Introduction to Partial Differential Equations in Physics

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Part I

Introduction

Chapter 1

Geometrical meaning of vector calculus

1.1 A very short introduction to diffusion (and dimensional analysis)

Let us consider the function

$$\rho(t, \mathbf{x}) \tag{1.1}$$

giving, for example, the density of a substance in still air as a function of time t and position $\mathbf{x}$ (a 3D vector). We may assume that at time $t = 0$ such density assumes a given distribution

$$\rho(0, \mathbf{x}) = \rho_0(\mathbf{x}) \tag{1.2}$$

and wonder how ρ will change with time. Let us make the hypothesis that at fixed $\mathbf{x} = \mathbf{x}_0$ the variation in time of ρ will depend on how much material is in $\mathbf{x}_0$ with respect to the neighbouring space. We may define a small volume $V_{\mathbf{x}_0}$ centred in $\mathbf{x}_0$ and measure the average of ρ in the volume

$$\overline{\rho}(t, \mathbf{x}_0) = \frac{\int_{V_{\mathbf{x}_0}} \rho(t, \mathbf{x}) d\mathbf{x}}{\int_{V_{\mathbf{x}_0}} d\mathbf{x}} \tag{1.3}$$

This quantity depends obviously on the details of the choice of $V_{\mathbf{x}_0}$, but we assume that it is uniquely defined if we let the size of $V_{\mathbf{x}_0}$ go to zero,

$$\overline{\rho}(t, \mathbf{x}_0) = \lim_{V_{\mathbf{x}_0} \to 0} \frac{\int_{V_{\mathbf{x}_0}} \rho(t, \mathbf{x}) d\mathbf{x}}{\int_{V_{\mathbf{x}_0}} d\mathbf{x}} \tag{1.4}$$

In a intuitive way, we may expect the amount of ρ to grow in time if $\overline{\rho} > \rho$, and to decrease if $\overline{\rho} < \rho$. Namely, the substance will diffuse in $\mathbf{x}_0$ if a larger

amount of it is in the surrounding small volume, and diffuse out of $\mathbf{x}_0$ if a smaller amount of it is in the volume.

Mathematically, we may express the change of ρ in time while keeping $\mathbf{x}$ fixed as the partial derivative in time

$$\frac{\partial \rho(t,\mathbf{x})}{\partial t} \equiv \partial_t \rho(t,\mathbf{x}) \equiv \partial_t \rho \tag{1.5}$$

In these notes, we will often use ∂_t as a short hand for the partial derivative with respect to variable t, and we will not write the list of variables when there is no risk of confusion.

We now assume that this variation in time is proportional to the difference between ρ and $\overline{\rho}$

$$\partial_t \rho(t,\mathbf{x}) = \kappa(\overline{\rho}(t,\mathbf{x}) - \rho(t,\mathbf{x})) \tag{1.6}$$

In this equation, we used $\mathbf{x}$ in place of $\mathbf{x}_0$ to stress that the equation is valid everywhere[1].

We note that the constant has "the dimension of inverse time", i.e., if time is measured in seconds, κ is measured in s^{-1}. This is due to the fact that on the left ρ is divided by time[2], while on the right ρ is multiplied by κ. As a result, if we want the equation to make sense if we change units, κ has to be the equivalent to a division by time.

Such a "dimensional analysis" is extremely useful in all physics problems, so that it may be useful to explain it better with a simple example. Let us assume we have a law[3] that relates the average velocity of walking v to the walked distance L,

$$v = \alpha/\sqrt{L} \tag{1.7}$$

Let us also assume that we know that if we measure distances in kilometres, and times in hours, we have $\alpha = 7.2$, meaning that we walk at 7.2 km/h over a 1 km distance. The law will then tell us that we walk at a 3.6 km/h velocity over a 4 km distance. Let us now use meters and seconds. 7.2 km equal 7200 m, an 1 hour is 3600 s, so that a velocity of 7.2 km/h corresponds to 2 m/s. We have now $2 = \alpha/\sqrt{1000}$ or $\alpha \approx 63.25$. It is clear that α is not a pure number, i.e. a number that does not change when we change a unit system. This is obvious, since on the left we have a velocity, and on the right α divided by the square of a length, so that α must have it's own "dimension", i.e. it mast be expressed as a function of length, time, mass,

[1] Or at least inside a proper domain in which we study the evolution of ρ.

[2] Since the (partial) derivative is given by the difference between two values of ρ at small time separation δt, divided by δt, or, more precisely given by $\lim_{\delta t \to 0} \frac{\rho(t+\delta t,\mathbf{x}) - \rho(t,\mathbf{x})}{\delta t}$.

[3] The actual law will be more complex, and dependent on individual fitness.

etc, so that also the right side will be a velocity. A velocity has to be equal to a velocity![4]

We may write an equation as

$$[V] = \frac{[L]}{[T]} = [L][T]^{-1} \tag{1.8}$$

that we read as "velocity has the dimensionality of length over time". This means that the physical quantity velocity is obtained as the ratio between a length and a time. Then, the dimensional equation corresponding to eq. (1.7) is

$$[L][T]^{-1} = [\alpha][L]^{-1/2} \tag{1.9}$$

that we solve as

$$[\alpha] = [L]^{3/2}[T]^{-1} \tag{1.10}$$

This means that α is measured in square roots of volumes divided by time. This looks quite complex, but as we know that a quantity measured in kilometres becomes 10^3 times bigger when we measure it in meters (i.e., when we pass to a unit that is 10^{-3} smaller) α will be scaled of a factor

$$(10^3)^{3/2}(3.6 \cdot 10^3)^{-1} = 10^{3/2}/3.6 \approx 8.784$$

passing from kilometres and hours to meters and seconds. Indeed,

$$7.2 \cdot 8.748 \approx 63.25$$

Let us go back to our original problem, eq. (1.6). In this form, the equation is very intuitive, and may already tell us something interesting. If, at time $t = 0$, we have $\rho(0, \mathbf{x}) \geq 0 \ \forall \mathbf{x}$, as we expect for the density of our substance, we will have $\rho(t, \mathbf{x}) \geq 0 \ \forall \mathbf{x}$, $t \geq 0$. Why? To have a negative ρ, we need (by eq. 1.6 and assuming the function and its derivatives to be continuous) a point with $\rho = 0$ and with $\overline{\rho} < 0$. This means that starting from $\rho \geq 0$ everywhere, we will never get a negative ρ.

Nevertheless, eq. (1.6) is written in a very peculiar way. It relates a partial derivative to the limit of an integral. It is possible to re-write it as an equation involving only partial derivative of ρ, i.e. as a *partial differential equation*. In our path of obtaining such a *diffusion equation* (or *heat equation*) we will also learn the geometrical and physical meaning of vector calculus, and how to write differential equations in different coordinate systems.

[4] So that the above expression $2 = \alpha/\sqrt{1000}$ is actually not correct, or better valid only after a specific set of units has been chosen.

1.2 Curvilinear coordinates

Let us consider to points on the plane, A and B. We assume their coordinates in a given Cartesian frame to be $A(x, y)$ and $B(x + \Delta x, y + \Delta y)$. By Pythagoras' theorem, we know that the distance between the two points is

$$\Delta s = \sqrt{\Delta x^2 + \Delta y^2} \tag{1.11}$$

We will often write this as

$$ds^2 = dx^2 + dy^2 \tag{1.12}$$

meaning that dx and dy are small and we are authorised to retain only leading terms in Taylor polynomials and the like.

We can also use other coordinates in the plane, e.g. polar coordinates (r, θ). The relation giving the Cartesian coordinates as functions of the polar ones is

$$x = r\cos\theta, \qquad y = r\sin\theta \tag{1.13}$$

Using a Taylor polynomial, we may write the change in x as a function of changes in r and θ, namely

$$\Delta x = \frac{\partial x}{\partial \theta}\Delta\theta + \frac{\partial x}{\partial r}\Delta r + \text{higher powers of } \Delta r, \Delta\theta \tag{1.14}$$

As stated above, assuming variations to be small we may also write this expression as

$$dx = \frac{\partial x}{\partial \theta}d\theta + \frac{\partial x}{\partial r}dr \tag{1.15}$$

We also have

$$dy = \frac{\partial y}{\partial \theta}d\theta + \frac{\partial y}{\partial r}dr \tag{1.16}$$

From eq. (1.13) we have

$$\frac{\partial x}{\partial r} = \cos\theta, \quad \frac{\partial x}{\partial \theta} = -r\sin\theta, \quad \frac{\partial y}{\partial r} = \sin\theta, \quad \frac{\partial y}{\partial \theta} = r\cos\theta \tag{1.17}$$

and substitution of eqs. (1.13,1.17) in eq. (1.12) gives

$$\begin{aligned} ds^2 &= \cos^2\theta dr^2 + r^2\cos^2\theta d\theta^2 - 2r\cos\theta\sin\theta + \sin^2\theta dr^2 + r^2\sin^2\theta d\theta^2 + 2r\sin\theta\cos\theta \\ &= r^2 d\theta^2 + dr^2 \end{aligned} \tag{1.18}$$

This equation tells us two important things

1. ds^2 may be written as a sum of quadratic terms in dr and $d\theta$, i.e. the polar coordinates are orthogonal and no mixed terms appear

2. the expression is anyway different from the one we obtained for Cartesian coordinates, since the contribution of $d\theta$ is weighted by a r^2 term. The reason of this should be evident from Fig. 1.1. For larger values of r, to same variation of θ corresponds a larger distance

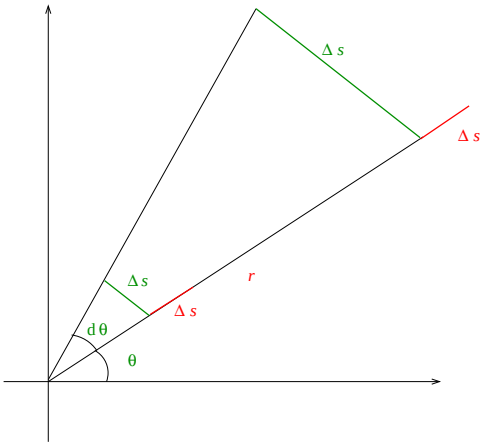

Figure 1.1: A variation in θ causes a larger displacement for larger r values.

In general, a point in 3D space may be identified by Cartesian coordinated (x, y, z) or more general *curvilinear coordinates* (q_1, q_2, q_3). We will have a relation expressing the former as a function for the latter

$$x(q_1, q_2, q_3), \quad y(q_1, q_2, q_3), \quad z(q_1, q_2, q_3) \tag{1.19}$$

We may also use the notation $x = x_1$, $y = x_2$, $z = x_3$, and write sometimes the relations 1.19 with the short hand $x_i(q_j)$.

We have

$$ds^2 = \sum_i dx_i^2 = \sum_{i,j,k} \left(\frac{\partial x_i}{\partial q_j} dq_j\right)\left(\frac{\partial x_i}{\partial q_k} dq_k\right) = \sum_{j,k} h_{j,k} dq_j dq_k \tag{1.20}$$

where we defined

$$h_{j,k} \equiv \sum_i \frac{\partial x_i}{\partial q_j}\frac{\partial x_i}{\partial q_k} \tag{1.21}$$

When, as in the case of polar coordinates, the variations in the q_i are orthogonal between them, the expression above simplifies to

$$ds^2 = \sum_i h_i^2 dq_i \tag{1.22}$$

The h_i are clearly functions of the q_i, so it is useful to write explicitly

$$ds^2 = h_1^2(q_1, q_2, q_3)dq_1^2 + h_2^2(q_1, q_2, q_3)dq_2^2 + h_3^2(q_1, q_2, q_3)dq_3^2 \tag{1.23}$$

In these notes we will focus on coordinates that allow us to use an expression in the form 1.23, and in particular on two useful coordinate systems;

1.2.1 Cylindrical coordinates

This coordinate system corresponds to choosing a plane, identified by Cartesian coordinates (x, y), and express it in polar coordinates (r, θ), while the z coordinate is left unchanged. The Cartesian coordinates are expressed as function of the cylindrical ones through

$$x = r\cos\theta, \qquad y = r\sin\theta, \qquad z = z \tag{1.24}$$

and it is straightforward to show that

$$ds^2 = dr^2 + r^2 d\theta^2 + dz^2 \tag{1.25}$$

so that

$$h_r = 1(= h_1), \qquad h_\theta = r(= h_2), \qquad h_z = 1(= h_3) \tag{1.26}$$

We will use this system of coordinates when we are facing a problem with a particular symmetry, namely rotation around a given axis (identified by the z coordinate).

1.2.2 Spherical coordinates

This coordinate system is used when we have a spherical symmetry in our problem, and somehow correspond to use a combination of two polar system. First we divide the component on the z axis from the component on the (x, y) plane by using r and the angle θ, and then we divide the x and y components introducing another angle, φ. In this "second application" of the polar transformation, the role of the distance is played by the component of r in the plane, $r\sin\theta$. The Cartesian coordinates are expressed as functions of the spherical ones through

$$x = r\sin\theta\cos\varphi, \qquad y = r\sin\theta\sin\varphi, \qquad z = r\cos\theta \tag{1.27}$$

Both from explicit computation or geometrical considerations (the two polar systems described above, one using r and the other one using $r\sin\theta$ as distance coordinates) we get

$$ds^2 = dr^2 + r^2 d\theta^2 + r^2\sin\theta^2 d\varphi^2 \tag{1.28}$$

so that

$$h_r = 1(= h_1), \qquad h_\theta = r(= h_2), \qquad h_\varphi = r\sin\theta(= h_3) \tag{1.29}$$

1.3 The gradient

The geometrical definition of the gradient operator $\boldsymbol{\nabla}$ is the following. Let us consider a function ϕ and its values in points A and B. Let us assume the separation between A and B being given by the vector

$$\boldsymbol{\Delta s} \equiv B - A \tag{1.30}$$

and define

$$\Delta\phi = \phi(B) - \phi(A) \tag{1.31}$$

Then we ask the gradient to satisfy

$$\Delta\phi = \boldsymbol{\nabla}\phi \cdot \boldsymbol{\Delta s} + \text{higher powers of the components of } \boldsymbol{\Delta s} \tag{1.32}$$

In Cartesian coordinates (2D) we have

$$\boldsymbol{\nabla}\phi \cdot \boldsymbol{\Delta s} = (\boldsymbol{\nabla}\phi)_x \Delta x + (\boldsymbol{\nabla}\phi)_y \Delta y \tag{1.33}$$

At the same time, in any coordinate system we have the Taylor expansion

$$\Delta\phi = \sum_i \frac{\partial\phi}{\partial q_i}\Delta q_i + \text{higher powers of } \Delta q_i \tag{1.34}$$

so that by comparison of eqs. (1.32,1.34) we obtain, *for Cartesian coordinates*,

$$(\boldsymbol{\nabla}\phi)_i = \frac{\partial\phi}{\partial x_i} \tag{1.35}$$

But this relation will not hold in curvilinear coordinates, if we want eq. (1.32) to hold when the displacement will have a less trivial dependence on coordinates (as in eq. 1.23).

Let us consider first the 2D polar case. The same $B - A = \boldsymbol{\Delta s}$ will be now given by (again, keeping only first order terms)

$$(\boldsymbol{\Delta s})_r = \Delta r, \qquad (\boldsymbol{\Delta s})_\theta = r\Delta\theta \tag{1.36}$$

where by $(\boldsymbol{\Delta s})_q$ we mean component of the vector along the variation of coordinate q. As a result, comparing eqs. (1.32,1.34) we get

$$(\boldsymbol{\nabla}\phi)_r \Delta r + (\boldsymbol{\nabla}\phi)_\theta r\Delta\theta \approx \Delta\phi \approx \frac{\partial\phi}{\partial r}\Delta r + \frac{\partial\phi}{\partial\theta}\Delta\theta \tag{1.37}$$

and

$$(\boldsymbol{\nabla}\phi)_r = \frac{\partial\phi}{\partial r}, \qquad (\boldsymbol{\nabla}\phi)_\theta = \frac{1}{r}\frac{\partial\phi}{\partial\theta} \tag{1.38}$$

The θ component of the gradient becomes smaller for large r to compensate for the growth of the displacement $(\boldsymbol{\Delta s})_\theta$.

In general, we will have for orthogonal coordinates

$$(\mathbf{\Delta s})_i = h_i(q_j)\Delta q_i \tag{1.39}$$

so that by comparing eqs. (1.32,1.34) we get

$$(\boldsymbol{\nabla}\phi)_i = \frac{1}{h_i(q_j)}\frac{\partial\phi}{\partial q_i} \tag{1.40}$$

1.3.1 Gradient for cylindrical coordinates

$$(\boldsymbol{\nabla}\phi)_r = \frac{\partial\phi}{\partial r}, \qquad (\boldsymbol{\nabla}\phi)_\theta = \frac{1}{r}\frac{\partial\phi}{\partial\theta}, \qquad (\boldsymbol{\nabla}\phi)_z = \frac{\partial\phi}{\partial z} \tag{1.41}$$

1.3.2 Gradient for spherical coordinates

$$(\boldsymbol{\nabla}\phi)_r = \frac{\partial\phi}{\partial r}, \qquad (\boldsymbol{\nabla}\phi)_\theta = \frac{1}{r}\frac{\partial\phi}{\partial\theta}, \qquad (\boldsymbol{\nabla}\phi)_\varphi = \frac{1}{r\sin\theta}\frac{\partial\phi}{\partial z} \tag{1.42}$$

1.3.3 Dimensional analysis

A gradient is physically a spatial derivative, so that its dimension should be

$$[\phi][L]^{-1} \tag{1.43}$$

Angles such as θ and φ are pure numbers. The correct dimensionality in eqs. (1.41,1.42) is given anyway by the division by r in front of derivations that involve angles. The dimensional analysis suggests thus the correctness of our results.

