17, we have

$$\int_V [u(\mathbf{r}) \nabla^2 G(\mathbf{r}, \mathbf{r}_0) - G(\mathbf{r}, \mathbf{r}_0) \nabla^2 u(\mathbf{r})] dV = \int_S \left[ u(\mathbf{r}) \frac{\partial G(\mathbf{r}, \mathbf{r}_0)}{\partial n} - G(\mathbf{r}, \mathbf{r}_0) \frac{\partial u(\mathbf{r})}{\partial n} \right] dS,$$

where the normal derivatives are defined as

$$\frac{\partial u(\mathbf{r})}{\partial n} = [\nabla u(\mathbf{r})] \cdot \mathbf{n} \quad \text{and} \quad \frac{\partial G(\mathbf{r}, \mathbf{r}_0)}{\partial n} = [\nabla_{\mathbf{r}} G(\mathbf{r}, \mathbf{r}_0)] \cdot \mathbf{n}.$$

When applied to Poisson's equation, i.e. using the fact that

$$\nabla^2 G(\mathbf{r}, \mathbf{r}_0) = \delta(\mathbf{r} - \mathbf{r}_0) \quad \text{and} \quad \nabla^2 u(\mathbf{r}) = \rho(\mathbf{r}),$$

the Green's theorem gives

$$\int_V (u(\mathbf{r})\delta(\mathbf{r} - \mathbf{r}_0) - G(\mathbf{r}, \mathbf{r}_0)\rho(\mathbf{r})) dV(\mathbf{r}) = \int_S \left( u(\mathbf{r}) \frac{\partial G(\mathbf{r}, \mathbf{r}_0)}{\partial n} - G(\mathbf{r}, \mathbf{r}_0) \frac{\partial u(\mathbf{r})}{\partial n} \right) dS(\mathbf{r}),$$

where  $dV(\mathbf{r})$  and  $dS(\mathbf{r})$  signify that the integration is carried out in the space of coordinates  $\mathbf{r}$ . Since  $\mathbf{r}_0$  is inside  $V$ ,

$$u(\mathbf{r}_0) = \int_V G(\mathbf{r}, \mathbf{r}_0)\rho(\mathbf{r})dV(\mathbf{r}) + \int_S \left( u(\mathbf{r}) \frac{\partial G(\mathbf{r}, \mathbf{r}_0)}{\partial n} - G(\mathbf{r}, \mathbf{r}_0) \frac{\partial u(\mathbf{r})}{\partial n} \right) dS(\mathbf{r}).$$

If  $u(\mathbf{r})$  satisfies homogeneous boundary conditions, i.e.,  $u(\mathbf{r}) = 0$  everywhere at the surface  $S$ , then the surface integral can be eliminated by demanding that the same conditions apply to  $G(\mathbf{r}, \mathbf{r}_0)$  and we obtain a familiar expression (see Eq. 7.16):

$$u(\mathbf{r}_0) = \int_V G(\mathbf{r}, \mathbf{r}_0)\rho(\mathbf{r})dV(\mathbf{r}).$$

**Boundary conditions.** Three types of boundary conditions are often considered:

1. *Dirichlet:* The value of  $u(\mathbf{r})$  is specified at each point of the boundary.
2. *Neumann:* The value of the normal derivative of  $u(\mathbf{r})$ , i.e.,

$$\frac{\partial u}{\partial n} = \nabla u \cdot \mathbf{n},$$

is specified at each point of the boundary.

3. *Cauchy:* Both  $u(\mathbf{r})$  and  $\partial u / \partial n$  are specified at each point of the boundary.

In the 3D case, these boundary conditions are specified on a 2D surface  $S$  bounding the volume  $V$ .

**Dirichlet boundary conditions.** Let us require that

$$u(\mathbf{r}) = f(\mathbf{r})$$

everywhere on the surface  $S$ . The expression for the function  $u(\mathbf{r}_0)$  can be simplified if we demand that  $G(\mathbf{r}, \mathbf{r}_0) = 0$  for all  $\mathbf{r} \in S$ . Then,

$$u(\mathbf{r}_0) = \int_V G(\mathbf{r}, \mathbf{r}_0) \rho(\mathbf{r}) dV(\mathbf{r}) + \int_S f(\mathbf{r}) \frac{\partial G(\mathbf{r}, \mathbf{r}_0)}{\partial n} dS(\mathbf{r}).$$

Since functions  $\rho(\mathbf{r})$  and  $f(\mathbf{r})$  are known, all that is left to do is to find  $G(\mathbf{r}, \mathbf{r}_0)$ , which satisfies Dirichlet boundary conditions.

To this end, consider  $G(\mathbf{r}, \mathbf{r}_0)$  as a sum of two contributions

$$G(\mathbf{r}, \mathbf{r}_0) = F(\mathbf{r}, \mathbf{r}_0) + H(\mathbf{r}, \mathbf{r}_0),$$

where function  $F(\mathbf{r}, \mathbf{r}_0)$ , called the *fundamental solution*, is defined so as

$$\nabla^2 G(\mathbf{r}, \mathbf{r}_0) = \nabla^2 F(\mathbf{r}, \mathbf{r}_0) = \delta(\mathbf{r} - \mathbf{r}_0),$$

i.e.  $F(\mathbf{r}, \mathbf{r}_0)$  corresponds to sources of, e.g., the electrostatic potential, *inside* volume  $V$ . However, it does not necessarily satisfy the boundary conditions. Therefore, function  $H(\mathbf{r}, \mathbf{r}_0)$  is chosen so as

$$\nabla^2 H(\mathbf{r}, \mathbf{r}_0) = 0$$

inside volume  $V$ , i.e., it corresponds to no sources inside  $V$  and it is fitted in such a way that the sum of  $F(\mathbf{r}, \mathbf{r}_0)$  and  $H(\mathbf{r}, \mathbf{r}_0)$  is required to satisfy the boundary conditions

$$G(\mathbf{r}, \mathbf{r}_0) = F(\mathbf{r}, \mathbf{r}_0) + H(\mathbf{r}, \mathbf{r}_0) = 0$$

for all  $\mathbf{r}$  at the surface  $S$  enclosing volume  $V$ .

**Method of images.** A practical method for finding such  $G(\mathbf{r}, \mathbf{r}_0)$  is called *method of images*. This method is applied in three steps as follows.

1. Determine the fundamental solution  $F(\mathbf{r}, \mathbf{r}_0)$  from

$$\nabla^2 F(\mathbf{r}, \mathbf{r}_0) = \delta(\mathbf{r} - \mathbf{r}_0)$$

and appropriate boundary conditions. For example, for a 3D case and  $F(\mathbf{r}, \mathbf{r}_0) \rightarrow 0$  for  $\mathbf{r} \rightarrow \infty$

$$F(\mathbf{r}, \mathbf{r}_0) = -\frac{1}{4\pi|\mathbf{r} - \mathbf{r}_0|}.$$

2. Add image sources *outside*  $V$ : position the sources at the points  $\mathbf{r}_n$  and assign them amplitudes of  $q_n$  where  $n = 1, 2, \dots, N$  and  $N$  is some integer. These sources can be represented as a superposition of  $\delta$ -functions:

$$\sum_{n=1}^N q_n \delta(\mathbf{r} - \mathbf{r}_n).$$

Note that at this point the values of  $q_n$  and  $\mathbf{r}_n$  ( $n = 1, 2, \dots, N$ ) are undefined.

3. Note that the sources *outside*  $V$  satisfy the Laplace's (not Poisson's) equation *inside*  $V$ . Hence, we can write

$$G(\mathbf{r}, \mathbf{r}_0) = F(\mathbf{r}, \mathbf{r}_0) + \sum_{n=1}^N q_n F(\mathbf{r}, \mathbf{r}_n)$$

and fit parameters  $q_n$  and  $\mathbf{r}_n$  ( $n = 1, 2, \dots, N$ ) so as to guarantee that  $G(\mathbf{r}, \mathbf{r}_0) = 0$  for  $\mathbf{r} \in S$ .

**Neumann boundary conditions.** Here we request that the normal derivative of the function  $u(\mathbf{r})$  is known everywhere at the surface  $S$ :

$$\frac{\partial u}{\partial n} = f(\mathbf{r}) \quad \text{for } \mathbf{r} \in S.$$

Use this to simplify the general expression for  $u(\mathbf{r}_0)$

$$u(\mathbf{r}_0) = \int_V G(\mathbf{r}, \mathbf{r}_0) \rho(\mathbf{r}) dV(\mathbf{r}) + \int_S \left( u(\mathbf{r}) \frac{\partial G(\mathbf{r}, \mathbf{r}_0)}{\partial n} - G(\mathbf{r}, \mathbf{r}_0) \frac{\partial u(\mathbf{r})}{\partial n} \right) dS(\mathbf{r})$$

obtained earlier. Also, notice that, according to the divergence theorem:

$$\int_S f(\mathbf{r}) dS = \int_S \nabla u \cdot \mathbf{n} dS = \int_V \nabla^2 u dV = \int_V \rho(\mathbf{r}) dV.$$

The same condition for the corresponding Green's function reads:

$$\int_S \frac{\partial G(\mathbf{r}, \mathbf{r}_0)}{\partial n} d^2\mathbf{r} = \int_S \nabla G \cdot \mathbf{n} d^2\mathbf{r} = \int_V \nabla^2 G d^3\mathbf{r} = \int_V \delta(\mathbf{r} - \mathbf{r}_0) d^3\mathbf{r} = 1.$$

Therefore, we cannot request that

$$\frac{\partial G(\mathbf{r}, \mathbf{r}_0)}{\partial n} = 0 \quad \text{for } \mathbf{r} \in S.$$

However, in order to choose as simple  $\partial G(\mathbf{r}, \mathbf{r}_0)/\partial n$  as possible, we can request that

$$\frac{\partial G(\mathbf{r}, \mathbf{r}_0)}{\partial n} = \frac{1}{A} \quad \text{for } \mathbf{r} \in S,$$

where  $A$  is the total area of the bounding surface  $S$ .