1.4 The divergence

1.4.1 Definition

We consider now the vector field (i.e., a function from $\mathbb{R}^3$ to $\mathbb{R}^3$, assigning a vector to each point in space) $\boldsymbol{A}(\boldsymbol{x})$. We geometrically define its divergence as

$$\mathrm{div}\boldsymbol{A}(\mathbf{x}_0) \equiv \boldsymbol{\nabla}\cdot\boldsymbol{A}(\boldsymbol{x}_0) = \lim_{V_{\boldsymbol{x}_0}\to 0}\frac{\int_{S_{V_{\boldsymbol{x}_0}}}\boldsymbol{A}(\boldsymbol{x})\cdot\boldsymbol{n}\,dS}{\int_{V_{\boldsymbol{x}_0}}d\boldsymbol{x}} \tag{1.44}$$

A few explanations are due. First of all, the notation $\boldsymbol{\nabla}\cdot\boldsymbol{A}$ for the divergence recalls us of the usual Cartesian expression $\sum_i \partial_i A_i$. Nevertheless, in these note we prefer to write div to recall the geometrical definition and the different forms assumed in different coordinate systems. As we did above for eq. (1.4), we define an integral in a small volume $V_{\boldsymbol{x}_0}$ centred around

$\boldsymbol{x}_0$, and let this volume go to zero (see below for a practical example of how this is done). $S_{V_{\boldsymbol{x}_0}}$ is the surface delimiting the volume, $\boldsymbol{n}$ is the unit vector that is orthogonal in each point to the surface, and $\boldsymbol{A}(\boldsymbol{x}) \cdot \boldsymbol{n}\, dS$ stands for the integration of the scalar product of the vectors $\boldsymbol{A}$ and $\boldsymbol{n}$. We are thus measuring on the whole surface the outgoing component of $\boldsymbol{A}$, and then dividing by the volume. This definition originates from fluid dynamics (how much fluid is flowing out of a volume).

1.4.2 Cartesian coordinates

Let us do this for the Cartesian coordinates. We operate on a small cube centred in (x_0, y_0, z_0) with sides $\Delta x = \Delta y = \Delta z = a$ (Fig 1.2). We have

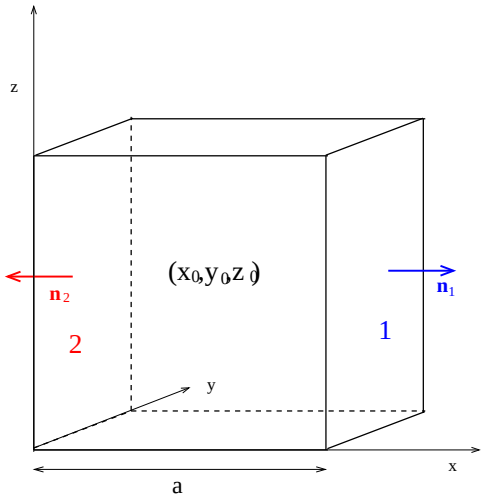

Figure 1.2: Small cube for divergence integral.

obviously

$$\int_{V_{\boldsymbol{x}_0}} d\boldsymbol{x} = \Delta x \Delta y \Delta z = a^3 \tag{1.45}$$

The limit $V_{\boldsymbol{x}_0} \to 0$ corresponds to sending $a \to 0$ [5].

We now need to integrate $\boldsymbol{A}(\boldsymbol{x}) \cdot \boldsymbol{n}$ on all faces of the cube. Let us name this faces $1, \ldots, 6$ and the corresponding integrals $I_1, \ldots, I_6$. If, as in Fig. 1.2 we name the face in the direction of growing x as 1, we have (due to

[5] If we use different values of Δx, Δy, Δz, the derivation would be unchanged provided that we send each of these to zero. Our proof is actually performed keeping explicit values of these variations, so that the need to send all of them to zero results evident. One way of getting the limit is to multiply the possibly different Δx_i by a, and then send a to 0.

$\boldsymbol{A} \cdot \boldsymbol{n}_1 = A_x$)

$$I_1 = \int_{-\frac{\Delta z}{2}}^{\frac{\Delta z}{2}} dz \int_{-\frac{\Delta y}{2}}^{\frac{\Delta y}{2}} A_x \left(x_0 + \frac{\Delta x}{2}, y_0 + y, z_0 + z \right) dy \tag{1.46}$$

Now we use the Taylor expansion

$$\begin{aligned} & A \left(x_0 + \frac{\Delta x}{2}, y_0 + y, z_0 + z \right) = \\ =& A \left(x_0 + \frac{\Delta x}{2}, y_0, z_0 \right) + \partial_y A_x \left(x_0 + \frac{\Delta x}{2}, y_0, z_0 \right) y + \\ & \partial_z A_x \left(x_0 + \frac{\Delta x}{2}, y_0, z_0 \right) z + O(y^2, z^2) \end{aligned} \tag{1.47}$$

where $O(y^2, z^2)$ stands for terms like x^2, y^2, zy or higher powers. If we compute an integral such as

$$\overline{I} = \int_{-\frac{\Delta z}{2}}^{\frac{\Delta z}{2}} dz \int_{-\frac{\Delta y}{2}}^{\frac{\Delta y}{2}} C y^2 dy \tag{1.48}$$

we obtain (using for simplicity a for the value of all sides)

$$\overline{I} = C \frac{a^4}{12} \tag{1.49}$$

Once we divide this contribution by the volume a^3, we get $Ca/12 \to 0$ as $a \to 0$. This is true of all quadratic terms (and higher). A quadratic term, integrated on the surface, will give a quartic term that will go to zero when divided by the volume.

We may now consider

$$\begin{aligned} I^* = & \int_{-\frac{\Delta z}{2}}^{\frac{\Delta z}{2}} dz \int_{-\frac{\Delta y}{2}}^{\frac{\Delta y}{2}} \partial_y A_x \left(x_0 + \frac{\Delta x}{2}, y_0, z_0 \right) y \, dy = \\ = & \partial_y A_x \left(x_0 + \frac{\Delta x}{2}, y_0, z_0 \right) \int_{-\frac{\Delta z}{2}}^{\frac{\Delta z}{2}} dz \int_{-\frac{\Delta y}{2}}^{\frac{\Delta y}{2}} y \, dy = 0 \end{aligned} \tag{1.50}$$

since

$$\int_{-\frac{\Delta x}{2}}^{\frac{\Delta x}{2}} y \, dy = \frac{a^2}{8} - \frac{a^2}{8} \tag{1.51}$$

Namely we are integrating an odd function on a symmetrical interval, so we get 0. The same will happen for the integral involving $\partial_z A_x(x_0, y_0, z_0) z$. Taking in account the only remaining term we have

$$I_1 = A_x \left(x_0 + \frac{\Delta x}{2}, y_0, z_0 \right) \Delta y \Delta z + O(a^4) \tag{1.52}$$

In a similar way

$$I_2 = -A_x\left(x_0 - \frac{\Delta x}{2}, y_0, z_0\right)\Delta y \Delta z + O(a^4) \tag{1.53}$$

the different sign being due to $\boldsymbol{A}\cdot\boldsymbol{n}_2 = -A_x$.

Now we have

$$\begin{aligned}
&I_1 + I_2 = \\
&= \left[A_x\left(x_0 + \frac{\Delta x}{2}, y_0, z_0\right) - A_x\left(x_0 - \frac{\Delta x}{2}, y_0, z_0\right)\right]\Delta y\Delta z + O(a^4) = \\
&= \Bigg[A_x\left(x_0, y_0, z_0\right) + \partial_x A_x(x_0, y_0, z_0)\frac{\Delta x}{2} \\
&\quad - \left(A_x\left(x_0, y_0, z_0\right) - \partial_x A_x(x_0, y_0, z_0)\frac{\Delta x}{2}\right) + O(a^2)\Bigg]\Delta y\Delta z + O(a^4) = \\
&= \partial_x A_x(x_0, y_0, z_0)\Delta x\Delta y\Delta z + O(a^4)
\end{aligned} \tag{1.54}$$

We may repeat this for the other faces of the cube just changing names of the variables, and we get

$$\mathrm{div}\boldsymbol{A}(\mathbf{x}) = \lim_{a\to 0}\frac{[\partial_x A_x(\mathbf{x}) + \partial_y A_y(\mathbf{x}) + \partial_z A_z(\mathbf{x})]\Delta x\Delta y\Delta z + O(a^4)}{\Delta x\Delta y\Delta z} \tag{1.55}$$

and thus, in *Cartesian coordinates*

$$\mathrm{div}\boldsymbol{A} = \sum_i \partial_i A_i \tag{1.56}$$

1.4.3 Gauss theorem

From the (coordinate independent) definition eq. (1.44) we have, for an infinitesimal cubic volume δV

$$\mathrm{div}\boldsymbol{A}(\mathbf{x})\delta V = \int_{S_{\delta V}} \boldsymbol{A}(\boldsymbol{x})\cdot\boldsymbol{n}\, dS \tag{1.57}$$

The integral over a finite volume may be defined as the integral over a partition of very small cubes, in the limit of the volume of all cubes going to zero. Namely, for a finite volume V we have

$$\int_V \mathrm{div}\boldsymbol{A}(\mathbf{x})d\mathbf{x} = \sum_i \mathrm{div}\boldsymbol{A}(\mathbf{x})\delta V_i = \sum_i \int_{S_{\delta V_i}} \boldsymbol{A}(\boldsymbol{x})\cdot\boldsymbol{n}dS \tag{1.58}$$

In general, the sum of the integrals over the surfaces $S_{\delta V_i}$ of the cubes that give the total volume V would be different from an integral over the

surface S_V, due to the contribution of the internal surfaces of the cubes. But due to the nature of the integrand, all internal terms will be present in two neighbouring cubes that have opposite $\boldsymbol{n}$, and thus all these terms will cancel, leaving only the integral over the external surface. This result is called Gauss theorem

$$\int_V \mathrm{div}\boldsymbol{A}(\mathbf{x})\, d\mathbf{x} = \int_{S_V} \boldsymbol{A}(\boldsymbol{x}) \cdot \boldsymbol{n}\, dS \tag{1.59}$$

1.4.4 Curvilinear coordinates

To understand how to generalise in the curvilinear coordinate case, let us check the cylindrical case described in Fig. 1.3. Our small volume will be

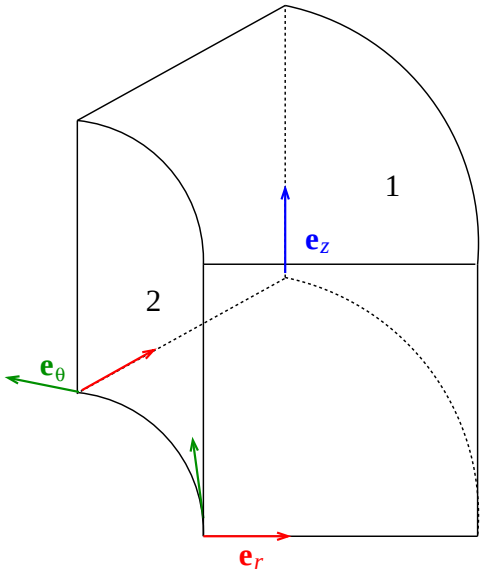

Figure 1.3: Small volume for divergence integral in the cylindrical coordinate case.

now characterised by having faces that are surfaces with constant r, θ or z. In each point of 3D space, vectors orthogonal to such surfaces define a set of orthonormal vectors, that we may call $\mathbf{e}_r$, $\mathbf{e}_\theta$, $\mathbf{e}_z$. These vectors (with the exception of $\mathbf{e}_z$) are different in different point of space, but at any given point they define a basis for the vector space at the location. Thus any vector $\mathbf{A}$ may be written as

$$\mathbf{A} = A_r\mathbf{e}_r + A_\theta\mathbf{e}_\theta + A_z\mathbf{e}_z \tag{1.60}$$

We may name again the faces of our small volume from 1 to 6, and for example, as shown in Fig. 1.3, name 1 and 2 the faces at constant r. We

will clearly have $\mathbf{n}_1 = \mathbf{e}_r$ and $\mathbf{n}_2 = -\mathbf{e}_r$. We may repeat the operations performed above in the Cartesian case remembering that all considerations involving Taylor expansions will be unchanged since for a general function $g(q)$

$$\Delta g = \partial_q g \Delta q \tag{1.61}$$

applies also to curvilinear coordinates. On the other hand, integration in a curvilinear coordinate has to be multiplied by h_q to take in account the fact that the displacement in the curvilinear direction is $h_q \Delta q$ [6]. For example, an integral in θ will involve a multiplication by the locally constant value of r.

If our volume is centred in (r_0, θ_0, z_0) we have

$$I_1 = A_r \left(r_0 + \frac{\Delta r}{2}, \theta_0, z_0 \right) \left[r_0 + \frac{\Delta r}{2} \right] \Delta\theta \Delta z + O(a^4) \tag{1.62}$$

and

$$I_2 = A_r \left(r_0 - \frac{\Delta r}{2}, \theta_0, z_0 \right) \left[r_0 - \frac{\Delta r}{2} \right] \Delta\theta \Delta z + O(a^4) \tag{1.63}$$

If we now consider the auxiliary function

$$f_r(r, \theta, z) = A_r(r, \theta, z) r \tag{1.64}$$

we may write

$$\begin{aligned} I_1 + I_2 = & \left[f_r(r_0 + \frac{\Delta r}{2}, \theta_0, z_0) - f_r(r_0 - \frac{\Delta r}{2}, \theta_0, z_0) \right] \Delta\theta \Delta z + O(a^4) = \\ & = \partial_r f(r_0, \theta_0, z_0) \Delta r \Delta\theta \Delta z + O(a^4) \end{aligned} \tag{1.65}$$

The contribution of these two faces to the divergence is thus

$$\lim_{a \to 0} \frac{I_1 + I_2}{\int_{V_{\boldsymbol{x}_0}} d\boldsymbol{x}} = \lim_{a \to 0} \frac{I_1 + I_2}{r_0 \Delta r \Delta\theta \Delta z} = \frac{1}{r_0} \partial_r \left(r A_r(r_0, \theta_0, z) \right) \tag{1.66}$$

How can we generalise to other curvilinear systems? The volume will be given in general by

$$\int_{V_{\boldsymbol{x}_0}} d\boldsymbol{x} = h_1(q_1, q_2, q_3) h_2(q_1, q_2, q_3) h_3(q_1, q_2, q_3) \tag{1.67}$$

[6] Obviously, this result agrees with the more formal and rigorous one that performs the integration taking in account the Jacobian determinant of the coordinate transformation. Such a determinant is indeed trivially $h_1 h_2 h_3$ for orthogonal coordinates.

while the auxiliary function f_i generated by the integral on the two faces at constant q_i has contribution h_j with $j \neq i$ to the integral, so that

$$f_i(q_j) = A_i(q_j) \prod_{j \neq i} h_j(q_k) \tag{1.68}$$

and finally

$$\mathrm{div}\boldsymbol{A} = \frac{\sum_i \partial_i f_i}{\prod_i h_i} \tag{1.69}$$

or, in an explicit way

$$\begin{aligned} \mathrm{div}\boldsymbol{A}(q_1,q_2,q_3) = & \frac{1}{h_1(q_1,q_2,q_3)h_2(q_1,q_2,q_3)h_3(q_1,q_2,q_3)} \\ & \Big[\partial_1[A_1(q_1,q_2,q_3)h_2(q_1,q_2,q_3)h_3(q_1,q_2,q_3)] + \\ & + \partial_2[A_2(q_1,q_2,q_3)h_1(q_1,q_2,q_3)h_3(q_1,q_2,q_3)] + \\ & + \partial_3[A_3(q_1,q_2,q_3)h_1(q_1,q_2,q_3)h_2(q_1,q_2,q_3)]\Big] \end{aligned} \tag{1.70}$$

Cylindrical coordinates

For cylindrical coordinates eq. (1.70) gives

$$\mathrm{div}\boldsymbol{A} = \frac{1}{r}\Big[\partial_r[rA_r] + \partial_\theta[A_\theta] + \partial_z[rA_z]\Big] \tag{1.71}$$

where $\boldsymbol{A}$ and its components are functions of (r,θ,z). Taking out some variables from the partial derivative we get

$$\mathrm{div}\boldsymbol{A}(r,\theta,z) = \frac{1}{r}\partial_r[rA_r(r,\theta,z)] + \frac{1}{r}\partial_\theta[A_\theta(r,\theta,z)] + \partial_z A_z(r,\theta,z) \tag{1.72}$$

Spherical coordinates

For spherical coordinates eq. (1.70) gives

$$\mathrm{div}\boldsymbol{A} = \frac{1}{r^2\sin\theta}\Big[\partial_r[r^2\sin\theta A_r] + \partial_\theta[r\sin\theta A_\theta] + \partial_\varphi[rA_\varphi]\Big] \tag{1.73}$$

where $\boldsymbol{A}$ and its components are functions of (r,θ,φ). Taking out some variables from the partial derivative we get

$$\mathrm{div}\boldsymbol{A}(r,\theta,\varphi) = \frac{1}{r^2}\partial_r[r^2A_r(r,\theta,\varphi)] + \frac{1}{r\sin\theta}\partial_\theta[\sin\theta A_\theta(r,\theta,\varphi)] + \frac{1}{r\sin\theta}\partial_\varphi A_\varphi(r,\theta,\varphi) \tag{1.74}$$

1.4.5 Dimensional analysis

You can easily check that the divergence has the expected dimensionality of

$$[A][L]^{-1} \tag{1.75}$$

1.5 The Laplacian

Since the gradient, when applied on a function, generates a vector, we may apply the divergence operator on the gradient. In such a way, we will define a new operator, the Laplacian

$$\mathrm{div}(\boldsymbol{\nabla}\phi) \equiv \nabla^2\phi \tag{1.76}$$

Since both the gradient and the divergence have been defined in a geometrical, coordinate independent way, also the Laplacian will have a geometrical, coordinate independent definition. Before investigating it, let us obtain its expression in an arbitrary (orthogonal) coordinate system From (eq. 1.40)

$$(\boldsymbol{\nabla}\phi) = \sum_i \frac{1}{h_i}\partial_i\phi \tag{1.77}$$

and (eq. 1.69)

$$\mathrm{div}\boldsymbol{A} = \frac{\sum_i \partial_i f_i}{\prod_i h_i} \tag{1.78}$$

where the f_i were defined in eq. (1.68), we obtain

$$\nabla^2\phi = \frac{\sum_i \partial_i \left[\frac{\prod_{j\neq i} h_j}{h_i}\partial_i\phi\right]}{\prod_i h_i} \tag{1.79}$$

The above is a short hand for

$$\nabla^2\phi = \frac{1}{h_1h_2h_3}\left[\partial_1\left[\frac{h_2h_3}{h_1}\partial_1\phi\right] + \partial_2\left[\frac{h_1h_3}{h_2}\partial_2\phi\right] + \partial_3\left[\frac{h_1h_2}{h_3}\partial_3\phi\right]\right] \tag{1.80}$$

where again we should remember that the h and ϕ are functions of the q_i.

1.5.1 Cartesian coordinates

In Cartesian coordinates all the h_i equal to 1 and we have

$$\nabla^2\phi(x,y,z) = \partial_x^2\phi(x,y,z) + \partial_y^2\phi(x,y,z) + \partial_z^2\phi(x,y,z) \tag{1.81}$$

1.5.2 Cylindrical coordinates

In cylindrical coordinates, substituting the values of the h_i and bringing out of derivatives variables when possible, we get

$$\nabla^2\phi(r,\theta,z) = \frac{1}{r}\partial_r(r\partial_r\phi(r,\theta,z)) + \frac{1}{r^2}\partial_\theta^2\phi(r,\theta,z) + \partial_z^2\phi(r,\theta,z) \tag{1.82}$$

1.5.3 Spherical coordinates

In spherical coordinates, substituting again the values of the h_i and bringing out of derivatives variables when possible, we get

$$\nabla^2\phi(r,\theta,\varphi) = \frac{1}{r^2}\partial_r(r^2\partial_r\phi(r,\theta,\varphi)) + \frac{1}{r^2\sin\theta}\partial_\theta(\sin\theta\partial_\theta\phi(r,\theta,\varphi)) + \frac{1}{r^2\sin^2\theta}\partial^2_\varphi\phi(r,\theta,\varphi) \tag{1.83}$$

1.5.4 Dimensional analysis

You can easily check that the divergence has the expected dimensionality of

$$[\phi][L]^{-2} \tag{1.84}$$

1.5.5 Geometrical meaning

In section 1.1 we suggested the form

$$\partial_t\rho(t,\mathbf{x}) = \kappa(\overline{\rho}(t,\mathbf{x}) - \rho(t,\mathbf{x})) \tag{1.85}$$

for a diffusion equation, where $\overline{\rho}$ stands for an average over a small volume centred in $\mathbf{x}$. Since then we got a good experience on small volume integrations and Taylor expansions. Let us try to compute $\overline{\phi}$ for a cube of size a centred in $\mathbf{x}_0 = (x_0, y_0, z_0)$. Using Cartesian coordinates we have

$$\begin{aligned}&\phi(x,y,x) = \phi(\mathbf{x}_0) + \partial_x\phi(\mathbf{x}_0)(x-x_0) + \partial_x\phi(\mathbf{y}_0)(y-y_0) + \partial_z\phi(\mathbf{x}_0)(z-z_0) + \\ &\partial_x\partial_y\phi(\mathbf{x}_0)(x-x_0)(y-y_0) + \partial_x\partial_z\phi(\mathbf{x}_0)(x-x_0)(z-z_0) + \partial_y\partial_z\phi(\mathbf{x}_0)(y-y_0)(z-z_0) + \\ &\frac{1}{2}\partial_x^2\phi(\mathbf{x}_0)(x-x_0)^2 + \frac{1}{2}\partial_y^2\phi(\mathbf{x}_0)(y-y_0)^2 + \frac{1}{2}\partial_z^2\phi(\mathbf{x}_0)(z-z_0)^2 \\ &+ \text{cubic terms}\end{aligned} \tag{1.86}$$

Now we write, remembering that the volume of the cube is a^3, and calling $\Delta x \equiv x - x_0$, $\Delta y \equiv y - y_0$, $\Delta z \equiv z - z_0$,

$$\begin{aligned}&\overline{\phi} = \frac{1}{a^3}\int_{-\frac{a}{2}}^{\frac{a}{2}} dx \int_{-\frac{a}{2}}^{\frac{a}{2}} dy \int_{-\frac{a}{2}}^{\frac{a}{2}} \phi(x,y,z)\, dz = \\ &\quad = \phi(x_0,y_0,z_0) + \frac{1}{a^3}\Big(\int\int\int \text{linear terms in } \Delta x, \Delta y, \Delta z d(\Delta x)d(\Delta y)d(\Delta z) + \\ &\quad \int\int\int \text{terms of the form } (\Delta x\Delta y), (\Delta y\Delta z), (\Delta x\Delta z) d(\Delta x)d(\Delta y)d(\Delta z) + \\ &\quad \frac{1}{2}\int\int\int \left(\partial_x^2\phi(\mathbf{x}_0)\Delta x^2 + \partial_y^2\phi(\mathbf{x}_0)\Delta y^2 + \partial_z^2\phi(\mathbf{x}_0)\Delta z^2\right) d(\Delta x)d(\Delta y)d(\Delta z)\Big)\end{aligned} \tag{1.87}$$

From the trivial result

$$\int_{-\frac{a}{2}}^{\frac{a}{2}} q dq = 0 \tag{1.88}$$

(and Fubini's theorem, namely the possibility of integrating first in one variable, etc.) we obtain that integrals involving the linear terms and terms such as xy give zero. We are left with integrals in the form (thanks again to Mr. Fubini, since the integral in the two variables unrelated to the integrand gives the face area a^2)

$$\frac{a^2}{2} \int_{-\frac{a}{2}}^{\frac{a}{2}} \partial_q^2 \phi(\mathbf{x}_0) q^2 dq = \frac{a^2}{2} \partial_q^2 \phi(\mathbf{x}_0) \left[\frac{q^3}{3} \right]_{-\frac{a}{2}}^{\frac{a}{2}} = \frac{a^5}{24} \tag{1.89}$$

Substituting in eq. 1.87 we get, at the lowest order in a,

$$\overline{\phi}(\mathbf{x}_0) - \phi(\mathbf{x}_0) = \frac{a^2}{24} \sum_i \partial_i^2 \phi(\mathbf{x}) = \frac{a^2}{24} \nabla^2 \phi(\mathbf{x}) \tag{1.90}$$

Thanks to our geometrical definitions, this will be true in any coordinate system, and the diffusion equation may be written as

$$\partial_t \rho = \gamma \nabla^2 \rho \tag{1.91}$$

A simple dimensional analysis shows now that

$$[\gamma] = [L]^2 [T] \tag{1.92}$$

1.6 Another approach to diffusion

Let us consider a fixed volume V. The amount of our "substance" in V is given by the integral of ρ over the volume[7].

$$Q_V(t) = \int_V \rho(t, \mathbf{x})\, d\mathbf{x} \tag{1.93}$$

Q_V is a function of the only time. Its time derivative is

$$\frac{dQ_V(t)}{dt} = \int_V \partial_t \rho(t, \mathbf{x})\, d\mathbf{x} \tag{1.94}$$

If we assume that the substance is "locally conserved" meaning that it cannot disappear but only move to a different place, then the change in time of

[7]For example, ρ may be the electric charge density. The dimensional analysis tells us then that if the dimension of charge is $[Q]$, the dimension of ρ has to be $[Q][L]^{-3}$, so that the integral in eq. (1.93) has the proper dimension. ρ gives a charge only after integration.

Q_V has to be given by the flux of it trough the surface of V. Imagine now that ρ gives the density of a liquid. This liquid moves in a cylinder (pipe) of section A with velocity v. This means that in time T an amount $\rho v T A$ of fluid will exit the pipe (Fig. 1.4). Once we divide by time, the "change of amount of water in time" is $\rho v A$. If now the "mouth of the pipe" is not orthogonal to the flow of water, although the surphace increases, the flow of water does not change. We can thus see that the flow is not given by the product of the velocity by the area, but by $A\rho\mathbf{v}\cdot\mathbf{n}$, where $\mathbf{n}$ is the outgoing unit vector orthogonal to the surphace A. The product $A\mathbf{v}\cdot\mathbf{n}$ gives us, indeed, the projection of the area in the direction of the water flow and leads us back to the same flow obtained for the orthogonal mouth (refer also to Fig. 1.4). In the discussion above we considered uniform velocities and flat surphaces, but we can generalise by taking an integral over "many infinitesimal flat surphaces and uniform velocities" (the usual Riemann definition of integral).

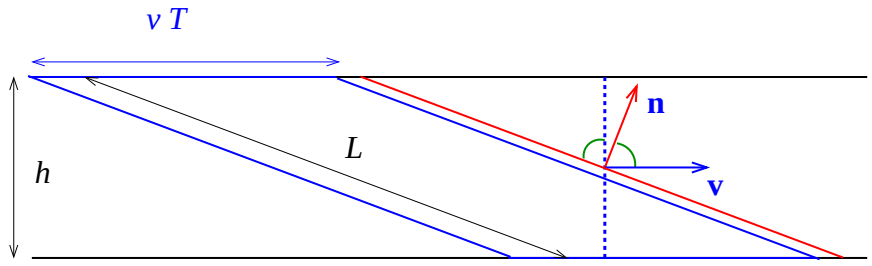

Figure 1.4: The amount of water that will exit the pipe with the oblique red mouth in time T is given by the blue parallelogram. The height of the parallelogram is $h = L\cos\theta$, where $\cos\theta = (\mathbf{v}\cdot\mathbf{n})/v$.

We define a flux vector

$$\mathbf{\Phi}(t,\mathbf{x}) = \rho(t,\mathbf{x})\mathbf{v}(t,\mathbf{x}) \tag{1.95}$$

and write

$$\frac{dQ_V(t)}{dt} = -\int_{S_V} \mathbf{\Phi}(t,\mathbf{x})\cdot\mathbf{n}\,dS \tag{1.96}$$

The sign is negative because a positive flux in the direction of $\mathbf{n}$ causes Q to decrease. Now we use Gauss theorem (eq. 1.59) to obtain

$$\frac{dQ_V(t)}{dt} = -\int_{V} \mathrm{div}\mathbf{\Phi}(t,\mathbf{x})\,d\mathbf{x} \tag{1.97}$$

so that, using eq. (1.93)

$$\int_V \partial_t \rho(t,\mathbf{x})\, d\mathbf{x} = -\int_V \mathrm{div}\boldsymbol{\Phi}(t,\mathbf{x})\, d\mathbf{x} \Rightarrow \int_V \left(\partial_t \rho(t,\mathbf{x}) + \mathrm{div}\boldsymbol{\Phi}(t,\mathbf{x})\right)\, d\mathbf{x} = 0 \tag{1.98}$$

This has to be true regardless of the volume V, so that we need to have[8].

$$\partial_t \rho(t,\mathbf{x}) + \mathrm{div}\boldsymbol{\Phi}(t,\mathbf{x}) = 0 \tag{1.99}$$

From eq. (1.32) we know that the gradient gives us the direction in which we have the maximum growth of the function[9]. We previously suggested that ρ locally grows if its integral in a small surrounding volume is higher than the local value. We may also think that "ρ flows where ρ is minimum, or

$$\boldsymbol{\Phi} = -\gamma \boldsymbol{\nabla} \rho \tag{1.100}$$

Here the dimensional analysis tell us that

$$[\rho][L][T]^{-1} = [\gamma][L]^{-1}[\rho] \Rightarrow [\gamma] = [L]^2[T]^{-1} \tag{1.101}$$

Substituting eq. (1.100) in eq.(1.99) we obtain the same form of the diffusion equation

$$\partial_t \rho = \gamma \nabla^2 \rho \tag{1.102}$$

This equation is often called heat equation since ρ may stand for termic energy (temperature).

[8] Otherwise, we could integrate in a small volume around the area where the integrand is not zero, and obtain a non zero integral (these kind of arguments are not completely rigorous due to the possibility of having the integrand different from zero an a set of zero measure

[9] Imagine to use vectors of fixed length $\Delta s = 1$ in eq. (1.32). The maximum growth will be given for a $\boldsymbol{\Delta s}$ in the same direction of the gradient.

Part II

Separation of variables

Chapter 2

Separation of variables in the heat equation

2.1 Boundary conditions

Let us consider the diffusion equation in Cartesian coordinates

$$\partial_t \rho(t,x,y,z) = \gamma\Big[\partial_x^2\rho(t,x,y,z) + \partial_y^2\rho(t,x,y,z) + \partial_z^2\rho(t,x,y,z)\Big] \qquad (2.1)$$

This equation express a relation between partial derivatives. A function ρ that represents a solution of the (modelled) physical problem needs to satisfy this relation in every point of a given area of space and time[1].

We may for example consider the time evolution of the temperature on a metal bar. The bar has a finite length L. The initial temperature ($t = 0$) is known for each $x \in [0, L]$ [2]. We also need to provide, in order to obtain a unique solution for the temperature at $t > 0$, information about "what

[1]Modern physics speaks about space-time. This is due to the fact that in Relativistic physics, time plays a role similar (although not exactly equal) to the other coordinates. As we may "mix" the spatial coordinates x, y, z by performing a rotation, according to Relativity we may also "mix" time and space, just by moving at constant velocity. We do not realise that this mixing happens because the effect is related to the ratio v/c where v is the velocity of movement and c the velocity of light, and $v \ll c$ for common life velocities. The physics of Newton is obtained indeed from the physics of Einstein in the $c \to \infty$ limit. Eq. (2.1) deals with time and space derivatives in a different way, and thus it is not a relativistic equation. Indeed, according to eq. (2.1), diffusion may happen at infinite velocity. The wave equation of electromagnetism (light propagation), $[\partial_t^2 - c(\partial_x^2 + \partial_y^2 + \partial_z^2)]\mathbf{A} = 0$, is a relativistic equation (the minus generates the difference between, time and space in Relativity, while a dimensional analysis easily shows that c is a velocity). It was indeed reasoning about light that Lorentz, Poincaré and Einstein developed the (Special, i.e. not including Gravitation) Relativity theory.

[2]We approximate the problem as a 1D one, i.e.we consider the bar "infinitely thin".

happens at the bars ends", $x = 0, x = L$. This information will be needed and will be enough to solve the problem. Why?

Let us remember the situation that we face when we want to solve an *ordinary* differential equation. For a first order differential equation, such as the equation for radioactive decay

$$\frac{dN(t)}{dt} = -\gamma N(t) \tag{2.2}$$

we have a general solution

$$N(t) = Ae^{-\gamma t} \tag{2.3}$$

The solution for a specific problem is obtained by noticing that $N(0) = A$. So if initially we have N_0 atoms of the radioactive material, the solution is

$$N(t) = N_0 e^{-\gamma t} \tag{2.4}$$

If we have a second order equation such as the Harmonic oscillator one

$$\frac{d^2X(t)}{dt^2} = -\omega^2 X(t) \tag{2.5}$$

the general solution is

$$X(t) = A\sin\omega t + B\cos\omega t \tag{2.6}$$

We have now two constants, so we need two conditions to specify our solution. The usual way of doing it is to notice that[3]

$$X(0) = B, \qquad \frac{dX(0)}{dt} = \omega\, A \tag{2.7}$$

so that, calling $X(0) = X_0$ and $\frac{dX(0)}{dt} = V_0$, the solution for a specific problem is

$$X(t) = \frac{V_0}{\omega}\sin\omega t + X_0\cos\omega t \tag{2.8}$$

But we can solve the oscillator problem in another way, for example by asking to have $X(0) = X_0$ and $X(T) = X_T$ so that

$$X_T = A\sin\omega T + X_0\cos\omega T \Rightarrow A = \frac{X_T - X_0\cos\omega T}{\sin\omega T} \tag{2.9}$$

provided that $\omega T \neq n\pi$. In the latter case, we have to check the equation *before* dividing by the sine, and we get

$$X_T = X_0 \tag{2.10}$$

[3]You should perform a dimensional analysis for each equation you see. They are always useful in checking the validity of your results.

so that no other condition may be satisfied.