With this, the solution of the Neumann's boundary problem becomes

$$u(\mathbf{r}_0) = \int_V G(\mathbf{r}, \mathbf{r}_0) \rho(\mathbf{r}) d^3\mathbf{r} + \frac{1}{A} \int_S u(\mathbf{r}) d^2\mathbf{r} - \int_S G(\mathbf{r}, \mathbf{r}_0) f(\mathbf{r}) d^2\mathbf{r}.$$

Note that

$$\frac{1}{A} \int_S u(\mathbf{r}) d^2\mathbf{r}$$

is a constant equal to the average value of  $u(\mathbf{r})$  at the surface  $S$ . If, for infinite volume  $V$ , we request that  $u(\mathbf{r}) \rightarrow 0$  as  $|\mathbf{r}| \rightarrow \infty$ , this term can be eliminated.

## Problem solving class: Partial Differential Equations.

1. Verify that that any function of  $p$ , where  $p = x^2 + 2y$  is a solution of

$$\frac{\partial u}{\partial x} = x \frac{\partial u}{\partial y}.$$

Then determine whether  $v(x, y)$  is a solution of this PDE if

1.  $v(x, y) = x^4 + 4x^2y + 4y^2$
2.  $v(x, y) = x^4 + 2x^2y + y^2$
3.  $v(x, y) = x^2(x^2 - 4) + 4y(x^2 - 2) + 4(y^2 - 1)$

2. Find solutions of the PDE

$$\frac{1}{x} \frac{\partial u}{\partial x} + \frac{1}{y} \frac{\partial u}{\partial y} = 0,$$

for which

1.  $u(0, y) = y$  (one-dimensional boundary condition);
2.  $u(1, 1) = 1$  (zero-dimensional boundary condition).

3. Find solutions of the PDE

$$\sin x \frac{\partial u}{\partial x} + \cos x \frac{\partial u}{\partial y} = \cos x,$$

for which

1.  $u(\pi/2, y) = 0$ ;
2.  $u(\pi/2, y) = y(y + 1)$ .

4. Find the general solution of the PDE

$$\frac{\partial^2 u}{\partial x^2} - 3 \frac{\partial^2 u}{\partial x \partial y} + 2 \frac{\partial^2 u}{\partial y^2} = 0.$$

Then,

1. find  $u(x, y)$ , for which  $u(x, 0) = -x^2$  and  $\partial u / \partial y(x, 0) = 0$
2. find the value of  $u(0, 1)$  for such  $u(x, y)$ .



# Chapter 8

## Fluid Mechanics

This short set of lectures is intended to provide a basic introduction to the mathematics of fluid flow, as a preparation for module MATH2301 Fluid Mechanics, which is available to Theoretical Physicists as a third year option. There are many books on fluid mechanics, some written for mathematicians, some for physicists, and some for engineers. I recommend Tritton's *Physical Fluid Dynamics*, but almost any book on the subject will allow you to explore topics beyond these brief notes. The following notes are modified from notes kindly provided by Prof Ian Ford.

### 8.1 Introduction

It is not at all common for Physics or Theoretical Physics degree programmes to contain a substantial amount of fluid mechanics, which is strange considering the amount of particle, solid, molecular, classical and quantum mechanics that is typically covered. Fluid mechanics has somehow become the preserve of mathematicians or of mechanical engineers. Nevertheless industrial, atmospheric and astrophysical models are often founded upon a representation of fluid flow, and in order to work with these it is necessary to have a basic appreciation of the fluid mechanics principles.

The mechanics of fluids is controlled by macroscopic properties such as viscosity and compressibility, properties that are described at a microscopic level within the field of condensed matter physics. Then there are important mathematical issues present in the study of fluids, such as the onset of an instability in a flow when a particular aspect of the system is changed, for

example the dimensions of a pipe, or the typical scale of velocity of a flow. This is the transition from a steady, smooth ‘laminar’ flow to an unsteady, turbulent flow, often regarded as the embodiment of the onset of chaos. We shall not be able to look deeply into these microscopic aspects and mathematical issues, but will confine ourselves to establishing the basic partial differential equations, and associated conservation principles, that are used to describe fluid mechanics on a macroscopic scale. We shall see that a variety of mathematical tools prove to be useful: tensors, vector calculus and the solution to partial differential equations in particular.

The first job is to decide what is the task in hand. *Fluids* can include both gases and liquids. The key issue is whether the substance can or cannot sustain a shear strain for an extended time: roughly speaking, if a material can generate a restoring force that acts against being twisted then it is not a fluid. The main objective in fluid mechanics is to determine the vector velocity field  $\mathbf{v}(\mathbf{r}, t)$  describing the motion. This is a specification of the velocity of a small *packet* of fluid situated in the vicinity of position  $\mathbf{r}$  at time  $t$ . The flow might be time-independent, in which case we should write simply  $\mathbf{v}(\mathbf{r})$ .

We are typically interested in the behaviour of a fluid contained within a region  $V$ , and the boundary of this region might be open to fluid input or loss, or it might be impenetrable. There might be moving boundaries, such as a paddle, that drive the fluid into motion. There might be other forces acting on the packets of fluid as they move around the region. One might be gravity, acting (usually) in the same direction and with the same strength throughout the region. Another might be a pressure gradient. Thus a fluid can be driven along a pipe if there is a pressure drop from one end to the other. Then there are Coriolis forces for a fluid moving in a rotating system. More exotic forces can operate, for example the flow of a liquid containing fine iron particles in suspension can be affected by magnetic fields, and the mixture is then described as a *ferrofluid*.

Fluids can carry other quantities as well as suspended particles. A fluid packet possesses a quantity of *internal energy* (essentially the total energy minus the kinetic energy of its bulk flow) that is characterised by a temperature. Thus the fluid can act as a transport medium for heat. The temperature field can affect the flow of the fluid, by changing the local density, thereby giving rise to buoyancy effects. For simplicity, however, we shall not consider deviations from constant temperature in these notes. Further quantities that may be transported by a fluid flow include dissolved species such as salt, or

more complicated thermodynamic quantities such as entropy.

These species can be carried or *adverted* by the fluid, but there is another more subtle transport mechanism. Consider a static fluid in which salt is dissolved, but with some parts of the fluid carrying a denser concentration than others. The concentration of salt will eventually even itself out, not by fluid motion, but by motion at the molecular scale: this is called *diffusion*. The rate at which the spreading out takes place is characterised by a diffusion coefficient. The transport of dissolved substances, suspended particles, or heat, is achieved in a fluid by a combination of advection (often called convection) and diffusion. In the case of heat transfer, the rate of molecular-scale spreading out is characterised by the coefficient of thermal conductivity.

A less obvious quantity that can be transported diffusively by a fluid is momentum. Packets of fluid can be brought into motion (i.e. acquire momentum) by being in the proximity of other packets that are already in motion. Such a momentum transfer is brought about by a diffusive process, and the quantity that characterises the spreading out has a name too: it is called viscosity.

We shall find that certain non-linear partial differential equations describe the velocity field  $\mathbf{v}(\mathbf{r}, t)$  and the associated scalar pressure field  $p(\mathbf{r}, t)$ . The solution to these equations requires boundary conditions provided by the specific nature of the problem. Obtaining a full understanding of these solutions is a Millennium Prize problem, for which an award of \$1 million is available from the Clay Mathematics Institute: so it is not a trivial matter!

## 8.2 Bernoulli's equation

It is easiest to begin our work by studying an equation established by Daniel Bernoulli in 1738. It is a connection between the time-independent velocity and pressure fields along so-called fluid streamlines (and in some circumstances across them too). A streamline is simply a trajectory of an infinitesimal fluid packet carried along by the flow. Bernoulli's principle is based upon the conservation of energy, but it is only valid if diffusive transport of momentum and energy are neglected. This means it is limited to the discussion of so-called *inviscid* fluids, defined to have zero viscosity, and for fluids where thermal conductivity is negligible. In its simplest form, it is also restricted to the discussion of *incompressible* fluids. These have a density  $\rho$

that is independent of the local pressure, temperature etc. Liquids are fairly incompressible, and so are gases, as long as the typical flow velocities are small compared with the speed of sound.

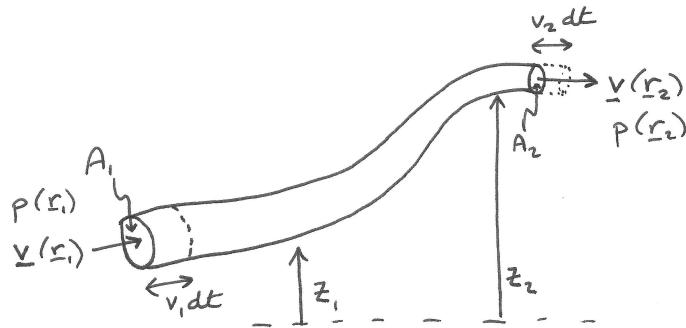


Figure 8.1: A fluid tube around a streamline used to derive Bernouilli's equation.

Consider a *streamtube* of fluid surrounding a streamline in a flow as illustrated in Figure 8.1. The key assumption is that fluid, momentum and energy are not exchanged across the sides of the tube, by definition, but only through the ends. Let us consider a time-independent velocity field  $\mathbf{v}(\mathbf{r})$ . In an interval of time  $dt$ , a mass  $\rho\mathbf{v}(\mathbf{r}_1).\mathbf{d}\mathbf{S}_1$  of fluid enters the tube through the cross-sectional area  $A_1$  perpendicular to the flow direction at position  $\mathbf{r}_1$ . The element of surface area  $\mathbf{d}\mathbf{S}_1$  is a vector of magnitude  $A_1$  oriented parallel to  $\mathbf{v}(\mathbf{r}_1)$ . The same mass of fluid exits through the outlet from the tube, where the cross-sectional area is  $A_2$  and the velocity is  $\mathbf{v}(\mathbf{r}_2)$ . Such conservation of mass implies that

$$\rho\mathbf{v}(\mathbf{r}_1).\mathbf{d}\mathbf{S}_1 = \rho\mathbf{v}(\mathbf{r}_2).\mathbf{d}\mathbf{S}_2, \quad (8.1)$$

and hence the diameter of the tube can vary in space, to accommodate a change in speed of the fluid, for example.

Let us compare the situation before and after the increment in time. A packet of fluid has moved a distance  $v_2 dt$  beyond the exit of the tube whilst a packet of fluid has moved a distance  $v_1 dt$  into the inlet. The speeds  $v_k$  are shorthand for  $|\mathbf{v}(\mathbf{r}_k)|$ . We can regard this as the creation of a packet at the exit and the elimination of a packet at the inlet. The kinetic energy densities

of the packets are  $\rho v_k^2/2$ . The change in kinetic energy of the fluid within the tube is therefore

$$dK = \frac{1}{2}\rho v_2^2 A_2 v_2 dt - \frac{1}{2}\rho v_1^2 A_1 v_1 dt. \quad (8.2)$$

Furthermore, the densities of fluid gravitational potential energy are  $\rho g z_k$  and the change in potential energy for the tube is

$$dV = \rho g z_2 A_2 v_2 dt - \rho g z_1 A_1 v_1 dt, \quad (8.3)$$

where  $z_k$  is the vertical component of position vector  $\mathbf{r}_k$ . The total energy of the tube has changed by  $dK + dV$ . We note that this change of energy has been supplied by the surrounding fluid, which has effectively pushed a piston into the inlet of the tube whilst having had a piston pushed into it at the outlet. The work done by the surrounding fluid at the inlet is the force times the displacement, namely  $p(\mathbf{r}_1)A_1 v_1 dt$  and the net work done on the tube is therefore

$$dW = p(\mathbf{r}_1)A_1 v_1 dt - p(\mathbf{r}_2)A_2 v_2 dt. \quad (8.4)$$

Neglecting diffusive losses through the tube walls, and any change in temperature of the fluid, energy conservation requires that  $dK + dV = dW$  or

$$\frac{1}{2}\rho v_2^2 A_2 v_2 + \rho A_2 v_2 g z_2 + p_2 A_2 v_2 = \frac{1}{2}\rho v_1^2 A_1 v_1 + \rho A_1 v_1 g z_1 + p_1 A_1 v_1, \quad (8.5)$$

where  $p_k = p(\mathbf{r}_k)$ . Now we use the condition for conservation of mass  $\rho \mathbf{v}(\mathbf{r}_1) \cdot \mathbf{dS}_1 = \rho \mathbf{v}(\mathbf{r}_2) \cdot \mathbf{dS}_2$  in the form  $v_1 A_1 = v_2 A_2$ , which yields

$$\frac{1}{2}\rho v_2^2 A_2 v_2 + \rho A_2 v_2 g z_2 + p_2 A_2 v_2 = \frac{1}{2}\rho v_1^2 A_1 v_1 + \rho A_1 v_1 g z_1 + p_1 A_1 v_1, \quad (8.6)$$

and thus

$$\frac{1}{2}\rho v_2^2 + \rho g z_2 + p_2 = \frac{1}{2}\rho v_1^2 + \rho g z_1 + p_1, \quad (8.7)$$

or

$$\frac{1}{2}\rho v^2 + \rho g z + p = \text{constant}, \quad (8.8)$$

along a streamline in a steady flow of an incompressible, inviscid, isothermal fluid. This is Bernoulli's equation. It can be generalised to  $\frac{1}{2}\rho v^2 + \rho \phi + p = \text{constant}$  for the case of flow in a region subject to a general scalar potential energy field (per unit mass) denoted by  $\phi(\mathbf{r})$ .

There are numerous straightforward illustrations of this principle. Consider the flow along a horizontal pipe that changes from a large diameter

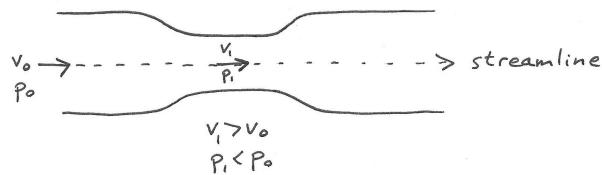


Figure 8.2: Pressure drop at a constriction in a pipe: the Venturi effect.

to a small diameter and back again. The velocity increases through the constriction, and therefore, neglecting gravity (since streamlines here are approximately horizontal), the pressure goes down: see Figure 8.2. This is the basis of the Venturi effect, whereby droplets of liquid, supplied from a side tube, can be drawn into an air flow at a constriction in a pipe. The effect can also be used in a Venturi meter to measure fluid flow velocity by measuring the pressure drop.

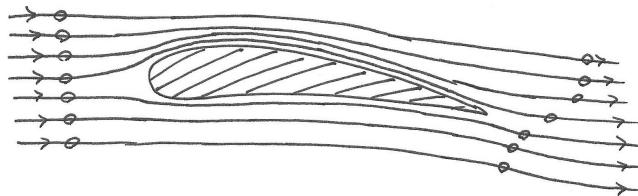


Figure 8.3: Streamlines in a flow around an aerofoil. Notice the squeezing together of the streamlines in the flow above the aerofoil, which means that the velocity there is greater than in the region beneath the aerofoil (indicated by the small circles that you can imagine advecting with the flow). Faster fluid has a lower pressure, and hence there is lift.

A frequently quoted example of the use of the Bernoulli equation is to consider flow around an aerofoil. The asymmetric shape of an aerofoil requires the upper part of the flow to move faster than the lower part. Streamlines in the incoming fluid are squeezed closer together if the fluid passes over the aerofoil compared with streamlines in the fluid passing below. It is assumed that the upstream pressure and speed of the fluid is approximately

constant with height. Fluid above the aerofoil moves faster than fluid below, and is therefore acquires a lower pressure. The overall effect is to create lift on the aerofoil, as illustrated in Figure 8.3. Notice that the fluid is sheared after passage above and below the aerofoil. The effect of an aerofoil is also to thrust downwards on the air, like a paddle, and this also contributes to the lift.

A third example is the Magnus effect. Consider the flow of a fluid around a spinning cylinder. The moving boundary drags the fluid along with it (through viscosity, which we have so far neglected) and causes it to move more slowly on one side of the cylinder than the other, spreading out and concentrating streamlines. This produces a pressure differential and a sideways force on the cylinder, as shown in Figure 8.4. A flow around a spinning sphere produces a sideways force which is sometimes called the Robins effect; one to master if you want to score spectacular goals!

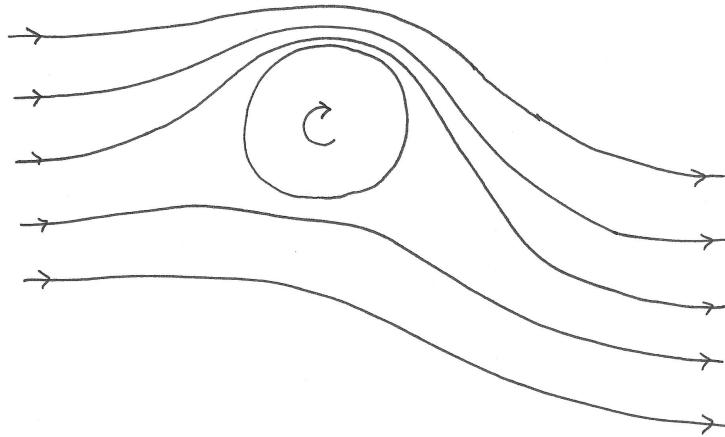


Figure 8.4: Flow streamlines around a spinning cylinder.

### 8.3 Channel flow

The discussion so far of Bernoulli's equation and the underlying principle of conservation of energy is, it has to be said, rather elementary. So let us

now raise our game a little and establish a differential equation to describe so-called *channel* flow. We consider the motion of an incompressible fluid down a parallel-sided channel or slot with a rectangular cross-section, driven by a pressure difference between the inlet to the channel and the outlet. At points in the channel far away from the inlet and outlet, we expect the velocity field to be approximately independent of distance  $x$  along the slot. For velocities that are not too large, we also expect a steady, smooth flow such that streamlines run parallel to the  $x$ -axis. If the channel width in the  $z$  direction (up and down, say) is much larger than that in the  $y$  direction, we expect furthermore that the velocity well away from these upper and lower boundaries (at  $z = \pm D/2$  say) is independent of  $z$ . The velocity field near  $z = 0$  is thus specified just by component  $v_x = u$  which is a function only of coordinate  $y$ , as shown in Figure 8.5. The pressure field is taken to depend only on coordinate  $x$ , i.e. there is a pressure gradient along the channel but none in directions perpendicular to the walls. This is the set-up for 2-d channel flow.