We have thus seen that for a second order ordinary differential equation we can get a solution either by specifying the initial value of the function and of its derivative[4], or by specifying its value at two different times. Nevertheless, while the first method always leads to a solution for our problem[5], as we have seen this is not true for the second approach. The second approach may nevertheless be useful to restrict the possible values that *the model's parameter may assume*. For example, let us ask $X_0 = 0$ and $X_{T=1} = 0$. If we want our solution to be different from zero everywhere we will need (left of eq. 2.9) $\omega = n\pi$. We will use this method very often in the following.

Before going back to partial differential equations, let us notice that from the general solution eq. (2.6) we may obtain the expression for the derivative

$$\frac{dX(t)}{dt} = \omega(A\cos\omega t - B\sin\omega t) \tag{2.11}$$

We may thus specify the state of our system also by asking $\frac{dX(0)}{dt} = V_0$, $\frac{dX(T)}{dt} = V_T$, i.e. by fixing the derivative (velocity) at two different points.

Let us analyse Fig. 2.1. We want to obtain the solution in the interior of the red area, where ρ will satisfy eq. (2.1). It looks reasonable that we may need to specify what happens on the *boundary* of the region (*boundary conditions* or BC). We need to know the initial state of the system

$$\rho(0, x) \tag{2.12}$$

but also what happens, for each t, at the borders. By studying the temperature of the bar, we are assuming that the bar itself follows the heat equation, but what happens around it may be changed in different ways. For example, we could put the bar in contact with one or two different external bodies at $x = 0$ and $x = L$. The temperature of these bodies could be fixed (for example, the bodies being much larger than the bar) or change in time (because connected to some thermic engine, or just because environmental temperature changes with time). Or we could insulate the ends in such a way that heat does not flow (or, in case the equation describes the diffusion of a gas: at the ends we could have walls that do not let the particles pass).

[4]For a physical particle, initial position and velocity. Since Newton's equation are second order, this means that the state of a system in classical physics is given by specifying the initial value of all particles and velocities (or, in a more general coordinate system, momenta).

[5]This is a very informal discussion, in which we assume all functions to be as well-behaved as possible. Refer to any book on differential equations for a more formal and rigorous treatment.

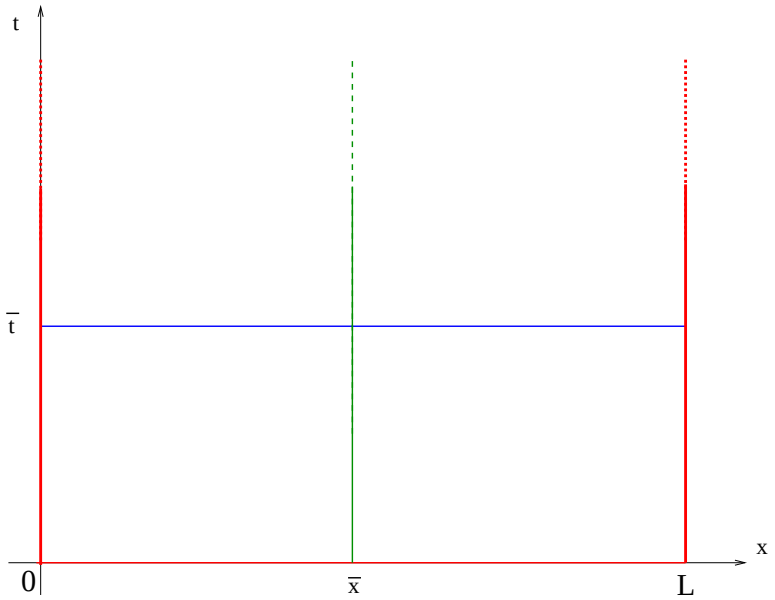

Figure 2.1: Space and time diagram for the problem of diffusion of heat on a 1D bar.

It is clear that, *for the same behaviour given by eq. (2.1) in the prescribed area*, the solution would be different given different boundary conditions, so that the importance of such conditions should be intuitive from a physical view point. Regarding which kind of boundary conditions are necessary we may, in a completely informal and not rigorous way, use the following argument based on a comparison with ordinary differential equations.

Let us wonder what happens at fixed $x = \overline{x}$, i.e. on the green line of Fig. 2.1. Since x is fixed, we may expect our equation to behave as

$$\frac{d\rho_{\overline{x}}(t)}{dt} = f_{\overline{x}}(t) \tag{2.13}$$

so that we need just an initial condition for it, $\rho(t = 0, \overline{x})$. But since we want to solve the problem *for all* $x \in [0, L]$, we actually need to provide the function

$$\rho(0, x) = f_{t=0}(x) \qquad x \in [0, L] \tag{2.14}$$

But obviously we are not dealing with a first order equation in t, since also what happens on x is "dynamical". If we try to think about what happens at fixed $t = \overline{t}$, i.e. on the blue line of Fig. 2.1, we expect an equation like

$$\frac{d^2\rho_{\overline{t}}(x)}{dx^2} = f_{\overline{t}}(x) \tag{2.15}$$

We thus need two conditions at fixed t to specify the solution, since we are dealing with a second order equation. For example, we can fix the temperature at $x = 0$ and $x = L$ for all values of $t > 0$

$$\rho(0,t) = f_{x=0}(t), \qquad \rho(L,t) = f_{x=L}(t), \qquad t > 0 \tag{2.16}$$

Or we can fix the flow of temperature on the ends. We have seen (eq. 1.100) that the flow is related to the gradient, i.e., for our 1D problem to the derivative. Fixing the flow amounts thus to provide the derivative

$$\frac{d\rho(0,t)}{dt} = g_{x=0}(t), \qquad \frac{d\rho(L,t)}{dt} = g_{x=L}(t), \qquad t > 0 \tag{2.17}$$

a choice motivated both by our understanding of the physical problem, and by our discussion on the conditions needed to specify second order problems. Insulating the bar, for example, would correspond to fix

$$g_{x=0}(t) = g_{x=L}(t) = 0 \qquad \forall t > 0 \tag{2.18}$$

2.2 1D heat equation with fixed temperature ends: dimensional analysis

We are almost ready to solve our first PDE problem, but before doing it let us define it properly. We want to study the diffusion of temperature on a 1D bar[6], while keeping the ends at a fixed (zero) temperature[7].

The problem is specified by the equation

$$\partial_{t'}\rho(t',x') = \gamma\partial^2_{x'}\rho(t',x') \tag{2.19}$$

initial condition

$$\rho(0,x') = f_{t=0}(x') \qquad x' \in [0,L] \tag{2.20}$$

and boundary conditions

$$\rho(0,t') = \rho(L,t') = 0, \qquad t' > 0 \tag{2.21}$$

As a first step, we start by simplifying our problem through an appropriate change of variables (this is the reason we called the above variables x' and t'... since we want to get rid of them as soon as possible!). As it will be

[6] These 1D problems are obviously idealisations, but they are very useful in understanding mathematical techniques in simple settings.

[7] Or at a given temperature $\overline{T}$. In such a case, we can re-define our temperature scale so that $\rho = T - \overline{T}$.

clear soon, in order to fix the the value of the function to zero at the ends, it will be handy to work on the interval $[0, \pi]$. Let us thus define

$$x = \frac{\pi}{L} x' \qquad \Rightarrow x' = \frac{L}{\pi} \tag{2.22}$$

so that x will assume values between 0 and L . Since we changed variables, also the form of the equation will change. Defining $\alpha = \pi/L$ we have

$$\frac{\partial}{\partial x'} = \frac{\partial}{\partial x}\frac{\partial x'}{\partial x} = \alpha \frac{\partial}{\partial x} \qquad \Rightarrow \partial^2_{x'} = \alpha \partial_x (\alpha \partial_x) = \alpha^2 \partial^2_x \tag{2.23}$$

and the equation becomes

$$\partial_{t'} \rho(t', x) = \gamma \alpha^2 \partial^2_x \rho(t, x) \tag{2.24}$$

Now we notice that if we if we define

$$t = \beta t' \qquad \Rightarrow \partial_{t'} = \beta \partial_t \tag{2.25}$$

the equation becomes

$$\partial_t \rho(t, x) = \frac{\gamma \alpha^2}{\beta} \partial^2_x \rho(t, x) \tag{2.26}$$

The trick is now to define $\beta = \gamma \alpha^2$ so that the change in the time variable is

$$t = \gamma \frac{\pi^2}{L^2} t' \qquad \Rightarrow t' = \frac{L^2}{\pi^2 \gamma} \tag{2.27}$$

and the equation becomes

$$\partial_t \rho(t, x) = \partial^2_x \rho(t, x) \tag{2.28}$$

We may call this the a-dimensional heat equation since, from eqs. (1.101,2.22,2.27),

$$[x] = \frac{[L]}{[L]} = [*]^0 \qquad [t] = [\gamma] \frac{[*]^0}{[L]^2} [T] = [*]^0 \tag{2.29}$$

where with the the notation $[*]^0$ we just mean a pure number, independent on unit systems.

The form of the equation got simplified. We will now proceed to find a solution for $\rho(t, x)$ from which we will be able to obtain the solution in the original dimensional variable through the transformation rules eqs. (2.22,2.27). Obviously, the same rules may also be used to express the boundary conditions eqs. (2.20,2.21) as functions of the a-dimensional variables (t, x).

2.3 Separation of variables for the 1D heat equation

The *separation of variables* method is based on assuming that the solution may be written as the product of a function of t and x

$$\rho(t,x) = T(t)X(x) \tag{2.30}$$

The method is basically based on trusting that the method will work. We will follow the consequence of the *ansatz*[8] eq. (2.30), perform a few doubtful steps like dividing by some function without worrying if it is zero or not, and finally arrive at a general solution for our equation. Only after we will reach the solution we will discuss about when this method may work or not. Let us substitute[9] eq. (2.30) in eq. (2.28)

$$\partial_t\big[T(t)X(x)\big] = \partial_x^2\big[T(t)X(x)\big] \qquad \Rightarrow X(x)\partial_t\big[T(t)\big] = T(t)\partial_x^2\big[X(x)\big] \tag{2.31}$$

Let us now divide both sides by $T(t)X(x)$ to obtain

$$\frac{\partial_t T(t)}{T(t)} = \frac{\partial_x^2 X(x)}{X(x)} \tag{2.32}$$

On the left we have a function of t, and on the right a function of x, and they are equal everywhere, i.e. *for each arbitrary* $x \in [0, L]$ and $t \geq 0$. From this follows that both sides of the equation have to be constants[10],

$$\frac{\partial_t T(t)}{T(t)} = C = \frac{\partial_x^2 X(x)}{X(x)} \tag{2.33}$$

and

$$\partial_t T(t) = CT(t) \tag{2.34}$$

$$\partial_x^2 X(x) = CX(x) \tag{2.35}$$

We reduced our problem to two independent ordinary differential equations!

We note that if eqs. (2.34,2.35) are true for all t, x we have

$$\partial_t \rho = \partial_t(XT) = X\partial_t T = CXT = T\partial_x^2 X = \partial_x^2(TX) = \partial_x^2 \rho \tag{2.36}$$

[8] A German word for an educated guess.

[9] We will use the partial derivative symbol also when it acts on a function of a single variable.

[10] Imagine we have $f(y) = g(z)$ for two independent variables y and z. Assume we have $f(y_1) = a \neq b = f(y_2)$, i.e. f is not constant. Now, if we pick up a value z_1, we want to have $g(z_1) = f(y_1) = a$, since the equality has to hold for arbitrarily picked values of y and z. But then $g(z_1) = a \neq b = f(y_2)$ and a contradiction arises.

so that we actually do not need to worry about divisions by zero.

Eq. (2.34) is trivially solved by

$$T(t) = A' e^{Ct} \tag{2.37}$$

We proceed now to study eq. (2.35). We know that the behaviour of this equation depends on the sign of C. Let us consider the three possible cases

(I) $C = 0$
We have

$$\partial_x^2 X(x) = 0 \Rightarrow \partial_x X(x) = \overline{A} \Rightarrow X(x) = \overline{A}x + \overline{B} \tag{2.38}$$

so that

$$\rho(t,x) = A' e^0 (\overline{A}x + \overline{B}) = Ax + B \tag{2.39}$$

where we defined $A = A'\overline{A}$, $B = A'\overline{B}$. If we want want eq. (2.21) to hold, we need to have

$$\rho(t,0) = B = 0, \quad \rho(t,\pi) = A\pi + 0 = 0 \quad \Rightarrow A = 0 \tag{2.40}$$

The $C = 0$ case led us to the solution $\rho = 0$. This is trivially a solution of the heat equation with the prescribed boundary conditions, but it can satisfy eq. (2.20) only if $f_{t=0}(x) = 0 \ \forall x \in [0,\pi]$.

(II) $C > 0$
Since C is positive, we re-name it as $C = \lambda^2$. Now we have from the theory of linear differential equations

$$\partial_x^2 X(x) = \lambda^2 X(x) \Rightarrow X(x) = \overline{A} e^{\lambda x} + \overline{B} e^{-\lambda x} \tag{2.41}$$

and

$$\rho(t,x) = A' e^{\lambda^2 t} X(x) = e^{\lambda^2 t} \left(A e^{\lambda x} + B e^{-\lambda x} \right) \tag{2.42}$$

thanks to usual re-definition of the constants. The term $e^{\lambda^2 t}$ is obviously positive, so the conditions eq. (2.21) are equivalent to ask for the term in the parenthesis to be null (we call this term X by absorbing A' in X)

$$0 = X(0) = A e^{\lambda 0} + B e^{-\lambda 0} \Rightarrow B = -A \tag{2.43}$$

and

$$0 = X(\pi) = A(e^{\lambda\pi} + B e^{-\lambda\pi}) \Rightarrow A = 0 \tag{2.44}$$

where the last result obviously follows since for $\lambda > 0$ we have $\lambda\pi \neq -\lambda\pi$ and the exponential is strictly growing. The only possible solution is again $\rho = 0$, that would nevertheless lead to a contradiction since we had asked $C > 0$. No solution is thus found for $C > 0$.

(III) $C < 0$

Since C is negative, we re-name it as $C = -\lambda^2$. Now we get

$$\partial_x^2 X(x) = -\lambda^2 X(x) \Rightarrow X(x) = \overline{A}\sin(\lambda x) + \overline{B}\cos(\lambda x) \tag{2.45}$$

and

$$\rho(t,x) = A' e^{-\lambda^2 t} X(x) = e^{-\lambda^2 t}\big(A\sin(\lambda x) + B\cos(\lambda x)\big) \tag{2.46}$$

Again, the time dependent factor is positive, so in order for eq. (2.21) to be true we need to ask $X = 0$ (and anyway, eq. (2.21) need to be true $\forall t > 0$, and thus is determined by X).

$$X(0) = B = 0 \Rightarrow X(x) = A\sin(\lambda x) \tag{2.47}$$

and

$$X(\pi) = A\sin(\lambda\pi) = 0 \tag{2.48}$$

If we want to avoid to get again a null solution, we have to ask $\lambda \in \mathbb{Z}$ so that $\sin(\lambda\pi) = 0$ (we now see the reason of our change of variables in x). We note anyway that $\lambda = 0$ has to be avoided because it will lead to the $C = 0$ case, while if $\lambda = -n < 0$ we have $(-n)^2 = (n^2)$ and

$$X(x) = A\sin(-nx) = -A\sin(nx) = A''\sin(nx) \tag{2.49}$$

so that negative integers just produce the same solutions given by positive ones. We may thus limit ourselves to

$$\rho(t,x) = Ae^{-n^2 t}\sin(nx), \qquad n \in \mathbb{N} \tag{2.50}$$

The $C < 0$ case just led us to solutions for our partial differential equation, eq. (2.50). This solution may also be re-written using the original variables (t', x') as[11]

$$\rho(t',x') = Ae^{-\frac{n^2\pi^2\gamma t'}{L^2}}\sin\left(\frac{n\pi}{L}x'\right), \qquad n \in \mathbb{N} \tag{2.51}$$

Nevertheless, eq. (2.50) gives, for $t = 0$,

$$\rho(0,x) = A\sin(nx) \tag{2.52}$$

and thus cannot satisfy eq. (2.20) unless $f_{t=0}$ is proportional to a sine function. This is better than a null function, but is not general at all!

[11] You may check that the arguments in the sine and exponential of eq. (2.51) have no dimension. This is correct and necessary (such functions may be written as power series of their arguments and thus it would make no sense to have arguments with dimensions).

2.3.1 Separation of variables and linearity

Nevertheless, we can use solutions in the form eq. (2.50) to build new solutions. *This is due to the fact that the heat equation is linear, and the problem that we have specified is homogeneous both in the equation and in the boundary condition.* Let us see what this means.

Linearity

Let us assume we have an equation such as

$$D\big[f(\mathbf{x})\big] = 0 \tag{2.53}$$

Here f is a function from $\mathbb{R}^n \to \mathbb{R}$ and D is an operator, i.e. a function that operates on a function to produce another function (e.g. a derivative). We say that D is linear if given two functions f and g and numbers α, β, the following holds

$$D\big[\alpha f(\mathbf{x}) + \beta g(\mathbf{x})\big] = \alpha D\big[f(\mathbf{x})\big] + \beta D\big[f(\mathbf{x})\big] \tag{2.54}$$

An example of a linear operator is the multiplication by a function $h(\mathbf{x})$

$$\begin{aligned} D\big[\alpha f(\mathbf{x}) + \beta g(\mathbf{x})\big] = h(\mathbf{x})\big[\alpha f(\mathbf{x}) + \beta g(\mathbf{x})\big] &= \alpha h(\mathbf{x}) f(\mathbf{x}) + \beta h(\mathbf{x}) f(\mathbf{x}) \\ &= \alpha D\big[f(\mathbf{x})\big] + \beta D\big[f(\mathbf{x})\big] \end{aligned} \tag{2.55}$$

A partial derivative, or a second partial derivative, is obviously also linear[12], and operators that include sums of derivatives of different orders and multiplications by functions are also linear, as can be easily checked.