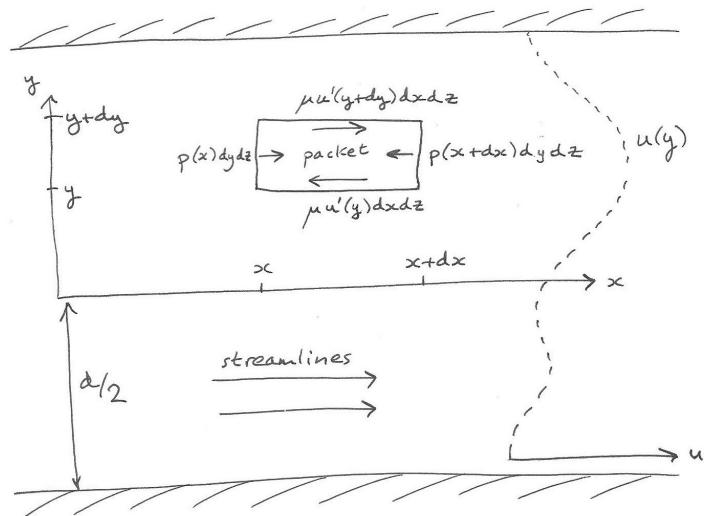


Figure 8.5: Illustration of the forces operating on a fluid packet in a two-dimensional channel flow.

It should be recognised that we are now considering a fluid that has viscosity. The velocity  $v_x$  for a given streamline is independent of  $x$ , but

there is a pressure gradient in that direction, so we are considering a pattern of flow where there is a clear violation of Bernouilli's equation, and this indicates that viscous effects are key to understanding channel flow. Let us now define viscosity  $\mu$  as the proportionality constant between the shear stress on an interface between packets of the fluid, and the gradient, in a direction normal to the interface, in the component of velocity parallel to the interface. Consider the situation shown in Figure 8.5. The non-zero velocity component in the  $x$  direction,  $u$ , has a gradient  $du/dy$  in the  $y$ -direction. This is expected to bring about a transfer of momentum, or equivalently it gives rise to a shear stress  $\tau$  acting in the  $x$  direction on the interface. The relationship between the shear stress and the velocity gradient is called a constitutive relationship, and the simplest possible relationship is linear, expressed as

$$\tau = \mu \frac{du}{dy}. \quad (8.9)$$

This is called Newton's law of viscosity and is empirically supported for many fluids. A proportionality between the gradient of the velocity field and the resulting shear stress is a property of a so-called Newtonian fluid. Non-Newtonian fluids are those that have a more complicated relationship between viscous stresses and velocity gradients. It is a task for condensed matter theory to correlate macroscopic viscous properties with microscopic intermolecular forces.

Now consider a small packet of fluid of length  $dx$ , thickness  $dy$  and height  $dz$ , situated at a distance  $y$  from the centre of the channel. We wish to determine the velocity in the  $x$  direction  $u(y)$  as a function of  $y$ . Let us consider the balance of forces on the packet. There is a pressure on the packet from behind, giving a forward force of  $p(x)dydz$ . Acting backwards on the front face of the packet is a force  $p(x+dx)dydz$ , and there are also a backward-acting shear force  $\mu u'(y)dxdz$  and a forward acting shear force  $\mu u'(y+dy)dxdz$ , where the prime indicates a derivative with respect to  $y$ . The quoted directions of the viscous forces are obtained for  $du/dy > 0$  without loss of generality. Equating the forces, for steady flow, we get

$$p(x)dydz + \mu u'(y+dy)dxdz = p(x+dx)dydz + \mu u'(y)dxdz, \quad (8.10)$$

which rearranges to

$$(p(x+dx) - p(x)) / dx = \mu (u'(y+dy) - u'(y)) / dy, \quad (8.11)$$

and this is nothing more than the second order differential equation

$$\frac{dp}{dx} = \mu \frac{d^2u}{dy^2}. \quad (8.12)$$

We next assume that the pressure gradient along the channel is negative. If the flow pattern is independent of  $x$ , then  $dp/dx$  must be equal to a constant  $-\alpha$ , and the solution for  $u(y)$  is then

$$u(y) = u(0) + Ay - (\alpha/2\mu)y^2. \quad (8.13)$$

We tidy this up by noting that the velocity profile ought to be symmetric about the centre of the channel at  $y = 0$ , so that  $A = 0$ . We then impose a boundary condition that the velocity at the walls at  $y = \pm d/2$  is zero. This is known as a no-slip boundary condition. Thus we find that

$$0 = u(0) - (\alpha/2\mu)d^2/4, \quad (8.14)$$

or  $u(0) = \alpha d^2/(8\mu)$ . The flow profile is parabolic:

$$u(y) = \frac{\alpha d^2}{8\mu} \left( 1 - \frac{4y^2}{d^2} \right), \quad (8.15)$$

and the volumetric flow rate down the channel is

$$Q = \int dz \int dy u(y) = D \frac{\alpha d^2}{8\mu} \left[ y - \frac{4y^3}{3d^2} \right]_{-d/2}^{d/2}, \quad (8.16)$$

where the width of the channel in the  $z$  direction is  $D$ , so

$$Q = D \frac{\alpha d^3}{12\mu}. \quad (8.17)$$

We note that the flow rate is proportional to the pressure gradient, and to the cube of the shorter cross-sectional dimension of the channel. It is inversely proportional to the viscosity.

We can also consider flow down a pipe with a circular cross-section with radius  $a$ . This is called Poiseuille flow. With just a little extra effort it can be shown that the velocity profile is again parabolic in distance  $r$  from the centre of the pipe, and that the volumetric flow rate is given by

$$Q = \frac{\pi \alpha a^4}{8\mu}. \quad (8.18)$$

## 8.4 Basic equations of fluid motion

Now we need to ratchet up the level of mathematics to derive differential equations to describe more general fluid flows. We shall need four such *partial* differential equations, together with appropriate boundary conditions, to determine the scalar pressure field  $p(\mathbf{r}, t)$  and the vector velocity field  $\mathbf{v}(\mathbf{r}, t)$ .

The first of these is known as the *continuity equation*, and it arises from the conservation of mass. Let us consider a compressible fluid, such that the mass density  $\rho(\mathbf{r}, t)$  is not a constant. It might be related to the pressure, for example, through an equation of state such as that of an ideal gas  $p = \rho kT/m$ , where  $m$  is the molecular mass. Consider a small cuboidal packet of fluid located in the vicinity of  $\mathbf{r}$  with volume  $dV = dx dy dz$ . The mass per unit time entering the packet from the negative  $x$  direction is  $\rho(x, y, z, t)v_x(x, y, z, t)dydz$ . The corresponding rate of loss of mass due to flow out of the packet towards the positive  $x$  direction is  $\rho(x + dx, y, z, t)v_x(x + dx, y, z, t)dydz$  and the difference between the two, contributing to the rate of change of mass inside the volume, is

$$(\rho(x, y, z, t)v_x(x, y, z, t) - \rho(x + dx, y, z, t)v_x(x + dx, y, z, t)) dy dz = -(\partial(\rho v_x)/\partial x)_{y,z} dx dy dz. \quad (8.19)$$

Taking into account flows into and out of the cuboid in the other two Cartesian directions, we obtain a total rate of change of mass inside the volume element. This must correspond to the quantity  $(\partial\rho/\partial t)_{x,y,z} dV$ . Putting this together, we obtain

$$\frac{\partial\rho}{\partial t} = -\nabla \cdot (\rho\mathbf{v}), \quad (8.20)$$

which is the desired continuity equation. For an ideal gas, we would employ  $p = \rho kT/m$  to turn this into an equation between the pressure and velocity fields, and perhaps involving a temperature field  $T$ .

If the fluid were incompressible, then the density would be constant and the continuity equation reduces to

$$\nabla \cdot \mathbf{v} = \frac{\partial v_x}{\partial x} + \frac{\partial v_y}{\partial y} + \frac{\partial v_z}{\partial z} = 0, \quad (8.21)$$

which is sometimes called a condition for solenoidal, or divergence-free flow. Note that incompressibility might seem to be incompatible with a variability in pressure across a flow: incompressibility is very much a convenient approximation.

We apply Newton's second law of motion to determine the other three partial differential equations describing the flow. We have already discussed the overall force on an elementary fluid packet due to a gradient in the pressure field  $\nabla p$ . The force in the  $x$  direction, for example, is  $-(\partial p / \partial x) dV$ . Let us ignore viscous forces for now. We next need to work out the rate of change of momentum of the fluid.

Fluid entering the volume element from the negative  $x$  direction at a mass per unit time of  $\rho(x, y, z, t)v_x(x, y, z, t)dydz$  injects (vector) momentum  $\mathbf{v}(x, y, z, t)$  per unit mass, making a contribution  $\rho(x, y, z, t)v_x(x, y, z, t)\mathbf{v}(x, y, z, t)dydz$  to the rate of change of momentum inside the element. Notice that a flow with a velocity component in the  $x$ -direction can carry momentum that has components in all three directions. The inward and outward flows therefore contribute overall a momentum  $-\partial_i(\rho v_i \mathbf{v})dxdydz$ . The rate of change of momentum of the volume element may be written  $(\partial(\rho \mathbf{v}) / \partial t) dV$  and so we can write

$$\frac{\partial(\rho \mathbf{v})}{\partial t} = -\partial_i(\rho v_i \mathbf{v}) - \nabla p, \quad (8.22)$$

for an inviscid fluid. We can also write

$$\partial_i(\rho v_i \mathbf{v}) = \rho v_i \partial_i \mathbf{v} + \mathbf{v} \partial_i(\rho v_i), \quad (8.23)$$

and using the continuity equation  $-\partial_i(\rho v_i) = \partial \rho / \partial t$  we can write  $\partial_i(\rho v_i \mathbf{v}) = \rho v_i \partial_i \mathbf{v} - \mathbf{v} \partial \rho / \partial t$ . We then get

$$\frac{\partial(\rho \mathbf{v})}{\partial t} = \mathbf{v} \frac{\partial \rho}{\partial t} - \rho \mathbf{v} \cdot \nabla \mathbf{v} - \nabla p, \quad (8.24)$$

where the second term on the right hand side, explicitly written out in Cartesian coordinates, is the vector

$$\mathbf{v} \cdot \nabla \mathbf{v} = \left( v_x \frac{\partial v_x}{\partial x} + v_y \frac{\partial v_x}{\partial y} + v_z \frac{\partial v_x}{\partial z}, v_x \frac{\partial v_y}{\partial x} + v_y \frac{\partial v_y}{\partial y} + v_z \frac{\partial v_y}{\partial z}, v_x \frac{\partial v_z}{\partial x} + v_y \frac{\partial v_z}{\partial y} + v_z \frac{\partial v_z}{\partial z} \right). \quad (8.25)$$

After one further simplification, we obtain

$$\rho \frac{\partial \mathbf{v}}{\partial t} + \rho \mathbf{v} \cdot \nabla \mathbf{v} = -\nabla p, \quad (8.26)$$

which is called the *Euler equation*. It provides three conditions on the pressure and velocity fields, which together with the continuity equation provide us with the means to solve for the motion of an inviscid, compressible fluid.

Notice the non-linearity of this partial differential equation. The second term contains products of velocities and velocity gradients. This means that if  $\mathbf{v}(\mathbf{r}, t)$  happens to be a solution, then it is *not* the case that  $\beta\mathbf{v}(\mathbf{r}, t)$ , where  $\beta$  is a constant, is also a solution. Similarly, if there are two solutions  $\mathbf{v}_a(\mathbf{r}, t)$  and  $\mathbf{v}_b(\mathbf{r}, t)$  then the sum  $\mathbf{v}_a(\mathbf{r}, t) + \mathbf{v}_b(\mathbf{r}, t)$  is not a solution. Scaling and superposition of solutions operates in systems of *linear* differential equations, but we are not so fortunate here. For this reason, solutions to Euler's equation are not easy to obtain. Furthermore, the non-linearity in the equation is thought to be the origin of the transition from steady, smooth, *laminar* flow to unsteady *turbulent* flow when a fluid is made to move faster by adjusting external parameters such as pressures or velocities at the boundaries.

Terms on the left hand side of Euler's equation (divided by  $\rho$ ) can be grouped together as

$$\frac{\partial \mathbf{v}}{\partial t} + \mathbf{v} \cdot \nabla \mathbf{v} = \frac{D\mathbf{v}}{Dt}, \quad (8.27)$$

which is known as the material or substantive derivative. Actually, the nomenclature *total* derivative is most appropriate, in my view, with the simple representation  $d\mathbf{v}/dt$ . Whilst the partial derivative  $\partial\mathbf{v}/\partial t$  refers to the rate of change in velocity of fluid contained within an elementary volume that is fixed in space, (the local velocity at that point changes but the actual fluid passes through and is replaced) the material derivative describes the rate of change of the velocity of a specific packet of fluid that moves with the flow. In a time interval  $dt$ , a packet initially in the vicinity of position  $\mathbf{r}$  moves to the vicinity of  $\mathbf{r} + \mathbf{v}dt$ . The change in its velocity component in the  $i$ th direction is

$$dv_i = v_i(\mathbf{r} + \mathbf{v}dt, t + dt) - v_i(\mathbf{r}, t) = \frac{\partial v_i}{\partial t}dt + \frac{\partial v_i}{\partial x_j}v_jdt, \quad (8.28)$$

with implied summation in the last term, so the total derivative is

$$\frac{dv_i}{dt} = \frac{\partial v_i}{\partial t} + v_j \frac{\partial v_i}{\partial x_j} = \left( \frac{\partial}{\partial t} + \mathbf{v} \cdot \nabla \right) v_i = \frac{Dv_i}{Dt}. \quad (8.29)$$

The  $\mathbf{v} \cdot \nabla \mathbf{v}$  term is often called the advective or inertial term, or the convective acceleration.

A treatment of the dynamics based on a fixed grid of coordinates, determining a vector field  $\mathbf{v}(\mathbf{r}, t)$  that satisfies the dynamical equations and the spatial and temporal boundary conditions, is a so-called *Eulerian* point of

view. One that examines the evolution of the velocity of a specific packet of fluid as time progresses is called a *Lagrangian* treatment, and requires us to determine the field  $\mathbf{v}(\mathbf{R}(t), t)$  where  $\mathbf{R}(t)$  traces out the trajectory of a packet situated at arbitrary position  $\mathbf{R}(0)$  at  $t = 0$ . A Lagrangian treatment is somewhat more complicated to obtain, but is analogous to the mechanics of individual particles and is convenient in numerical simulation.

Our discussion of the basic equations of fluid motion will be completed in a later section when we include viscous effects and derive the Navier-Stokes equation. We first delve deeper into the description of inviscid fluids.

## 8.5 The Bernouilli and Euler equations

We started these lectures by showing that Bernouilli's equation is valid in the limit of steady, incompressible inviscid flows, and then went on to derive Euler's equation for a similar regime. Let us see how these two results are related.

We start with the following identity in vector calculus:

$$\mathbf{v} \times (\nabla \times \mathbf{v}) = \frac{1}{2} \nabla(\mathbf{v} \cdot \mathbf{v}) - \mathbf{v} \cdot \nabla \mathbf{v}, \quad (8.30)$$

which can be proved in the following way. We know that  $(\mathbf{a} \times \mathbf{b})_i = \epsilon_{ijk} a_j b_k$  so

$$(\mathbf{v} \times (\nabla \times \mathbf{v}))_i = \epsilon_{ijk} v_j \epsilon_{klm} \partial_l v_m, \quad (8.31)$$

and using the identity

$$\epsilon_{ijk} \epsilon_{klm} = \epsilon_{kij} \epsilon_{klm} = \delta_{il} \delta_{jm} - \delta_{im} \delta_{jl}, \quad (8.32)$$

this becomes

$$(\mathbf{v} \times (\nabla \times \mathbf{v}))_i = (\delta_{il} \delta_{jm} - \delta_{im} \delta_{jl}) v_j \partial_l v_m = v_j \partial_i v_j - v_j \partial_j v_i = \frac{1}{2} \partial_i(v_j v_j) - \mathbf{v} \cdot \nabla v_i, \quad (8.33)$$

and the result is proved.

Thus Euler's equation for steady incompressible flow, with  $\partial \mathbf{v} / \partial t = 0$  and  $\rho = \text{constant}$  can be recast as

$$\rho \mathbf{v} \cdot \nabla \mathbf{v} = \frac{1}{2} \nabla(\rho \mathbf{v} \cdot \mathbf{v}) - \rho \mathbf{v} \times (\nabla \times \mathbf{v}) = -\nabla p. \quad (8.34)$$

If we take a dot product of both sides with  $\mathbf{v}$  and rearrange we get

$$\mathbf{v} \cdot \nabla \left( \frac{1}{2} \rho v^2 + p \right) = 0, \quad (8.35)$$

where  $v^2 = \mathbf{v} \cdot \mathbf{v}$  and having used  $\mathbf{v} \cdot (\mathbf{v} \times (\nabla \times \mathbf{v})) = 0$  by the rules of the triple vector product. The equation shows that the gradient of the quantity  $\frac{1}{2} \rho v^2 + p$  is perpendicular to the flow direction. In other words, this scalar quantity does not change its value along a streamline. This is, of course, Bernouilli's equation, valid as before for the steady flow of incompressible, inviscid fluids.

There is a generalisation of Bernouilli's result that would hold if the condition  $\nabla \times \mathbf{v} = 0$  happens to be satisfied. The above development, before taking the dot product with  $\mathbf{v}$ , would lead to

$$\nabla \left( \frac{1}{2} \rho v^2 + p \right) = 0, \quad (8.36)$$

which states that Bernouilli's equation holds at every point in the region, not just along streamlines. The condition  $\nabla \times \mathbf{v} = 0$  is referred to as curl-free flow, amongst other things, and it is not as uncommon as you might think, as we discuss next.

## 8.6 Vorticity and irrotational flow

One of the most noticeable phenomena arising from the complex dynamics of fluids is the production and evolution of vortices: examples include spinning whirlpools or tornados. A vortex line is the axis of a rotating region of fluid. A number of mathematical tools have been developed in order to describe vortex behaviour. The most useful of these is called vorticity, and is defined to be the curl of the velocity field:

$$\boldsymbol{\omega} = \nabla \times \mathbf{v}. \quad (8.37)$$

Let us evaluate the vorticity of some common flow patterns. For a constant, unidirectional flow,  $\boldsymbol{\omega} = 0$ . Next consider a shear flow  $\mathbf{v} = (u(y), 0, 0)$  in Cartesian coordinates. The components of vorticity are given by  $\omega_i = \epsilon_{ijk} \partial_j v_k$  and the only non-zero component is  $\omega_z = -\partial_y u$ . Shear flows therefore possess a vorticity perpendicular to the shear gradient and the direction of flow.

Consider next a flow pattern where packets of fluid are advected in a circular path around the origin. We consider first the cases where the fluid rotates in a rigid body fashion, for which the velocity field is  $\mathbf{v} = \boldsymbol{\Omega} \times \mathbf{r}$ , where  $\boldsymbol{\Omega}$  is the angular velocity of rotation. The vorticity is  $\boldsymbol{\omega} = \nabla \times (\boldsymbol{\Omega} \times \mathbf{r})$  and so

$$\begin{aligned}\omega_i &= \epsilon_{ijk} \partial_j \epsilon_{klm} \Omega_l x_m = \epsilon_{kij} \epsilon_{klm} \Omega_l \partial_j x_m = (\delta_{il} \delta_{jm} - \delta_{im} \delta_{jl}) \Omega_l \partial_j x_m \\ &= (\delta_{il} \delta_{jm} - \delta_{im} \delta_{jl}) \Omega_l \delta_{jm} = 3\Omega_i - \Omega_i = 2\Omega_i,\end{aligned}\quad (8.38)$$

and so the vorticity at all points in a ‘rigid body’ rotational flow is equal to twice the angular velocity.