Obviously, not all operators are linear. $D[f] = f^2$ is clearly not linear, since $D[\alpha f] = \alpha^2 D[f]$. Also *adding* a function $D[f] = f + h$ is not linear, since $D[f + g] = f + g + h \neq D[f] + D[g] = g + f + 2h$.

Nevertheless, our differential equation (2.28) is in the form eq. (2.53) with the *linear* operator[13]

$$D = \partial_t - \partial_x^2 \tag{2.56}$$

As a result, if we have two solutions for our problem , $D[f] = 0$ and $D[g] = 0$, we can get a third solution just by a combination of them, $D[\alpha f + \beta g] = 0$.

[12] Linearity is a property of derivation.

[13] In section 1.6 we assumed ρ to be conserved, namely not created or destroyed. If we quit this assumption we get a diffusion equation with a source, in the form $D'[f] = 0$, $D'[f] = D[f] - h$, and we lose linearity. Equations with such terms are called *not homogeneous*.

Homogeneous boundary conditions

Until now we did not touch the problem of the boundary conditions. We have seen that if we have two solutions ρ_1 and ρ_2 that satisfy eq. (2.28), then also

$$\rho_3(t,x) = \alpha\rho_1(t,x) + \beta\rho_2(t,x) \tag{2.57}$$

will satisfy eq. (2.28). But our problem includes also boundary conditions. If such conditions were, for example, in the form

$$\rho(t,0) = f_{x=0} \neq 0 \tag{2.58}$$

and if ρ_1 and ρ_2 satisfied such conditions, we would have

$$\rho_3(0,x) = \alpha\rho_1(0,x) + \beta\rho_2(0,x) = (\alpha+\beta)f_{x=0} \tag{2.59}$$

which is in general *not* equal to $f_{x=0}$.

The process of combining two solutions to obtain a third will thus be possible to apply only when we have *homogeneous boundary conditions* such as[14]

$$\rho(t,0) = \rho(t,L) = 0 \tag{2.60}$$

or

$$\partial_x\rho(t,0) = \partial_x\rho(t,L) = 0 \tag{2.61}$$

2.4 Fourier series and general solution to the 1D heat equation with homogeneous boundary conditions

2.4.1 General solution

For our problem we may thus combine different solutions in the form eq. (2.50) to obtain functions that are more general than simple sine functions. But, how general can we get?

At $t = 0$, eq. (2.50) becomes

$$\rho(0,x) = A\sin(nx), \qquad n \in \mathbb{N} \tag{2.62}$$

so that the most general initial condition that we may express with the method of separation of variables is

$$\rho(0,x) = \sum_{n=1}^{\infty} A_n \sin(nx) \tag{2.63}$$

[14] We may always deal with boundary conditions in the form $\rho(t,0) = f_{x=0} = c$ by re-defining the zero of our function, i.e. by studying $\rho' = \rho - c$. This function may assume also negative values, but it is described by the same equation that describes ρ.

An important theorem in functional analysis says that a function which is enough well behaved[15] and assumes $f(0) = f(\pi) = 0$ may be approximated to any degree by the *Fourier series* eq. (2.63). We will assume our initial conditions to satisfy these criteria[16]. We thus state that the general solution to our problem is written as

$$\rho(t, x) = \sum_{n=1}^{\infty} A_n e^{-n^2 t} \sin(nx) \tag{2.64}$$

in a-dimensional variables, and

$$\rho(t', x') = \sum_{n=1}^{\infty} A_n e^{-\frac{n^2 \pi^2 \gamma t'}{L^2}} \sin\left(\frac{n\pi}{L} x'\right) \tag{2.65}$$

in the original, dimensional, ones.

2.5 Computation of coefficients

The formula (2.64), although theoretically important, is by itself scarcely useful since initial conditions are not given in the form eq. (2.64). We need thus a way to obtain the coefficients A_n, that completely specify the solution, from the initial condition. The process is based on a formal analogy with the process that we may use to obtain the coefficients of a vector in a given basis through scalar products, and is based on the definition of a vector space of functions and a corresponding scalar product. We will deal with the theory, although in a largely non rigorous way, in a subsequent chapter, but for the moment we will limit ourselves to the introduction of the computation technique.

We first notice that

$$\int_0^{\pi} \sin(nx) \sin(mx) dx = \frac{\pi}{2} \delta_{nm} = \begin{cases} \frac{\pi}{2} \text{ if } n = m \\ 0 \text{ if } n \neq m \end{cases} \tag{2.66}$$

This result is based on the following trigonometric relations[17]

$$\sin(x + y) = \sin(x) \cos(y) + \sin(y) \cos(x) \tag{2.67}$$

$$\cos(x + y) = \cos(x) \cos(y) - \sin(x) \sin(y) \tag{2.68}$$

[15] For example, piece-wise continuous and differentiable

[16] Functions in classical physics are considered in general *smooth*, i.e. possible to differentiate infinite times, although sometimes piece-wise continuous functions may be used to model some initial conditions.

[17] A straightforward but tedious analytical proof may be based on Euler formulae.

From these we obtain, by substitution and using $\cos(-x) = \cos(x)$, $\sin(-x) = -\sin(x)$

$$\cos(x-y)-\cos(x+y) = 2\sin(x)\sin(y) \Rightarrow \sin(x)\sin(y) = \frac{1}{2}\Big[\cos(x-y)-\cos(x+y)\Big] \tag{2.69}$$

Our integral becomes

$$\int_0^\pi \sin(nx)\sin(mx)dx = \frac{1}{2}\int_0^\pi \cos((n-m)x)dx - \frac{1}{2}\int_0^\pi \cos((n+m)x)dx \tag{2.70}$$

Now, if $n \neq m$, we can use

$$\int_0^\pi \cos(kx) = \frac{1}{k}\Big[\sin(kx)\Big]_0^\pi = 0 \tag{2.71}$$

valid for integer $k \neq 0$, and obtain

$$\int_0^\pi \sin(nx)\sin(mx)dx = 0 \tag{2.72}$$

If $n = m$, eq. (2.69) becomes

$$\sin(x)^2 = \frac{1}{2}\Big[1 - \cos(2x)\Big] \tag{2.73}$$

so that

$$\int_0^\pi \sin^2(nx) = \frac{1}{2}\int_0^\pi dx - \frac{1}{2}\int_0^\pi \cos(2nx)dx = \frac{1}{2}(\pi + 0) = \frac{\pi}{2} \tag{2.74}$$

We may get rid of the factor $\pi/2$ by defining the functions

$$s_n(x) = \sqrt{\frac{2}{\pi}}\sin(nx) \tag{2.75}$$

so that

$$\int_0^\pi s_n(x)s_m(x)dx = \delta_{nm} \tag{2.76}$$

Now, just by redefining the A_n, we may re-write eqs. (2.63,2.64) as

$$\rho(0,x) = \sum_{n=1}^{\infty} A_n s_n(x) \tag{2.77}$$

$$\rho(t,x) = \sum_{n=1}^{\infty} A_n e^{-n^2 t} s_n(x) \tag{2.78}$$

The initial condition for our problem is given by

$$\rho(0,x) = f_{t=0}(x) = \sum_{n=1}^{\infty} A_n s_n(x) \tag{2.79}$$

We know that it can be written as a Fourier series, but we explicitly have only $f_{t=0}(x)$. We may compute the integral

$$\int_0^\pi s_m(x) f_{t=0}(x) = \int_0^\pi s_m(x) \sum_{n=1}^\infty A_n s_n(x) = \sum_{n=1}^\infty A_n \int_0^\pi s_m(x) s_n(x) = A_m \tag{2.80}$$

The general solution may be thus written as

$$\rho(t,x) = \sum_{n=1}^\infty \left[\int_0^\pi s_n(x) f(x)_{t=0} \right] e^{-n^2 t} s_n(x) \tag{2.81}$$

We used the a-dimensional equation in order to develop the theory, but we may now see how to write down a procedure to get the coefficients directly from the dimensional initial condition. Starting from eq. (2.66), and changing variables using eq. (2.22) we get, from $dx = \alpha dx'$

$$\delta_{nm} = \frac{2}{\pi} \int_0^L \sin(n\,\alpha\,x') \sin(m\,\alpha\,x') \alpha\, dx' \tag{2.82}$$

or

$$\int_0^L \sin\left(n\frac{\pi}{L}x'\right) \sin\left(m\frac{\pi}{L}x'\right) dx' = \frac{L}{2}\delta_{nm} \tag{2.83}$$

that has the proper dimension (an integral over distance of a pure number give a length). Defining

$$s_n^L(x') = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi}{L}x'\right) \tag{2.84}$$

we have

$$\int_0^L s_n^L(x') s_m^L(x') dx' = \delta_{nm} \tag{2.85}$$

and, repeating the discussion above, the general solution in dimensional variables may be written as

$$\rho(t',x') = \sum_{n=1}^\infty \left[\int_0^\pi s_n^L(x') f(x')_{t=0} \right] e^{-\frac{n^2\pi^2\gamma t'}{L^2}} s_n^L(x') \tag{2.86}$$

2.6 Time dependence

Let us write again the general solution in the form

$$\rho(t,x) = \sum_{n=1}^\infty A_n e^{-n^2 t} \sin(nx) \tag{2.87}$$

We have highlighted the time dependence in blue. Since $n \neq 0$, all this terms go to zero in the limit $t \to \infty$, the terms with high n decaying faster than those with low n. This shows that

$$\lim_{t\to\infty} \rho(t,x) = 0 \;\; \forall x \in [0,\pi] \tag{2.88}$$

and as a result, the identically zero function is the only stationary solution of the problem, where by stationary solution we mean a solution that does not depend on time

$$\rho(t,x) = \rho_{\text{stat}}(x) \tag{2.89}$$

This is not surprising, both from a mathematical and physical viewpoint.

Mathematically, we have

$$\partial_t \rho_{\text{stat}}(x) = 0 = \partial_x^2 \rho_{\text{stat}}(x) \Rightarrow \rho_{\text{stat}}(x) = Ax + B \tag{2.90}$$

but since we have $\rho = 0$ at 0 and π, we necessarily obtain zero everywhere.

Physically, we may expect the bar to continually lose energy at the ends until the zero solution is reached[18].

2.7 Flux boundary conditions

2.7.1 Stationary solution

Let us consider the solution for the stationary (time independent) problem in case the boundary conditions state that we have zero flux at the end, or (eq. 2.61)

$$\partial_x \rho(t,0) = \partial_x \rho(t,\pi) = 0 \tag{2.91}$$

The argument leading to eq. (2.90) does not depend on boundary conditions, so that the solution is in the form $\rho_{\text{stat}}(x) = Ax + B$, with $\partial_x \rho_{\text{stat}}(x) = A$. Fixing $A = 0$ satisfies the flux conditions at *both* ends, so that the solution for the stationary problem is

$$\rho_{\text{stat}} = B \tag{2.92}$$

There is no way to further specify the solution based on boundary conditions. If prepare the bar at constant temperature B, and insulate the ends, the

[18] The same applies obviously also if this is a "re-scaled" zero, for example if our boundary conditions for the heat equation correspond to keeping the ends at the zero of the Celsius scale, instead of the absolute zero. In this case, the bar may gain energy from the ends, since the function may assume negative values, but the validity of the result does not change.

bar will stay at B. This is obviously very understandable and intuitive also from a physical viewpoint. Nevertheless, in section 2.6 we have seen that the $\rho = 0$ stationary solution is also the $t \to \infty$ limit for *any* general solution of the problem in which the ends where kept at zero. Is also the solution eq. (2.92) a limit for large t? And if it is, how does B relate to the initial condition?

Physical intuition suggests that since the ends are insulated, the system will conserve its energy and reach a stationary, constant solution in which B equals the average energy of the initial condition, i.e.

$$B =< \rho(0,x) >_x = \frac{1}{\pi}\int_0^\pi \rho(0,x)\,dx \tag{2.93}$$

Nevertheless, we do not need to rely on physical intuition.

2.7.2 General solution

We use again the separation of variable method. The discussion leading to eqs. (2.34,2.35) is independent on boundary conditions, so that we can start from

$$\partial_t T(t) = CT(t) \tag{2.94}$$

with solution

$$T(t) = A' e^{Ct} \tag{2.95}$$

and

$$\partial_x^2 X(x) = CX(x) \tag{2.96}$$

We consider again the 3 possible cases for the sign of C

(I) $C > 0$
Since C is positive, we re-name it as $C = \lambda^2$, and solve for

$$\partial_x^2 X(x) = \lambda^2 X(x) \Rightarrow X(x) = \overline{A} e^{\lambda x} + \overline{B} e^{-\lambda x} \tag{2.97}$$

We now have[19]

$$\partial_x X(x) = \lambda\Big[\overline{A} e^{\lambda x} - \overline{B} e^{-\lambda x}\Big] \tag{2.98}$$

$$\partial_x X(0) = \lambda(\overline{A} - \overline{B}) = 0 \Rightarrow \overline{B} = \overline{A} \tag{2.99}$$

and

$$\partial_x X(\pi) = \overline{A}\Big(e^{\lambda x} - e^{-\lambda x}\Big) = 0 \tag{2.100}$$

But this latter equation is satisfied only for $\overline{A} = 0$, which would lead to $C = 0$, i.e., to a contradiction. There is thus no solution corresponding to $C > 0$.

[19] Obviously, for the conditions on ∂_x it is sufficient to analyse X.

(II) $C = 0$
We have

$$\partial_x^2 X(x) = 0 \Rightarrow \partial_x X(x) = \overline{A} \Rightarrow X(x) = \overline{A}x + \overline{B} \tag{2.101}$$

From

$$\partial_x X(x) = \overline{A} = 0 \tag{2.102}$$

we find, with the usual re-definition of constants, the solution

$$\rho(t,x) = T(t)X(x) = e^{0t}B = B \tag{2.103}$$

which is exactly the stationary solution of section 2.7.1.

(III) $C < 0$
Since C is negative, we re-name it as $C = -\lambda^2$, and find

$$\partial_x^2 X(x) = -\lambda^2 X(x) \Rightarrow X(x) = \overline{A}\sin(\lambda x) + \overline{B}\cos(\lambda x) \tag{2.104}$$

From

$$\partial_x X(x) = \lambda\big(\overline{A}\cos(\lambda x) - \overline{B}\sin(\lambda x)\big) \tag{2.105}$$

we get

$$\partial_x X(0) = \lambda\overline{A} \Rightarrow X(x) = \overline{B}\cos(\lambda x) \tag{2.106}$$

and

$$\partial_x X(\pi) = -\lambda\overline{B}\sin(\lambda\pi) = 0 \tag{2.107}$$

As before, to avoid a null solution, we have to ask $\lambda \in \mathbb{Z}$ so that $\sin(\lambda\pi) = 0$. $\lambda = 0$ corresponds to the $C = 0$ case, while if $\lambda = -n < 0$ we have $(-n)^2 = (n^2)$ and

$$X(x) = \overline{B}\cos(-nx) = \overline{B}\cos(nx) \tag{2.108}$$

so that negative integers just produce the same solutions given by positive ones. We may thus limit ourselves to

$$\rho(t,x) = Be^{-n^2 t}\cos(nx), \qquad n \in \mathbb{N} \tag{2.109}$$

If two solutions ρ_1, ρ_2 satisfy the boundary condition $\partial_x\rho(0) = \partial_x\rho(\pi) = 0$, also a linear combination of them will satisfy the same condition since

$$\partial_x(\alpha\rho_1 + \beta\rho_2) = \alpha\partial_x\rho_1 + \beta\partial_x\rho_2 \tag{2.110}$$

We may thus write the general solution as

$$\rho(t,x) = \sum_{n=0}^{\infty} B_n e^{-n^2 t}\cos(nx) = B_0 + \sum_{n=1}^{\infty} B_n e^{-n^2 t}\cos(nx) \tag{2.111}$$

where on the rightmost expression we singled out the time independent term corresponding to $C = 0$. This term will obviously be the only one to survive in the $t \to 0$ limit. As it happened for the case in which the ends temperature was kept to 0, time decay is faster for high n, but now we have also a t independent term.

This solution is, again according to the Fourier series theory, able to approximate any regular initial condition in agreement with eqs. (2.61)

2.7.3 Computation of coefficients

We want again to be able to compute the coefficients B_n from the initial condition $\rho_{t=0}(x)$. We use

$$\cos(x-y)+\cos(x+y) = 2\cos(x)\cos(y) \Rightarrow \cos(x)\cos(y) = \frac{1}{2}\Big[\cos(x-y)+\cos(x+y)\Big] \tag{2.112}$$

and

$$\int_0^\pi \cos(kx)dx = \frac{1}{k}\Big[\sin(kx)\Big]_0^\pi = 0 \tag{2.113}$$

provided that k is a non zero integer, so that if $m \neq n$

$$\int_0^\pi \cos(nx)\cos(mx)dx = \frac{1}{2}\int_0^\pi \cos((n-m)x)dx + \frac{1}{2}\int_0^\pi \cos((n+m)x)dx = 0 \tag{2.114}$$

The formula above applies also to the case $n = 0$, $\cos(nx) = 1$.