Next consider a rotating flow that has shear as well. Consider  $\mathbf{v} = (0, v_\theta(r), 0)$  in cylindrical polar coordinates. The curl of this vector, and hence the vorticity, is  $(0, 0, v_\theta/r + \partial_r v_\theta)$  in these coordinates. Notice that the pattern of rotation  $v_\theta(r) = K/r$  has zero vorticity at all radial positions, except perhaps at the origin. This is called a free vortex. Packets of fluid in such a flow are not in fact spinning, even though they are moving in a circle around the origin. They continue to ‘face’ the same way. But in fact there is a singularity of vorticity at the origin. This can be demonstrated by applying Stokes’ theorem along a circular path around the origin:

$$\int \boldsymbol{\omega} \cdot d\mathbf{S} = \int (\nabla \times \mathbf{v}) \cdot d\mathbf{S} = \oint \mathbf{v} \cdot d\mathbf{l} = \int_0^{2\pi} v_\theta r d\theta = 2\pi K, \quad (8.39)$$

and so it must be the case that  $\boldsymbol{\omega} = 2\pi K \delta(\mathbf{r}) \hat{\mathbf{e}}_z$  for this flow, where  $\delta(\mathbf{r})$  is a Dirac delta function: an infinite spike at precisely  $\mathbf{r} = 0$ . A free vortex is a rough model of the spinning fluid structures that are naturally generated in the atmosphere or (possibly) in a teacup: notice that the rotational motion is faster closer to the axis. The vorticity takes the form of a vector field defined only on a line running along the vortex axis.

The above discussion indicates that vorticity is associated with circular motion, with local spinning behaviour, and with shear flows. Let us now attempt to establish equations of motion for the vorticity for an inviscid fluid. We take the curl of the Euler equation to get

$$\rho \frac{\partial \boldsymbol{\omega}}{\partial t} + \rho \nabla \times (\mathbf{v} \cdot \nabla \mathbf{v}) = -\nabla \times \nabla p, \quad (8.40)$$

having passed the curl operator through the time derivative. We note that the curl of a gradient is zero, deduced from  $(\nabla \times \nabla p)_i = \epsilon_{ijk} \partial_j \partial_k p = \epsilon_{ijk} \partial_k \partial_j p =$

$\epsilon_{ikj}\partial_j\partial_k p = -\epsilon_{ijk}\partial_j\partial_k p$ , so the pressure term vanishes. Let us consider the second term on the left hand side. We employ an identity used earlier:

$$\nabla \times (\mathbf{v} \cdot \nabla \mathbf{v}) = \nabla \times \left( \frac{1}{2} \nabla(\mathbf{v} \cdot \mathbf{v}) - \mathbf{v} \times (\nabla \times \mathbf{v}) \right) = -\nabla \times (\mathbf{v} \times \boldsymbol{\omega}), \quad (8.41)$$

having again used the fact that the curl of a gradient is zero, and continue with

$$\begin{aligned} -(\nabla \times (\mathbf{v} \times \boldsymbol{\omega}))_i &= -\epsilon_{ijk}\partial_j\epsilon_{klm}v_l\omega_m = \epsilon_{kij}\epsilon_{kml}\partial_jv_l\omega_m \\ &= (\delta_{im}\delta_{jl} - \delta_{il}\delta_{jm})\partial_jv_l\omega_m \\ &= \partial_jv_j\omega_i - \partial_jv_i\omega_j \\ &= v_j\partial_j\omega_i + \omega_i\partial_jv_j - \omega_j\partial_jv_i - v_i\partial_j\omega_j \\ &= v_j\partial_j\omega_i + \omega_i\partial_jv_j - \omega_j\partial_jv_i - v_i\partial_j\epsilon_{jkl}\partial_kv_l \\ &= \mathbf{v} \cdot \nabla \omega_i + (\nabla \cdot \mathbf{v})\omega_i - \boldsymbol{\omega} \cdot \nabla v_i, \end{aligned} \quad (8.42)$$

having noticed that  $\partial_j\epsilon_{jkl}\partial_kv_l = -\partial_j\epsilon_{kjl}\partial_kv_l = -\partial_k\epsilon_{jkl}\partial_jv_l = -\partial_j\epsilon_{jkl}\partial_kv_l = 0$ . Hence

$$\frac{\partial \boldsymbol{\omega}}{\partial t} + \mathbf{v} \cdot \nabla \boldsymbol{\omega} + (\nabla \cdot \mathbf{v})\boldsymbol{\omega} - \boldsymbol{\omega} \cdot \nabla \mathbf{v} = 0, \quad (8.43)$$

and hence

$$\frac{D\boldsymbol{\omega}}{Dt} = \boldsymbol{\omega} \cdot \nabla \mathbf{v} - (\nabla \cdot \mathbf{v})\boldsymbol{\omega}. \quad (8.44)$$

This is an interesting equation with several features, but the point here is to demonstrate that a flow with zero vorticity remains curl-free, or *irrotational* at later times, if we can ignore viscous effects. Packets with zero vorticity advect with no change in vorticity. To see this, consider the advection of a fluid packet along a streamline. The right hand side in the above equation is effectively a source term for the vorticity of the fluid packet, and it vanishes if the local value of vorticity is zero. If the initial  $\boldsymbol{\omega}$  of the packet is zero, then it will remain zero.

This has the following consequence. Consider the flow of an incompressible, inviscid fluid through some complicated geometry, but with the upstream boundary condition that the velocity field is uniform, and hence irrotational. If we can ignore viscosity, then the flow remains irrotational as it passes through the complicated geometry and becomes spatially non-uniform. The development of vorticity is only due to viscous effects, which it turns out are relevant where the flow speeds are low, which is near boundaries.

Due to the consequent relative ubiquity of irrotational flow, it is fruitful to seek solutions to Euler's equation based on the representation of the velocity field as the gradient of a so-called *velocity potential*:

$$\mathbf{v} = -\nabla\Phi(\mathbf{r}, t). \quad (8.45)$$

This representation ensures that the flow is irrotational: its curl is zero. Inserting this form into Euler's equation gives an equation for  $\Phi$  and  $p$ , which is one direction that could be pursued. However, an equation of much greater value is obtained by inserting (8.45) into the continuity equation and assuming incompressibility:

$$-\nabla \cdot \mathbf{v} = 0 = \nabla^2\Phi, \quad (8.46)$$

which implies that we need to solve the Laplace equation, familiar from other areas of physics such as electrostatics!

Let us consider the flow of an inviscid fluid around a sphere of radius  $a$  using this approach. The asymptotic flow field, far from the sphere, is  $\mathbf{U}$ , directed along the  $z$  axis of spherical polar coordinates centred on the stationary sphere. We need to solve Laplace's equation in these coordinates, and we assume that the velocity potential has no dependence on the angle  $\phi$ . Thus we solve

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\Phi}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\Phi}{\partial\theta}\right) = 0, \quad (8.47)$$

subject to the boundary conditions  $v_r = -\partial\Phi/\partial r = 0$  at  $r = a$  and  $\nabla\Phi = -\mathbf{U}$  as  $r \rightarrow \infty$ . Notice that we do not employ a no-slip boundary condition at the sphere surface, since physically this is brought about by viscosity, which we have not yet included. The solution, obtained by a separation of variables technique, is

$$\Phi = -Ur\left(1 + \frac{a^3}{2r^3}\right)\cos\theta, \quad (8.48)$$

giving velocity components

$$\begin{aligned} v_r &= U\left(1 - \frac{a^3}{r^3}\right)\cos\theta \\ v_\theta &= -U\left(1 + \frac{a^3}{2r^3}\right)\sin\theta. \end{aligned} \quad (8.49)$$

This potential bears a resemblance to the electrostatic potential field around a dipole. A sketch of the streamlines is shown in Figure 8.6.

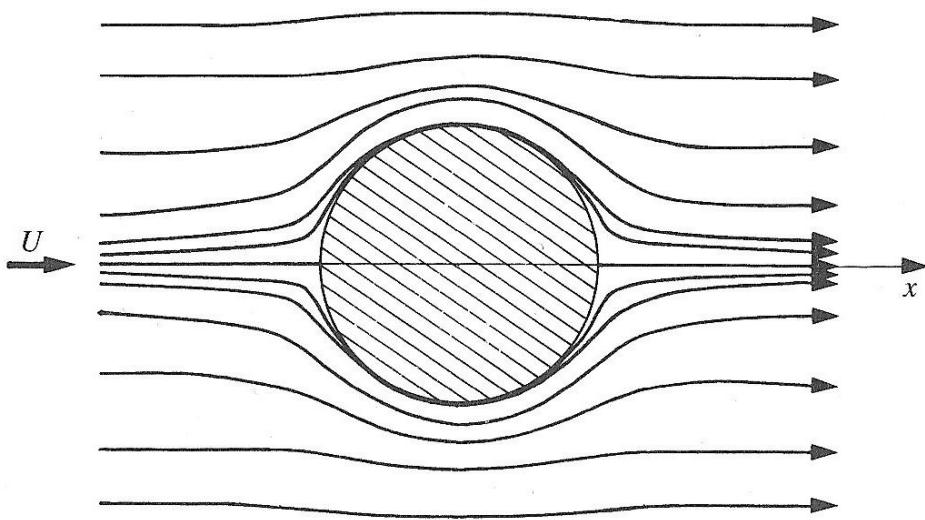


Figure 8.6: Sketch of potential flow field around a sphere.

## 8.7 Viscous flow

### 8.7.1 Navier-Stokes equation

We return to our derivation of the general evolution equations, now with the inclusion of viscous effects.