If $n = m \neq 0$ we have

$$\int_0^\pi \cos^2(nx)dx = \frac{1}{2}\int_0^\pi dx + \frac{1}{2}\int_0^\pi \cos(2nx)dx = \frac{1}{2}(\pi + 0) = \frac{\pi}{2} \tag{2.115}$$

while for $n = m = 0$ we have obviously

$$\int_0^\pi dx = \pi \tag{2.116}$$

Let us then define

$$c_0(x) = \frac{1}{\sqrt{\pi}}, \qquad c_n(x) = \sqrt{\frac{2}{\pi}}\cos(nx) \;\; n \in \mathbb{N} \tag{2.117}$$

so that we have

$$\int_0^\pi c_n(x)c_m(x) = \delta_{n,m} \tag{2.118}$$

We re-write the general solution as

$$\rho(t,x) = \sum_{n=0}^{\infty} B_n e^{-n^2 t} c_n(x) \tag{2.119}$$

where (see eq. 2.80)

$$B_n = \int_0^\pi c_n(x) f_{t=0}(x) dx \tag{2.120}$$

If you prefer working with the dimensional variables, you may define

$$c_0^L(x') = \sqrt{\frac{1}{L}}, \qquad c_n^L(x') = \sqrt{\frac{2}{L}} \cos\left(\frac{n\pi}{L} x'\right) \tag{2.121}$$

and

$$\rho(t', x') = \sum_{n=0}^{\infty} \left[\int_0^\pi c_n^L(x') f(x')_{t=0} \right] e^{-\frac{n^2 \pi^2 \gamma t'}{L^2}} c_n^L(x') \tag{2.122}$$

Let us explicitly compute

$$B_0 = \int_0^\pi \frac{1}{\sqrt{\pi}} f_{t=0}(x)\, dx = \sqrt{\pi} < f_{t=0} >_x \tag{2.123}$$

We thus have

$$\lim_{t\to\infty} \rho(t, x) = B_0 c_0 = \sqrt{\pi} < f_{t=0} >_x \frac{1}{\sqrt{\pi}} =< f_{t=0} >_x \tag{2.124}$$

confirming our physical intuition.

2.8 Diffusion on the circle

2.8.1 Periodic boundary conditions

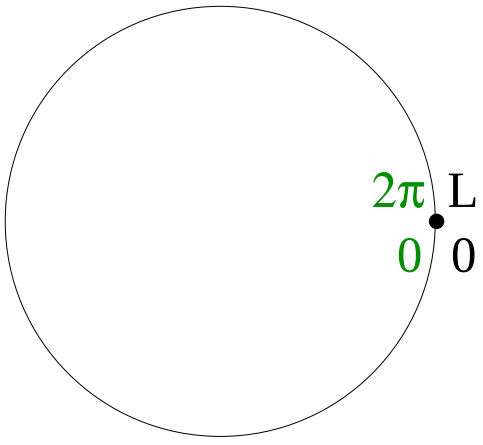

Figure 2.2: Diffusion on the circle

Let us now imagine that, without changing the physical properties of diffusion, we may bend the bar in a circle in such a way so that the two

ends will be unified in a single point (Fig. 2.2). It is useful then to make a change of variables, for this problem, from

$$x' \in [0, L] \to x \in [0, 2\pi] \tag{2.125}$$

namely

$$x = \alpha x', \qquad \alpha = \frac{2\pi}{L} \tag{2.126}$$

and the corresponding (see eq. 2.27)

$$t = \gamma\alpha^2 t' = \frac{4\pi^2\gamma}{L^2}t' \tag{2.127}$$

that leads to the usual

$$\partial_t \rho = \partial_x^2 \rho \tag{2.128}$$

expression for the differential equation.

The reason for this change of variables should be clear: x (we could have called it θ) is the angle that gives the position on the circle. Now, since we assume it to be purely 1D, the system is completely closed, since its ends interact with each other, and are actually the same point. The boundary conditions are now fixed in a natural way by asking the solution[20] to be periodic

$$\rho(t, x + 2\pi) = \rho(t, x) \tag{2.129}$$

These are the so called *periodic boundary conditions*.

2.8.2 Separation of variables

It is straightforward that if ρ_1 and ρ_2 are periodic then

$$\alpha\rho_1(t, x + 2\pi) + \beta\rho_2(t, x + 2\pi) = \alpha\rho_1(t, x) + \beta\rho_2(t, x) \tag{2.130}$$

so that we will be able to combine different solutions to the problem to obtain new solutions. We proceed again with the separation method, that leads as usual to

$$\partial_t T(t) = CT(t) \tag{2.131}$$

with solution

$$T(t) = A' e^{Ct} \tag{2.132}$$

and

$$\partial_x^2 X(x) = CX(x) \tag{2.133}$$

We consider again the 3 possible cases for the sign of C

[20] And by consequence all its derivatives.

(I) $C = \lambda^2 > 0$
The solution

$$X(x) = \overline{A}e^{\lambda x} + \overline{B}e^{-\lambda x} \tag{2.134}$$

is not periodic, regardless of the values of the constants, so that $C > 0$ will not satisfy the boundary conditions

(II) $C = 0$
The solution

$$X(x) = \overline{A}x + \overline{B} \tag{2.135}$$

is periodic only for $\overline{A} = 0$ so that we get the solution

$$\rho(t, x) = T(t)X(x) = e^{0t}B = B \tag{2.136}$$

We may already understand (and soon prove) that this stationary solution will be the $\lim_{t\to 0}$ of ρ, and its value will correspond to the initial average energy/temperature/density[21].

(III) $C = -\lambda^2 < 0$
This time may proceed in a different (but equivalent) way. We know that the general complex solution to

$$\partial_x^2 X(x) = -\lambda^2 X(x) \tag{2.137}$$

is

$$X(x) = A'e^{i\lambda x} + B'e^{-i\lambda x} \tag{2.138}$$

This solution will be periodic if $\lambda = n \in \mathbb{Z}$. To ask for the solution to be real we may notice that the complex conjugate X^* is

$$X^*(x) = (A')^* e^{-inx} + (B')^* e^{inx} \tag{2.139}$$

so that the solution is real if

$$A' = (B')^* \Rightarrow (A')^* = B' \tag{2.140}$$

or

$$A' = B'' + iA'', \qquad B' = B'' - iA'' \tag{2.141}$$

with A'', $B'' \in \mathbb{R}$, so that

$$X(x) = 2B''\frac{e^{inx} + e^{-inx}}{2} + 2iA''\frac{e^{inx} - e^{-inx}}{2i} = \overline{B}\cos(nx) + \overline{A}\sin(nx) \tag{2.142}$$

[21] The system is clearly conserving $\int \rho$ since it has no contact with the exterior world. The boundary from which ρ could flow, that before corresponded to the two ends, has now been reduced to no point.

2.8.3 Complex "orthogonal" solutions

The periodic complex solutions

$$e^{int}, n \in \mathbb{Z} \tag{2.143}$$

are extremely important and may shed some light also on the behaviour of real solutions, as we will see soon. Being of a simple exponential form, they are more easy to operate on than the trigonometric functions.

We start their study by computing the following integral[22]

$$\int_0^{2\pi} \left(e^{imx}\right)^* e^{inx} dx = \int_0^{2\pi} e^{-imx} e^{inx} dx = \int_0^{2\pi} e^{i(n-m)x} dx \tag{2.144}$$

In the $n = m$ case we have

$$\int_0^{2\pi} dx = 2\pi \tag{2.145}$$

while if $n \neq m$ we use

$$\int_0^{2\pi} e^{i(n-m)x} dx = \frac{1}{i(n-m)} \left[e^{i(n-m)x}\right]_0^{2\pi} = 0 \text{ if } n, m \in \mathbb{Z} \tag{2.146}$$

If we define

$$a_n(x) = \frac{1}{\sqrt{2\pi}} e^{inx} \tag{2.147}$$

we have

$$\int_0^{2\pi} a_n^*(x) a_m(x) dx = \delta_{n,m} \tag{2.148}$$

We may also define the following real functions for $n \in \mathbb{N}$ (p stands for periodic)

$$c_0^p(x) = a_0(x) = \frac{1}{\sqrt{2\pi}} \tag{2.149}$$

$$c_n^p(x) = \frac{1}{\sqrt{2}} \big(a_n(x) + a_{-n}(x)\big) = \frac{1}{\sqrt{\pi}} \cos(nx) \tag{2.150}$$

$$s_n^p(x) = \frac{1}{\sqrt{2}i} \big(a_n(x) - a_{-n}(x)\big) = \frac{1}{\sqrt{\pi}} \sin(nx) \tag{2.151}$$

[22] We will later learn that this integral corresponds to a scalar product in a function space.

We have[23]

$$\int_0^{2\pi} (c_n^p(x))^* c_m^p(x)dx = \int_0^{2\pi} c_n^p(x)c_m^p(x)dx =$$
$$\frac{1}{2}\int_0^{2\pi} (a_n(x)a_m(x) + a_{-n}(x)a_m(x) + a_n(x)a_{-m}(x) + a_{-n}(x)a_{-m}(x))$$
$$= \frac{1}{2}(\delta_{n,m} + 0 + 0 + \delta_{-n,-m}) = \frac{1}{2}(\delta_{n,m} + \delta_{n,m}) = \delta_{n,m} \tag{2.152}$$

and similarly

$$\int_0^{2\pi} (s_n^p(x))^* s_m^p(x)dx = \int_0^{2\pi} s_n^p(x)s_m^p(x)dx$$
$$=\frac{1}{2}\int_0^{2\pi} (a_n(x)a_m(x) + a_{-n}(x)a_m(x) - a_n(x)a_{-m}(x) - a_{-n}(x)a_{-m}(x)) = \delta_{n,m} \tag{2.153}$$

2.8.4 General solution

If we were studying a problem in which ρ was a complex function, its general solution would be written as

$$\rho(x,t) = \sum_{n=-\infty}^{+\infty} A_n e^{-n^2 t} a_n(x) \tag{2.154}$$

with

$$A_n = \int_0^{2\pi} a_n^*(x) f_{t=0}(x)dx \tag{2.155}$$

But since our initial condition is real, we have

$$A_n^* = \int_0^{2\pi} a_n(x) f_{t=0}(x)dx = \int_0^{2\pi} a_{-n}^*(x) f_{t=0}(x)dx = A_{-n} \tag{2.156}$$

so that

$$\rho(x,t) = A_0 a_0(x) + \sum_{n=1}^{\infty} \left(A_n a_n(x) + A_n^* a_{-n}(x)\right) =$$
$$A_0 a_0(x) + \sum_{n=1}^{\infty} \left(2\ \mathrm{Re}(A_n)(a_n(x) + a_{-n}(x)) + 2i\ \mathrm{Im}(A_n)(a_n(x) - a_{-n}(x))\right) \tag{2.157}$$

By defining

$$A_0 = C_0, \quad C_n = 2\sqrt{2}\ \mathrm{Re}(A_n), \quad S_n = 2i\sqrt{2}\ \mathrm{Im}(A_n) \tag{2.158}$$

[23] These relations may obviously be shown to hold also through trigonometric equalities.

we get the general solution in a-dimensional variables

$$\rho(t,x) = \sum_{n=0}^{\infty} C_n c_n^p(x) e^{-n^2 t} + \sum_{n=1}^{\infty} S_n s_n^p(x) e^{-n^2 t} \tag{2.159}$$

with

$$C_n = \int_0^{2\pi} c_n^p(x) f_{t=0}(x), \quad S_n = \int_0^{2\pi} s_n^p(x) f_{t=0}(x) \tag{2.160}$$

or

$$C_0 = \frac{1}{\sqrt{2\pi}} \int_0^{2\pi} f_{t=0}(x) = \sqrt{2\pi} < f_{t=0} >_x \tag{2.161}$$

$$C_n = \frac{1}{\sqrt{\pi}} \int_0^{2\pi} \cos(nx) f_{t=0}(x) \tag{2.162}$$

$$S_n = \frac{1}{\sqrt{\pi}} \int_0^{2\pi} \sin(nx) f_{t=0}(x) \tag{2.163}$$

In the $t \to \infty$ limit we have

$$\lim_{t\to\infty} \rho(t,x) = c_0^p \sqrt{2\pi} < f_{t=0}(x) >_x = < f_{t=0}(x) >_x \tag{2.164}$$

These formulae that can be re-conducted to the dimensional case through eqs. (2.126,2.127), namely defining

$$c_0^{L,p}(x') = \sqrt{\frac{1}{L}}, \quad c_n^{L,p}(x') = \sqrt{\frac{2}{L}} \cos\left(\frac{2n\pi}{L} x'\right), \quad s_n^{L,p}(x') = \sqrt{\frac{2}{L}} \sin\left(\frac{2n\pi}{L} x'\right) \tag{2.165}$$

$$C_n = \int_0^{L} c_n^{L,p}(x') f_{t=0}(x'), \quad S_n = \int_0^{L} s_n^{L,p}(x') f_{t=0}(x') \tag{2.166}$$

$$\rho(t',x') = \sum_{n=0}^{\infty} C_n e^{-\frac{4n^2\pi^2\gamma t'}{L^2}} c_n^L(x') + \sum_{n=1}^{\infty} S_n e^{-\frac{4n^2\pi^2\gamma t'}{L^2}} s_n^L(x') \tag{2.167}$$

Chapter 3

The Schrödinger equation

We will discuss briefly how the method of separation of variables may be used to solve simple problems in Quantum Mechanics, i.e. related to behaviours of particles at the atomic or sub-atomic level. The context for the equation describing quantum behaviour will be provided using an historical perspective, i.e. trying to describe how the leading physicists of the time developed and understood these ideas at the beginning of the 20th century. The discussion would be nevertheless extremely simplified and distorted to fit in this short chapter, and should not be considered as a loyal description of facts and opinions, but just as an invitation to the subject.

3.1 Historical remarks

3.1.1 Plank

In 1900, the great German physicist Max Planck proposed a solution to one of the most important physical problem of the time, the law at which a non-light reflecting body ("black body") emits radiation when it is at thermal equilibrium[1]. The details of the problem go beyond the purpose of this course, but in order to find the correct law Planck had to do a very revolutionary hypothesis: light (more properly, electromagnetic radiation), which Maxwell theory had shown to be a continuous wave phenomenon, had to be found in the body only under the form of discrete units (quanta). Light with wave frequency ν could be found only in "packets" with energy

$$E = h\nu \tag{3.1}$$

[1]This may be a good model of the energy emitted by a star as a function of the star's temperature.

where h is the Planck constant. We know that energy has the dimensionality of mass multiplied by a squared velocity, while v is an inverse time, so that h is an *action*, i.e. a quantity with dimension

$$[h] = [M][L]^2[T]^{-1} \tag{3.2}$$

If we measure masses in kilograms, lengths in meters and time in seconds, i.e. if energy is measured in Joules, the value of h is

$$h \approx 6.63 \cdot 10^{-34} \text{J s} \tag{3.3}$$

Planck, who was a conservative man in life and science[2] introduced this law not because he believed light to be formed by particles of energy $h\nu$, but simply because the hypothesis allowed him to find the right solution. At the time he proposed his law, it was still not understood that the hypothesis was *necessary* to find the correct law, and that a continuous distribution of energy would lead to non-sensical results (this was proven later by the British Rayleigh and Jeans, and, independently, by Einstein).

3.1.2 Einstein

Photoelectric effect

As we have just seen, Albert Einstein had arrived to the conclusion that Planck's law was not just a mathematical trick, since he could prove that if the radiation had a continuous energy distribution, the black body would need an infinite energy before arriving at thermal equilibrium. Einstein had also learned about experiments saying that the energy of electrons released by a metal when electromagnetic radiation (light) was sent on it were independent on the radiation intensity, a very surprising fact since the energy of a wave is related to its intensity.

[2]Max Planck, who received the Nobel prize in 1918 for his work on the black body radiation, strongly disliked Nazism but tried to convince German physicists to remain to work in Germany under the regime. He never openly opposed Nazi policies, but tried (with no success) to use his authority in order to defend some Jewish colleagues, talking once to the same Hitler (these are Planck' memories of their talk *"In response to my comment that it would essentially be a self-inflicted catastrophe if valuable Jews were forced to emigrate, as we urgently need their scientific work, and that this will otherwise benefit primarily other countries, he (Hitler) did not comment any further. He turned instead to general chitchat and concluded by saying: People say that I occasionally suffer from neurasthenia. This is slander. I have nerves of steel. He then slapped his knee hard, spoke at an increasingly faster rate and worked himself up into such a rage that there was nothing else for me to do but to remain silent and leave."*). Planck's son Erwin was sentenced to death in 1944 for taking part to a plot aimed at killing Hitler.

Einstein thus stated that light was composed of particles of energy $h\nu$, where ν is the frequency of the wave. The intensity of the wave was related to the *number* of particles in the wave. Nevertheless, when interacting with individual electrons, it would be the energy of the particle (*photon*) to decide if the electron received enough energy to leave the metal. The energy of the released electron would be, according to Einstein's prediction,

$$E = h\nu - \phi \tag{3.4}$$

ϕ being the minimum energy needed to release the electron from the metal. Intensity, Einstein predicted, would be related to the number of released electrons, not to their energy.

Einstein wrote his theory in 1905, and his predictions were experimentally confirmed in 1916. The theory was not easily accepted. Einstein did not explain why light usually behaved like a wave, and not as a particle, in other situations. The particle theory of light, proposed in the past by Newton, had been rejected empirical data. For these reasons even the most prominent physicists of the time considered Einstein's theory as wrong, and even when data supporting it emerged, most phycisits believed the quantization to be due to interaction with matter, and not intrinsic in light itself. Only after the quantum theory for particles (as electrons) was developed, and was understood that the particle-wave duality is universal in nature, was it possible to better understand Einstein's theory[3].

3.1.3 Relativity

In the same year, Einstein proposed his relativity theory, which extends some results previously introduced by the Dutch physicist Lorentz, and largely parallels a theory introduced at the same time by the French mathematician Poincaré[4]. In non relativistic physics, the energy of a particle in a potential U is given by

$$E = \frac{1}{2}mv^2 + U(\mathbf{x}) \tag{3.5}$$

This is often written in physics as

$$H(\mathbf{x}, \mathbf{p}) = \frac{p^2}{2m} + U(\mathbf{x}) \tag{3.6}$$

[3]The quantum theory of light , being inherently relativistic, presents more difficulties than the quantum theory of electrons, and was developed only in a second time.

[4]The difference between their approaches is subtle and debated between historians. Most nevertheless agree that Einstein was the first one to state clearly that the new dynamics and kinematics derived just by asking that all laws of physics, including the value of the velocity of light, were the same in all inertial frames.

where H is the Hamiltonian function of position $\mathbf{x}$ and momentum $\mathbf{p}$, a function that plays a fundamental role in the theoretical study of mechanics. The momentum $\mathbf{p}$ is, for this simple system, defined as

$$\mathbf{p} = m\mathbf{v} \tag{3.7}$$

so that Newton's second law may be written as

$$\frac{dp_i}{dt} = -\partial_{x_i} H(\mathbf{x}, \mathbf{p}) = -\partial_{x_i} U(\mathbf{x}) = F_i(\mathbf{x}) \tag{3.8}$$

In relativistic physics we still have

$$\frac{dp_i}{dt} = F_i(\mathbf{x}) \tag{3.9}$$

but now the momentum is given by

$$\mathbf{p} = \frac{m\mathbf{v}}{\sqrt{1 - \frac{v^2}{c^2}}} \tag{3.10}$$

where c is the velocity of light (this causes the inertia of a particle to diverge when the velocity approaches c, so that no force may bring a particle to a velocity higher than c.) The energy of a free particle (i.e in absence of force) is now defined by

$$E = \sqrt{m^2c^4 + p^2c^2} \tag{3.11}$$

which may be solved for

$$E = \frac{mc^2}{\sqrt{1 - \frac{v^2}{c^2}}} \tag{3.12}$$

so that

$$\frac{p}{E} = \frac{v}{c^2} \tag{3.13}$$

Let us now assume there is a particle without mass, $m = 0$. Eq. (3.11) becomes

$$E = pc \tag{3.14}$$

and substituting in (3.13) gives

$$v = c \tag{3.15}$$

For this reason, the "light particles" that Einstein introduced in his work on the photoelectric effect have necessarily zero mass (since they move with velocity c [5]). The theory of Relativity was soon accepted by the leading physicists of the time[6].

[5] It is clear from eq. (3.11) that if $m > 0$ then $E > pc$.

[6] In particular those of Einstein's generation or younger. Others, while agreeing with the mathematical results, maintained a different philosophical approach, closer to the one

3.1.4 De Broglie

With is 1924 Ph. D. thesis, the French physicist Luis de Broglie made an important step in understanding the relation between wave and particle behaviour.

About waves

Let us first start with some notation. If we have a periodic phenomenon (in our case the oscillation of a wave) with period T, its frequency is given by

$$\nu = \frac{1}{T} \tag{3.16}$$

We often express periodic phenomena through trigonometric functions[7],

$$f(t) = A\cos(\omega t + \phi) = A\cos(\omega(t+T) + \phi) = f(t+T) \tag{3.17}$$

This implies

$$\omega T = 2\pi \Rightarrow \omega = 2\pi\nu \tag{3.18}$$

where ω is called the angular velocity. Relation (3.1) may thus be written as

$$E = \hbar\omega, \qquad \hbar = \frac{h}{2\pi} \tag{3.19}$$

where we have defined the useful constant $\hbar$ (h-bar).

If a wave has velocity c, it will cover a distance cT in time T. This distance is called the wave length

$$\lambda = \frac{c}{\nu} \tag{3.20}$$

Let us write a function which is periodic in space and time

$$\Phi(t,x) = A\cos(kx - \omega t + \phi) \tag{3.21}$$

At a fixed point $\overline{x}$ this function will be oscillating in time with a period T such that $\omega T = 2\pi$, as discussed above. If observed at fixed t, the function

of Lorentz and Poincare. It is nevertheless interesting that less important physicists had an harder time to accept relativity theory. The Nobel Prize committee received, in the years following the publishing of Einstein's Special and General (Gravitation) Relativity theory, many endorsements to give the prize to Einstein, but the members of the committee were reluctant to give the prize for relativity theory, and eventually decided to give him the prize for the photoelectric effect in 1921. Interestingly, a few of the eminent physicists proposing Einstein were actually doubtful with regards to the correctness of the revolutionary theory according to which light is composed by particles!.

[7] $\cos(\omega t + \phi) = \cos(\phi)\cos(\omega t) - \sin(\phi)\sin(\omega t) = C_1\cos(\omega t) + C_2\sin(\omega t)$

looks like oscillating with a period (distance between two crests) λ such that $k\lambda = 2\pi$, or

$$k = \frac{2\pi}{\lambda} \tag{3.22}$$

where k is called the *wave number*. Is this the same λ in equation (3.20)?

We have mentioned above that the oscillation of a (1D) wave is described by a differential equation in the form

$$\partial_t^2 \Phi(t,x) = c^2 \partial_x^2 \Phi(t,x) \tag{3.23}$$

If we substitute Φ from eq. (3.21) in eq. (3.23) we obtain

$$\omega^2 \Phi(t,x) = c^2 k^2 \Phi(t,x) \tag{3.24}$$

i.e. we have a solution provided that

$$\omega = \pm ck \Rightarrow 2\pi\nu = \pm c\frac{2\pi}{\lambda} \Rightarrow \lambda = \frac{c}{\nu} \tag{3.25}$$

(we have assumed to define ν and λ as positive), so that λ appearing in the periodic solution is indeed the distance the wave covers in T.

De Broglie's matter waves

De Broglie noticed that for a photon, using eqs. (3.14,3.20,3.22), we have

$$p = \frac{h\nu}{c} = \frac{h}{\lambda} = \hbar k \Rightarrow \lambda = \frac{h}{p} \tag{3.26}$$

and made the hypothesis that a wave length λ was associated to any particle of momentum p according to the law above.

De Broglie's idea was very easy to test[8]: it was enough to have a beam of electrons with momentum p through a crystal with lattice distance b and see if the beam generated a diffraction pattern corresponding to a wave of wavelenght λ. It did, and de Broglie (1929) and experimental physicists Davisson and Thomson (1937, for two different experiments performed in USA and Britain) got the Nobel prize.

3.1.5 Heisenberg

In 1925, the 23 year old German physicist Werner Heisenberg formulated the first successful and completely consistent description of atomic phenomena,

[8] In principle, performing actual experiments nobody did before is never easy.

through a quite obscure model called *matrix mechanics*. The model was perfectioned and mathematically brushed up in collaboration with Max Born[9] and Pascual Jordan, two other German physicists, and used by the Austrian Wolfang Pauli[10] to find the the spectrum (possible energies of electrons) of the Hydrogen atom.

Despite its early success, the model, who lead Heisenberg to the 1932 Nobel Prize[11], was not extremely loved by contemporary physicists. Many just disliked its mathematical formalism, but a few disliked the underlying philosophy: Heisenberg claimed that there was nothing more in physics that what could be directly observed, no underlying substrate, and based his theory on this philosophical principle.

3.1.6 Schrödinger

Between those that did not like the philosophical principles underlying Heisenberg model there was Albert Einstein, who believed that the truth was in the direction shown by de Broglie's ideas. Through Einstein, the Austrian mathematical physicist Erwin Schrödinger learned about de Broglie waves, namely that a free (non interacting particle) could be described through relations (3.1,3.26) by a periodic function

$$\Psi(t, \mathbf{x}) = e^{i\left(\frac{\mathbf{p}\cdot\mathbf{x}}{\hbar} - \frac{Et}{\hbar}\right)} \tag{3.27}$$

Here we used the complex formulation (whose real part gives a cosine and imaginary part a sine), and generalised to the 3D case[12] the relations

$$\frac{E}{\hbar} = \omega, \qquad \frac{\mathbf{p}}{\hbar} = \mathbf{k} \tag{3.28}$$

[9] 1954 Nobel Prize for his interpretation of the statistical nature of Quantum Mechanics, to be discussed later.

[10] 1945 Nobel Prize for his exclusion principle, that describes the impossibility of two electrons to be in the same physical state.

[11] Heisenberg trajectory during the dark years of National Socialism may recall the experience of the much older Planck. A proud and patriotic German, never thought of leaving the country. He was nevertheless accused of being a "white Jew", since he taught Einstein's theories in his university courses. Eventually, due to his scientific stature, he was put in charge of theoretical work related to the development of the German Atom bomb, a role that made him be partially ostracised from the scientific community at the end of teh conflict, and ruined his relation with his mentor, the Danish Jew Niels Bohr. Nevertheless, Heisenberg always stated that he worked only to develop civil nuclear power. After being arrested by Allied forces, and detained in Britain with other fellow scientists, he gave to his fellow inmates a lecture on the functioning of the Hiroshima bomb, showing, according to some historians, that he actually did his best *not* to build a Nazi bomb.

[12] Using $\nabla^2 e^{i\mathbf{k}\cdot\mathbf{x}} = -k^2 e^{i\mathbf{k}\cdot\mathbf{x}}$.

He started lecturing about this idea, in opposition to Heisenberg formulation, until someone commented that "a wave needs a wave equation". Schrödinger, who was at the time 38, an age at which in general theoretical physicists have already produced their best works, decided to spend a few days in a mountain cabin on the Alps with a woman that was not exactly his wife[13] and used (part of) his time to write down the wave equation that takes is name. He started from the Hamiltonian function (3.6)

$$E = H(\mathbf{x}, \mathbf{p}) = \frac{p^2}{2m} + U(\mathbf{x}) \tag{3.29}$$

He noticed that, according to eq. (3.27), the energy is obtained by operating on Ψ using the following differential operator $\hat{E}$

$$E\Psi = \hat{E}\Psi = i\hbar\partial_t\Psi \tag{3.30}$$

In a equivalent way, the (x component of the) momentum is obtained by

$$p_x\Psi = \hat{p}_x\Psi = -i\hbar\partial_x\Psi \tag{3.31}$$

He thus replaced the quantities E and p in eq. 3.29 with these differential operators acting on Ψ. In order to replace p^2, he used

$$p^2 = \mathbf{p}\cdot\mathbf{p} \Rightarrow \hat{p}^2 = \sum_i (-i\hbar\partial_i)(-i\hbar\partial_i) = -\hbar^2\nabla^2 \tag{3.32}$$

He was left with the potential U, that he decided to introduce as an operator that multiplies Ψ by U, since, as we saw with eq. (2.55), such a choice gives a linear operator.

He thus introduced the following equation that takes his name

$$\hat{E}\Psi(t,\mathbf{x}) = \hat{H}\Psi(t,\mathbf{x}) = \frac{\hat{p}^2}{2m}\Psi(t,\mathbf{x}) + U(\mathbf{x})\Psi(t,\mathbf{x}) \tag{3.33}$$

or, explicitly

$$i\hbar\partial_t\Psi(t,\mathbf{x}) = -\frac{\hbar^2}{2m}\nabla^2\Psi(t,\mathbf{x}) + U(\mathbf{x})\Psi(t,\mathbf{x}) \tag{3.34}$$

Before discussing the meaning of this equation is better to find its solution, just as Schrödinger did.

[13] In 1939, Schrödinger moved to Dublin, invited by the Irish Prime Minister (later President) De Valera, when he had to leave Austria due to his positions against the Nazi party (smart people had a tendency to dislike Nazism), where he openly lived with his wife and the mother of one of his daughters. While in Dublin, he had other two daughters from different women.

3.2 A simple 1D problem in Quantum mechanics: a trapped particle

Let us suppose we have a particle trapped in a area of length L. We will assume, for reasons of mathematical simplicity, the problem to be 1D.

3.2.1 Boundary conditions

This trap is realised by asking that the particle moves freely ($U = 0$) in the $[0, L]$ area, but it cannot exit it. Namely we will study the equation in such interval with the boundary conditions

$$\Psi(t, 0) = \Psi(t, L) = 0 \tag{3.35}$$

Although we still did not discuss the meaning of Ψ, we are implying that Ψ somehow tells us where the particle is, for example Ψ may be related to the particle's "density" (reality is more complex, see section 3.3). Since the equation is second order in space, these conditions should be enough to fix the behaviour of the solution. The equation is first order in time, so that knowledge of

$$\Psi(0, x), \quad x \in [0, L] \tag{3.36}$$

should suffice[14].

3.2.2 Separation of variables: the Time-independent Schrödinger equation

The equation is linear and the boundary conditions are homogeneous, so we will proceed with separation of variables.

$$\Psi(t, x) = T(t)X(x) \tag{3.37}$$

This leads to

$$X(x)\big(i\hbar\partial_t T(t)\big) = T(t)\left(-\frac{\hbar^2}{2m}\partial_x^2 X(x)\right) \tag{3.38}$$

and, dividing by Ψ,

$$\frac{i\hbar\partial_t T(t)}{T(t)} = C = \frac{-\frac{\hbar^2}{2m}\partial_x^2 X(x)}{X(x)} \tag{3.39}$$

Let us reflect on the role of C. We introduced the operator

$$\hat{E} = i\hbar\partial_t \tag{3.40}$$

[14] Schrödinger equation is basically a diffusion equation with a $-i$ in front of the time derivative.

because it gave the energy when applied to Ψ in the form of a de Broglie wave, eq. (3.27). Here we have

$$\hat{E}\Psi(t,x) = i\hbar\partial_t T(t)X(x) = X(x)i\hbar\partial_t T(t) = CX(x)T(t) = C\Psi(t,x) \tag{3.41}$$

it looks thus reasonable to name $C = E$, the *energy of the particle*.

We are thus left with two equations

$$i\hbar\partial_t T(t) = ET(t) \tag{3.42}$$

and

$$-\frac{\hbar^2}{2m}\partial_x^2 X(x) = EX(x) \tag{3.43}$$

The first equation is solved as

$$T(t) = A'e^{-i\frac{E}{\hbar}t} \tag{3.44}$$

This is obviously the time part of eq. (3.27), but now we obtained it from a wave equation, so that Schrödinger's critics could be silenced. It should be clear that, provided the potential U is time-independent, the procedure leading to eq. (3.44) will not depend on U. The time dependence of Ψ for a particle with a given energy E will be always given by eq. (3.44). We will thus be left with the problem of finding the space dependence of Ψ, which is given by the *Time-independent Schrödinger equation*, eq. (3.43).

We may notice, given the discussion above, that, when dealing with the Schrödinger equation, the separation of variable process has a deep physical meaning, since leads us to obtaining *physical states with a defined energy.*

3.2.3 Solution of the time-independent Schrödinger equation

The equation may be written as

$$\partial_x^2 X(x) = -\frac{2mE}{\hbar^2}X(x) \tag{3.45}$$

We have as usual 3 cases depending on the sign of the energy

(I) $E < 0$, $\frac{2mE}{\hbar^2} = \lambda^2$
The solution to

$$\partial_x^2 X(x) = \lambda^2 X(x) \tag{3.46}$$

is

$$X(x) = Ae^{\lambda x} + Be^{-\lambda x} \tag{3.47}$$

Clearly

$$X(0) = 0 \Rightarrow B = -A \tag{3.48}$$

and

$$X(L) = A(e^{\lambda L} - e^{-\lambda L}) \tag{3.49}$$

cannot be zero for $A \neq 0$, so that there is no solution for negative energy.

This is not surprising. The energy for a classical particle is

$$E = \frac{1}{2}v^2 + U(x) \geq U(x) \tag{3.50}$$

so that by fixing the potential $U = 0$ we are (from a classical view point) forcing the energy to be $E \geq 0$. We have just seen that this result applies also to the quantum problem.

(II) $E = 0$, $\frac{2mE}{\hbar^2} = 0$
The solution is

$$X(x) = Ax + B \tag{3.51}$$

and as usual the boundary conditions impose $A = B = 0$. But if Ψ tells us where the particle is, $\Psi = 0$ means no particle at all[15].

While in the classical physics case we could have zero energy states, corresponding to the particle standing still somewhere between 0 and L, this is not possible in Quantum Mechanics. According to **Heisenberg indeterminacy principle**, it is impossible to know the position and velocity of a particle at the same time, and thus it is impossible for a particle to stand still somewhere[16].