Consider the viscous stress tensor  $\tau_{ij}$ , defined to be the viscous force per unit area acting in direction  $i$  on an interface in the fluid with a normal vector pointing in the direction  $j$ . The concept is illustrated in Figure 8.7. For a Newtonian fluid one proposes the relationship

$$\tau_{ij} = \Lambda_{ijkl}\dot{\epsilon}_{kl} = \Lambda_{ijkl}\frac{1}{2} \left( \frac{\partial v_k}{\partial x_l} + \frac{\partial v_l}{\partial x_k} \right), \quad (8.50)$$

where  $\dot{\epsilon}_{ij}$  is called the rate of strain tensor. Clearly the expression  $\tau = \mu du/dy$  used earlier is just a special case of this one. It is usual to relate  $\tau_{ij}$  to  $\dot{\epsilon}_{kl}$  rather than  $\partial v_k / \partial x_l$  since  $\dot{\epsilon}_{kl}$  is symmetric under exchange of suffices, which is useful in analysis.

The fourth rank tensor  $\Lambda_{ijkl}$  is a set of 81 constants relating viscous stresses to rates of strain. It is a property of the fluid material. Isotropic fluids

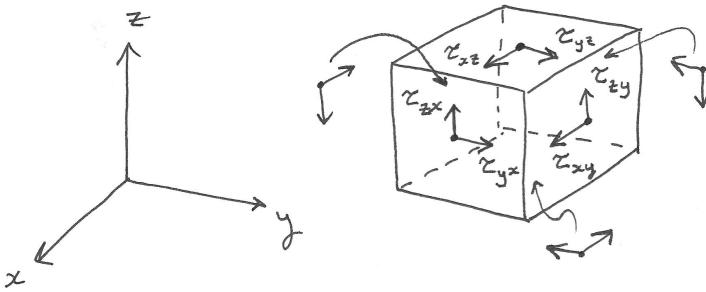


Figure 8.7: Viscous shear stresses acting on a cuboidal fluid element.  $\tau_{ij}$  is the force per unit area in the  $i$ th direction acting on the face with outward normal pointing in the  $j$ th direction. Note that the rear faces are subject to shear stresses in the opposite directions to those present on the adjacent fluid elements (equal action and reaction at those points).

have properties that are independent of the choice of orientation of coordinate axes. This class includes most common fluids, but excludes such exotica as liquid crystals. We shall assume, for simplicity, that  $\Lambda_{ijkl}$  is an isotropic tensor, namely one that transforms into itself under a rotation of coordinates. It turns out that isotropic fourth rank tensors can be constructed out of products of the isotropic second rank tensor, namely the Kronecker delta. We write

$$\Lambda_{ijkl} = A\delta_{ij}\delta_{kl} + B\delta_{ik}\delta_{jl} + C\delta_{il}\delta_{jk}, \quad (8.51)$$

where  $A$ ,  $B$  and  $C$  are scalar fluid properties, such that

$$\tau_{ij} = A\delta_{ij}\nabla \cdot \mathbf{v} + (B + C)\frac{1}{2} \left( \frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i} \right), \quad (8.52)$$

or equivalently

$$\tau_{ij} = \lambda\delta_{ij}\nabla \cdot \mathbf{v} + \mu(\partial_j v_i + \partial_i v_j), \quad (8.53)$$

which is written in terms of the so-called shear and bulk viscosities,  $\mu$  and  $\lambda$ . The force in the  $i$ th direction on the elementary fluid packet is, as we found earlier when we considered pressure alone, proportional to a gradient in the stress, and for viscous forces this is given by  $\partial_j \tau_{ij} dV$ , with implied

summation over  $j$  but with  $\tau_{xx} = \tau_{yy} = \tau_{zz} = 0$ . Newton's equations of motion now take the form

$$\rho \frac{\partial v_i}{\partial t} + \rho \mathbf{v} \cdot \nabla v_i = -\partial_i p + \partial_j \tau_{ij} = -\partial_i p + \lambda \partial_i (\nabla \cdot \mathbf{v}) + \mu \partial_j \partial_j v_i + \mu \partial_i (\nabla \cdot \mathbf{v}), \quad (8.54)$$

assuming that  $\mu$  and  $\lambda$  are constants, which may be written

$$\rho \frac{\partial \mathbf{v}}{\partial t} + \rho \mathbf{v} \cdot \nabla \mathbf{v} = -\nabla p + (\lambda + \mu) \nabla (\nabla \cdot \mathbf{v}) + \mu \nabla^2 \mathbf{v}, \quad (8.55)$$

and for an incompressible fluid, for which  $\nabla \cdot \mathbf{v} = 0$ , this becomes

$$\rho \frac{\partial \mathbf{v}}{\partial t} + \rho \mathbf{v} \cdot \nabla \mathbf{v} = -\nabla p + \mu \nabla^2 \mathbf{v} + \mathbf{F}, \quad (8.56)$$

where we have added, for completeness, a further 'body' force per unit volume  $\mathbf{F}$ , for which the prototype is the gravitational  $\mathbf{F} = -\rho g \hat{\mathbf{e}}_z$ . This is the *Navier-Stokes equation*, the general solution to which is worth \$1m.

The Navier-Stokes equation reduces to the equation we established earlier for steady channel flow. If we assume a form  $\mathbf{v} = (v_x(y), 0, 0)$  in Cartesian coordinates (a form that together with the continuity equation implies fluid incompressibility), then

$$\mathbf{v} \cdot \nabla \mathbf{v} = \left( v_x \frac{\partial v_x}{\partial x} + v_y \frac{\partial v_x}{\partial y} + v_z \frac{\partial v_x}{\partial z}, v_x \frac{\partial v_y}{\partial x} + v_y \frac{\partial v_y}{\partial y} + v_z \frac{\partial v_y}{\partial z}, v_x \frac{\partial v_z}{\partial x} + v_y \frac{\partial v_z}{\partial y} + v_z \frac{\partial v_z}{\partial z} \right) = 0, \quad (8.57)$$

and if  $\mathbf{F} = 0$  and  $p$  is a function of  $x$  only, the N-S equation reduces to

$$0 = -\frac{dp}{dx} + \mu \frac{d^2 v_x}{dy^2}, \quad (8.58)$$

as before. The Poiseuille solution, for flow down a pipe with circular bore of radius  $a$ , is obtained by solving the Navier-Stokes equation appropriate to a solution of form  $\mathbf{v} = (0, 0, v_z(r))$  in cylindrical polar coordinates. The advective term still vanishes, and we have to solve

$$0 = -\frac{dp}{dz} + \mu \frac{1}{r} \frac{d}{dr} \left( r \frac{dv_z}{dr} \right), \quad (8.59)$$

and if  $dp/dz = -\alpha$  is constant, then the appropriate solution subject to the no-slip boundary condition  $v_z(a) = 0$  and the requirement that  $v_z(0)$  is finite is  $v_z(r) = \alpha(a^2 - r^2)/(4\mu)$ .

### 8.7.2 Reynolds number

Earlier we discussed solutions to the flow equations for inviscid fluids and now we have included viscous effects. It is important to be able to judge when viscous forces are significant. We can do this by comparing the expected magnitudes of contributions to the Navier-Stokes equation. The best way to do this is to contrast the viscous force term  $\mu \nabla^2 \mathbf{v}$  with the advective term  $\rho \mathbf{v} \cdot \nabla \mathbf{v}$ . On this basis, we should be able to neglect the viscous term and regard the fluid as inviscid if the fluid speed is large or the viscosity is low. This can be stated more precisely. If we have a solution to the Navier-Stokes equation we can always cast it in dimensionless quantities, namely by putting  $\mathbf{r} = L \mathbf{r}'$ , and  $\mathbf{v} = u \mathbf{v}'$  where  $L$  is a particular length scale (such as the diameter of a channel) and  $u$  is a particular scale of speed. The primed variables are dimensionless. Now the viscous and advective terms take the form

$$\frac{\mu u}{L^2} \nabla'^2 \mathbf{v}' \quad \text{and} \quad \frac{\rho u^2}{L} \mathbf{v}' \cdot \nabla' \mathbf{v}', \quad (8.60)$$

where we take derivatives with respect to dimensionless distances. From this we conclude that we can definitely ignore the viscous terms in obtaining the solution if

$$\frac{\mu u}{L^2} \ll \frac{\rho u^2}{L} \quad \text{or} \quad \frac{\mu}{L u \rho} = \frac{1}{\text{Re}} \ll 1, \quad (8.61)$$

which defines an important dimensionless number characterising the flow: the *Reynolds number*  $\text{Re} = L u \rho / \mu$ . Flows are inviscid for  $\text{Re} \gg 1$ , and viscous for Reynolds numbers of order unity and below. An identification of the precise cross-over between regimes, if one exists, requires a specification of the length scale and speed, but the qualitative association of viscous and inviscid flow regimes with small and large Reynolds number, respectively, is quite general.

In the limit of small Reynolds number, we can simplify the Navier-Stokes equations considerably by ignoring the advective term. This eliminates the non-linearity, and allows us to study some important cases.

### 8.7.3 Stokes flow around a sphere

Consider the flow of a fluid around a sphere of radius  $a$  that is moving at (low) speed  $U$  through a stagnant, incompressible fluid. It is easier to discuss this problem using a coordinate system with an origin that remains

at the centre of the sphere, namely moving at speed  $U$ , in which frame the fluid takes a steady flow pattern with constant speed  $-U$  at infinity. Let us use spherical polar coordinates where the direction of fluid motion is defined by  $\theta = 0$ . We seek a solution to the Navier-Stokes equations of the form  $\mathbf{v} = (v_r(r, \theta), v_\theta(r, \theta), 0)$ . We assume the component  $v_\phi$  to be zero by symmetry, and that there is no dependence of velocity components  $v_r$  and  $v_\theta$  on angle  $\phi$  for the same reason. The inner boundary conditions are  $v_r(a, \theta) = 0$  denoting the impenetrability of the sphere of radius  $a$ , and  $v_\theta(a, \theta) = 0$  which represents a no-slip boundary condition. Apart from the latter, these are the same ingredients we used to study the irrotational flow around the sphere in the inviscid regime earlier. The outer boundary conditions are  $v_r \rightarrow U \cos \theta$  and  $v_\theta \rightarrow -U \sin \theta$  as  $r \rightarrow \infty$ . Furthermore, the pressure field tends towards a constant value  $p_0$  as  $r \rightarrow \infty$ . The geometry is illustrated in Figure 8.8.

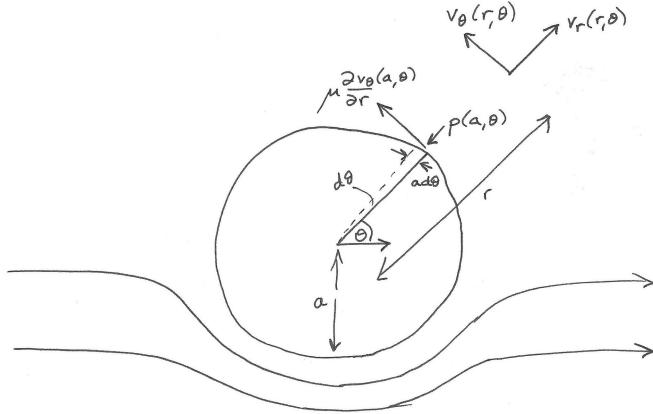


Figure 8.8: Geometry of Stokes flow around a sphere.

Neglecting the advective term, and in the absence of body forces, the Navier-Stokes equation reduces to

$$\rho \frac{\partial \mathbf{v}}{\partial t} = -\nabla p + \mu \nabla^2 \mathbf{v} = 0, \quad (8.62)$$

and for the presumed form of the solution, this leads to the differential equa-

tions

$$0 = -\frac{\partial p}{\partial r} + \mu \left( \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial v_r}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial v_r}{\partial \theta} \right) - \frac{2v_r}{r^2} - \frac{2v_\theta}{r^2} \cot \theta - \frac{2}{r^2} \frac{\partial v_\theta}{\partial \theta} \right), \quad (8.63)$$

and

$$0 = -\frac{1}{r} \frac{\partial p}{\partial \theta} + \mu \left( \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial v_\theta}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial v_\theta}{\partial \theta} \right) - \frac{v_\theta}{r^2 \sin^2 \theta} + \frac{2}{r^2} \frac{\partial v_r}{\partial \theta} \right), \quad (8.64)$$

whilst the continuity equation, for an incompressible fluid, is written

$$\frac{1}{r^2} \frac{\partial(r^2 v_r)}{\partial r} + \frac{1}{r \sin \theta} \frac{\partial(\sin \theta v_\theta)}{\partial \theta} = 0. \quad (8.65)$$

Notice the that the effect of the Laplacian operator on a vector differs from its effect on a scalar.

Yikes! What a mass of complication is hidden within the compact form of the Navier-Stokes equation! The above equations need not be memorised, by the way, nor do you need to know how the various terms are generated. A discussion of the vector calculus may be found in maths books. We cut through all the complication by stating that the velocity and pressure fields that satisfy these equations and the boundary conditions, are

$$\begin{aligned} v_r &= U \cos \theta \left( 1 - \frac{3a}{2r} + \frac{a^3}{2r^3} \right) \\ v_\theta &= -U \sin \theta \left( 1 - \frac{3a}{4r} - \frac{a^3}{4r^3} \right) \\ p &= p_0 - \frac{3\mu U a}{2r^2} \cos \theta. \end{aligned} \quad (8.66)$$

This is Stokes' solution for so-called *creeping* flow around a sphere, approximately valid at not too high an asymptotic fluid speed  $U$ , and not too large a sphere radius  $a$ . The Reynolds number for flow around a sphere may be constructed from speed and length scales  $U$  and  $a$  in the form  $\text{Re} = aU\rho/\mu$  and for Stokes flow to hold, this ratio must be rather smaller than unity. If the Reynolds number were increased, a complicated wake would form behind the sphere, brought about by the neglected advective term.

We can use the Stokes solution to determine the drag force on a sphere around which a fluid is slowly moving. The force on the sphere in the direction of the asymptotic flow velocity arises from a combination of the fluid

pressure and viscous stress (due to the radial gradient of  $v_\theta$ ), both evaluated at the spherical surface. We write

$$F_{\text{drag}} = \int_0^\pi 2\pi a^2 \sin \theta d\theta \left( -p(a, \theta) \cos \theta - \mu \sin \theta \left. \frac{\partial v_\theta}{\partial r} \right|_{r=a} \right) = 6\pi\mu a U, \quad (8.67)$$

and the drag force is therefore proportional to the speed of relative motion between the sphere and the flow (a common assumption made when calculating the frictional drag on a projectile moving through the air, for example). The Stokes drag force is also proportional to radius: one might perhaps expect proportionality to cross-sectional area, but this only emerges at high Reynolds number.

## 8.8 Summary

The dynamical behaviour of fluids is remarkably diverse, and we have only touched upon some of the most basic cases. But we have identified the main reason for the diversity: the non-linearity of the Navier-Stokes equation for the velocity field. When we have to add additional features such as complicated boundaries, the effects of heat input and temperature variation, and perhaps even the effect of suspended objects in the flow, obtaining theoretical predictions of behaviour becomes extremely challenging. This is why physical problems involving flow, such as weather forecasting, are rather hard to model. The solution of fluid mechanical problems relies heavily on numerical methods and fast computers.

Apart from learning some elements of fluid mechanics from these lectures, I hope you have gained an appreciation of the nature of a classical field theory, a model that describes a spatially distributed collection of physical quantities that are coupled to one other. The velocity field of a fluid is easy to visualise and to experience, and its dynamics are expressed in terms of partial differential equations and conservation principles that are a representation of Newton's laws of motion. Another field theory you will encounter describes the electric and magnetic fields: this also satisfies some (rather simpler) differential equations, but is a little less easy to visualise.

## Exercises for discussion

1. State the conditions under which the following theoretical tools are valid descriptions of fluid flow:
  - Bernouilli's equation along a streamline
  - Bernouilli's equation throughout the region
  - the continuity equation
  - Euler's equation
  - Laplace's equation for a scalar field
  - the Navier-Stokes equation
  - Laplace's equation for a vector field
2. Using the properties of  $\epsilon_{ijk}$  prove that  $\nabla \times (\nabla V) = 0$  where  $V$  is a scalar field.
3. The advective term in cylindrical polar coordinates is

$$\begin{aligned}(\mathbf{v} \cdot \nabla \mathbf{v})_r &= v_r \frac{\partial v_r}{\partial r} + \frac{v_\theta}{r} \frac{\partial v_r}{\partial \theta} + v_z \frac{\partial v_r}{\partial z} - \frac{v_\theta^2}{r} \\(\mathbf{v} \cdot \nabla \mathbf{v})_\theta &= v_r \frac{\partial v_\theta}{\partial r} + \frac{v_r v_\theta}{r} + \frac{v_\theta}{r} \frac{\partial v_\theta}{\partial \theta} + v_z \frac{\partial v_\theta}{\partial z} \\(\mathbf{v} \cdot \nabla \mathbf{v})_z &= v_r \frac{\partial v_z}{\partial r} + \frac{v_\theta}{r} \frac{\partial v_z}{\partial \theta} + v_z \frac{\partial v_z}{\partial z}\end{aligned}$$

Show that for a flow field of the form  $\mathbf{v} = (0, 0, v_z(r))$  each component of the advective term is equal to zero. Thus calculate the Poiseuille volumetric flow rate along a cylindrical pipe of radius  $a$ , subject to an axial pressure gradient  $-\alpha$ .

4. Figure 8.6 illustrates the flow of an inviscid fluid around a sphere. The drag force on the sphere may be written as an integral involving the local pressure on the surface. What is the magnitude of the drag force? (Hint: you might think that you need to substitute the derived potential flow solution into Euler's equation to obtain the pressure at the surface, and then perform the integral, but the answer (which might not be what you expect) can be obtained by a simpler route based on imagining a reversal of all velocities.)

5. Show that the flow field  $\mathbf{v} = (0, K(2\pi r)^{-1}(1 - \exp(-r^2\rho/(4\mu t))), 0)$  in cylindrical polars satisfies the Navier-Stokes equation for an incompressible fluid. You may assume that  $\nabla^2\mathbf{v}$  (the vector Laplacian) in cylindrical polars takes the form:

$$\begin{aligned}(\nabla^2\mathbf{v})_r &= \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial v_r}{\partial r} \right) + \frac{1}{r^2} \frac{\partial^2 v_r}{\partial \theta^2} - \frac{v_r}{r^2} + \frac{\partial^2 v_r}{\partial z^2} - \frac{2}{r^2} \frac{\partial v_\theta}{\partial \theta} \\(\nabla^2\mathbf{v})_\theta &= \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial v_\theta}{\partial r} \right) + \frac{1}{r^2} \frac{\partial^2 v_\theta}{\partial \theta^2} - \frac{v_\theta}{r^2} + \frac{\partial^2 v_\theta}{\partial z^2} + \frac{2}{r^2} \frac{\partial v_r}{\partial \theta} \\(\nabla^2\mathbf{v})_z &= \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial v_z}{\partial r} \right) + \frac{1}{r^2} \frac{\partial^2 v_z}{\partial \theta^2} + \frac{\partial^2 v_z}{\partial z^2}\end{aligned}$$

Calculate the radial pressure gradient. Calculate the vorticity. Don't be afraid to use Mathematica! Describe what is going on physically in this flow field.