(III) $E > 0$, $\frac{2mE}{\hbar^2} = -\lambda^2$
Since we are dealing with a equation that includes a complex term (i in front of ∂_t) it is better to write the solution in complex form

$$X(x) = \overline{A}e^{i\lambda x} + \overline{B}e^{-i\lambda x} \tag{3.52}$$

Anyway, from $X(0) = 0$ we get $B = -A$ or

$$X(x) = A' \sin(\lambda x) \tag{3.53}$$

To have $X(L) = 0$ we require $\lambda L = n\pi$, $n \in \mathbb{N}$ or

$$\lambda = \frac{n\pi}{L} \Rightarrow E = \frac{\lambda^2\hbar^2}{2m} = \frac{n^2\pi^2\hbar^2}{2mL^2} = \frac{n^2h^2}{8mL^2} = n^2E_0 \tag{3.54}$$

[15] This statement will be justified in section 3.3.
[16] Heisenberg's name popped out as a result of Schrödinger's theory... more on this later.

where we defined

$$E_0 = \frac{n^2 h^2}{8mL^2} \tag{3.55}$$

Classically, the particle's energy could assume any value $mv^2/2 \geq 0$, but a quantum particle described by Schrödinger's equation can only assume *discrete* values of the energy, such as

$$E_0, \quad 4E_0, \quad 9E_0, \quad 16E_0, \quad 25E_0, \text{ etc.} \tag{3.56}$$

3.2.4 General solution

Eq. (3.53) may be written as (refer to eq. 2.84)

$$X(x) = A' \sin\left(\frac{n\pi}{L}x\right) = A s_n^L(x) \tag{3.57}$$

so that a general solution may be written as

$$\Psi(x,t) = \sum_{n=0}^{\infty} A_n e^{-i\frac{E_n}{\hbar}t} s_n^L(x) \tag{3.58}$$

with

$$A_n = \int_0^L s_n^L(x)\Psi(0,t)dx \tag{3.59}$$

Since the functions s_n^L represent the solutions of the time independent equation corresponding to the energy E_n, we will call them also ψ_{E_n} and write the general solution as

$$\Psi(x,t) = \sum_{n=0}^{\infty} A_n e^{-i\frac{E_n}{\hbar}t} \psi_{E_n}(x) \tag{3.60}$$

But, what does this mean?

3.3 The Philosophy of Quantum Mechanics

What Schrödinger actually did in the days spent on the Alps with (one of) his mistress(es) was to compute the possible energy states of the hydrogen atom. As we will see in a following chapter, also these states can assume only discrete values[17]. That energies of electrons in atoms assume discrete values was well know by experiments. The Danish physicist Niels Bohr had proposed in 1912 a model, that was based on some ad hoc assumptions following Planck quantum hypothesis, that constrained electrons to move only

[17] From this discreteness comes the name quantum. *Quantum* is the Latin for *how much*, and it is related to the English *quantity*.

on some specific orbits, and could explain the energies of some atoms[18]. But now Schrödinger was able to derive the same results from a completely consistent model, and had written an equation to derive the energy of an electron in any physical problem, just by knowing the potential U. Furthermore, he was able to derive Heisenberg's theory from his own, showing, he believed, that there was no need of such a theory with its philosophical implications. For his work on Wave Mechanics[19] he received the 1933 Nobel prize.

But he still had to provide an interpretation for his *wave function* Ψ. The wave function is a complex function, and cannot be directly observed. One can nevertheless define a real quantity from it

$$\rho(t, \mathbf{x}) = \Psi^*(t, \mathbf{x})\Psi(t, \mathbf{x}) \tag{3.61}$$

Other real quantities could obviously be defined, such as $\mathrm{Re}\Psi$ and $\mathrm{Im}\Psi$. Nevertheless, the quantity defined in eq. (3.61) satisfies a conservation law similar to eq. (1.99), and thus leads to Schrödinger's interpretation of it as "a particle density".

This interpretation soon showed to have a few conceptual problems[20]. In 1926, Max Born suggested that ρ, if better defined as

$$\rho(t, \mathbf{x}) = \frac{\Psi^*(t, \mathbf{x})\Psi(t, \mathbf{x})}{\int_V \Psi^*(t, \mathbf{x})\Psi(t, \mathbf{x})d\mathbf{x}} \tag{3.62}$$

so that its integral over all space V is one, ρ gives the *probability* of finding a particle in $\mathbf{x}$. The quantum world is no more *deterministic*, as the classical one, in which the initial state (position and velocity) determines all the evolution of the system. Schrödinger equations are still deterministic regarding the evolution of Ψ, but when an experiment is performed, the result of the experiment is probabilistic[21].

This framework is very general. The British physicist Paul Dirac, who shared the 1933 Nobel Prize with Schrödinger, showed that both wave and matrix mechanics may be derived from a more general formalism. Let us consider for example a de Broglie wave, eq. (3.27). If we apply the operator $\hat{p}$ to it, we obtain

$$\hat{p}\Psi = p\Psi \tag{3.63}$$

But if we apply it to eq. (3.53) we get

$$\hat{p}\Psi = -i\hbar\partial_x \sin\left(\frac{n\pi}{L}x\right) = -i\hbar\frac{n\pi}{L}\cos\left(\frac{n\pi}{L}x\right) \tag{3.64}$$

[18] Bohr won the 1922 Nobel Prize for this model.

[19] Quantum Mechanics using Schrödinger's formalism.

[20] E.g., when used to describe more than a particle.

[21] The dimensionality of Ψ is, in D dimensions, $[\Psi] = [L]^{-D/2}$. Why?

The operator $\hat{p}$ has no more the effect of multiplying Ψ by a number, so that the physical state has no defined momentum. What will be the result of an experiment? From eq. (3.49) we see that the sine is the sum of two terms that have a specified momentum , each of them with a different sign. An experiment that measures the momentum of the particle in a state of given energy will give one of these two values, each one with probability 1/2. If the experiment measures the position, it will give a value between 0 and L with probability proportional to $\sin^2(\frac{n\pi}{L}x)$. When we have the general solution eq. (3.60), that includes many different energies, the probability of an experiment to give a given energy is

$$p_{E_n} = \frac{A_n^* A_n}{\sum_n A_n^* A_n} \tag{3.65}$$

Macroscopic objects are composed of many particles, whose dynamics is described by Quantum Mechanics. So Quantum Mechanics should be more fundamental than Classical Mechanics, and should be applied to any object. The reason we do not realise the weird quantum behaviour in our everyday life is related to the small value of h. The minimum energy of a particle in a trap is discrete,

$$E_0 = \frac{n^2 h^2}{8mL^2} \tag{3.66}$$

If we use as mass the electron mass, of order 10^{-31} Kg, and as $L = 10^{-10}$ m, comparable to the size of an atom, we get $E_0 \approx 10^{-17}$ J. This is a relevant energy for an electron, that has an electrostatic energy of $\approx 10^{-19}$ J when in a field of 1 V. But if we consider a ball of 1 Kg moving in a trap of 1 m, we get $E_0 \approx 10^{-67}$, which is basically zero from a macroscopic point of view, so that the energy appears to be continuum.

The standard interpretation of Quantum Mechanics has been developed by Niels Bohr's group (including Heisenberg). It makes a distinction between the mathematical structure of the wave equation, and the results of experiments. Only the latter are observable, and questions about what happens to the particle before the experiment result are meaningless. The predictions of Quantum Mechanics are in perfect agreement with the experiments, that are the only thing that may be tested.

This interpretation baffled Schrödinger (and Einstein). Also the experimental equipment, and the experimenter themselves, are composed of particles. How can we make the distinction between Quantum and not Quantum? Schrödinger came out with this example. A nucleus may be in different energy states. The passage between two different states (two ψ_E) corresponds to the emission of radiation. Observing the emission of radiation is an experiment, and has a probabilistic outcome. Now, says Schrödinger, let us

connect a mechanism to the emission of radiation, and let us have this mechanism kill a cat closed in a box with the atom and mechanism, in case the atom decays. Our experimental result is the cat being dead or alive. According to Schrödinger, if Bohr's interpretation is correct, we should have a quantum function describing the whole system, and thus the cat being both alive and dead, until we open the box[22].

The predictions of Quantum Mechanics are very reliable. So reliable that in general for long time many physicists adopted a "compute and shut up" approach, i.e. they ignored philosophical questions, leaving them to people like Einstein, Schrödinger, Bohr and other Nobel prizes that did not need to care too much about how they used their time since they already obtained so much[23]. Nevertheless, physicists have come to apply Quantum Mechanics outside the realm of atoms and nuclei (for example, to study the whole universe) so that questions such as "what happens before the experiment is performed" became quite relevant. The philosophical debate is not over.

3.4 Getting rid of $\hbar$

To get a clear idea of what our results imply, we worked using the original variables t and x with dimensions of time and length. Nevertheless, many physicists, in particular theoretical physicists, like to work in a unit system in which $\hbar = 1$. This not only allows them to get rid of $\hbar$ in their expressions, but introduces also a "natural" unit system, i.e. a system based not on human conventions but on Nature's rules[24].

Let us write the 1D Schrödinger equation

$$i\hbar\partial_t\Psi(t,\mathbf{x}) = -\frac{\hbar^2}{2m}\partial_x^2\Psi(t,x) + U(\mathbf{x})\Psi(t,x) \tag{3.67}$$

[22] In his words, *One can even set up quite ridiculous cases. A cat is penned up in a steel chamber, along with the following device (which must be secured against direct interference by the cat): in a Geiger counter, there is a tiny bit of radioactive substance, so small, that perhaps in the course of the hour one of the atoms decays, but also, with equal probability, perhaps none; if it happens, the counter tube discharges and through a relay releases a hammer that shatters a small flask of hydrocyanic acid. If one has left this entire system to itself for an hour, one would say that the cat still lives if meanwhile no atom has decayed. The psi-function of the entire system would express this by having in it the living and dead cat (pardon the expression) mixed or smeared out in equal parts.*

[23] And in general, this approach went in favour of Bohr's school of thinking that you shouldn't ask yourself what happens in the microscopic system.

[24] Since it uses a universal constant as a unit measure. In an equivalent way, the velocity of light c is usually fixed to one (this accounts to measure distances in time, as for the celebrated "light year")

and perform the change

$$t' = \frac{t}{\hbar} \Rightarrow \partial_t = \frac{1}{\hbar}\partial_{t'} \tag{3.68}$$

$$x' = \frac{x}{\hbar} \Rightarrow \partial_x = \frac{1}{\hbar}\partial_{x'} \tag{3.69}$$

The equation in the new variables becomes

$$i\partial_{t'}\Psi(t', x') = -\frac{1}{2m}\partial^2_{x'}\Psi(t', x') + U(x')\Psi(t', x') \tag{3.70}$$

i.e. we got rid of $\hbar$. To better understand how this happened, let us remember (eq. 3.2) that $\hbar$ had the dimensionality of an action, i.e. energy multiplied by time. Actions are extremely important in physics, since it may be shown that a classical (i.e., not quantum) particle moves on a trajectory that minimises[25] a quantity S, called indeed action, with the dimension of energy multiplied by time.

If we define a quantity S', given by an energy multiplied by time *in the new scaled coordinates*, we have that

$$[S'] = [M][L']^2[T']^{-2}[T'] = [M][L']^2[T']^{-1} = [M][L]^2[\hbar]^{-2}[T]^{-1}[\hbar] = [S][\hbar]^{-1} = [*]^0 \tag{3.71}$$

This equation tells us two things

1. The new action is a-dimensional (the $[*]^0$ term)
2. Its value is given in units of $\hbar$ (the $[S][\hbar]^{-1}$ term)

Indeed our change of coordinates introduces a "natural" system in which actions are counted as multiples of $\hbar$.

By working in such a system, we would have found, for the energy of the system

$$E'_n = n^2 E'_0 \tag{3.72}$$

with

$$E'_0 = \frac{\pi^2}{2mL'^2} \tag{3.73}$$

How can we regain from this expression the one including the $\hbar$ factors?

One way of doing it is to notice that

$$L' = \frac{L}{\hbar} \tag{3.74}$$

[25] Actually extremises.

and substitute. But in some situations, we may not have such a simple expression. A more general approach is to write

$$E_0 = \frac{\pi^2}{8mL^2}\hbar^k \tag{3.75}$$

and determine k by dimensional analysis

$$[M][L]^2[T]^{-2} = [E_0] = [E]^k[T]^k[L]^{-2}[M]^{-1} = [M]^{k-1}L^{2k-2}[T]^{-k} \tag{3.76}$$

that implies $k = 2$.

3.5 The particle in a 3D box

Let us solve our first 3D problem, by asking our particle to be trapped inside a 3D box. We have

$$U(\mathbf{x}) = 0 \text{ for } x \in [0, L_x] \text{ and } y \in [0, L_y] \text{ and } z \in [0, L_z] \tag{3.77}$$

and

$$\Psi(t, 0, y, z) = \Psi(t, L_x, y, z) = \Psi(t, 0, x, y) = \Psi(t, x, L_y, z) = \Psi(t, x, y, 0) = \Psi(t, x, y, L_z) = 0 \tag{3.78}$$

Let us use the separation of variables technique by asking

$$\Psi(t, x, y, z) = T(t)X(x)Y(y)Z(z) \tag{3.79}$$

so that the Schrödinger equation becomes

$$X(x)Y(y)Z(z)(i\hbar\partial_t T(t)) = \\ -\frac{\hbar^2}{2m}\Big(T(t)Y(y)Z(z)\partial_x^2 X(x) + T(t)X(x)Z(z)\partial_y^2 Y(y) + T(t)X(x)Y(y)\partial_z^2 Z(z)\Big) \tag{3.80}$$

we divide by Ψ and obtain as usual[26]

$$\frac{i\hbar\partial_t T(t)}{T(t)} = E = -\frac{\hbar^2}{2m}\left(\frac{\partial_x^2 X(x)}{X(x)} + \frac{\partial_x^2 Y(y)}{Y(y)} + \frac{\partial_x^2 Z(z)}{Z(z)}\right) \tag{3.81}$$

As we stated above, provided that U is time independent, the solution of the time function is always

$$T(t) = A' e^{-i\frac{E}{\hbar}t} \tag{3.82}$$

[26] Since the two sides of the equal are functions of unrelated variables.

To solve the time independent equation that gives the physical state (wave function) corresponding to the energy E we write

$$E + \frac{\hbar^2}{2m}\frac{\partial_x^2 Z(z)}{Z(z)} = -\frac{\hbar^2}{2m}\left(\frac{\partial_x^2 X(x)}{X(x)} + \frac{\partial_x^2 Y(y)}{Y(y)}\right) \tag{3.83}$$

Now, the two sides of the equality are functions of unrelated variables, and they have to be constant. We name such constant E_{xy}. We have

$$-\frac{\hbar^2}{2m}\frac{\partial_x^2 Z(z)}{Z(z)} = E - E_{xy} \equiv E_z \tag{3.84}$$

We already solved this equation in the 1D case. We get $E_z > 0$,

$$E_z = n_z^2 E_0^z, \qquad E_0^z = \frac{h^2}{8mL_z^2} \tag{3.85}$$

with $n_z \in \mathbb{N}$, and[27]

$$Z(z) = s_{n_z}^{L_z}(z) \tag{3.86}$$

We proceed in the same way and get from

$$E_{xy} = -\frac{\hbar^2}{2m}\left(\frac{\partial_x^2 X(x)}{X(x)} + \frac{\partial_x^2 Y(y)}{Y(y)}\right) \tag{3.87}$$

the equation

$$E_{xy} + \frac{\hbar^2}{2m}\frac{\partial_x^2 Y(y)}{Y(y)} = E_x = -\frac{\hbar^2}{2m}\frac{\partial_x^2 X(x)}{X(x)} \tag{3.88}$$

and, solving for X

$$E_x = n_x^2 E_0^x, \qquad E_0^x = \frac{h^2}{8mL_x^2} \tag{3.89}$$

with $n_x \in \mathbb{N}$, and

$$X(x) = s_{n_x}^{L_x}(x) \tag{3.90}$$

Finally, from

$$-\frac{\hbar^2}{2m}\frac{\partial_x^2 Y(y)}{Y(y)} = E_{xy} - E_x \equiv E_y \tag{3.91}$$

we get

$$E_y = n_y^2 E_0^y, \qquad E_0^y = \frac{h^2}{8mL_y^2} \tag{3.92}$$

with $n_y \in \mathbb{N}$, and

$$Y(y) = s_{n_y}^{L_y}(y) \tag{3.93}$$

[27] We do not write the multiplicative constant. It is usual in Quantum mechanics to use functions that have integral of their square modulus equal to 1, as our s functions are, due to the probabilitic interpretation eq. (3.62).

Clearly, from our definitions we have

$$E = E_x + E_y + E_z = n_x^2 E_0^x + n_y^2 E_0^y + n_z^2 E_0^z \tag{3.94}$$

where the n are *positive* integers. For a cube, it simplifies to

$$E = n^2 E_0, \quad n^2 = n_x^2 + n_y^2 + n_z^2 \tag{3.95}$$

The general solution[28] is

$$\Psi(t,x,y,z) = \sum_{n_x=1}^{\infty}\sum_{n_y=1}^{\infty}\sum_{n_z=1}^{\infty} A_{n_x,n_y,n_z} e^{-i\frac{n_x^2 E_0^x + n_y^2 E_0^y + n_z^2 E_0^z}{\hbar}t} s_{n_x}^{L_x}(x) s_{n_y}^{L_y}(y) s_{n_z}^{L_z}(z) \tag{3.96}$$

with

$$A_{n_x,n_y,n_z} = \int_0^{L_x} dx \int_0^{L_y} dy \int_0^{L_z} dz \Big(\Psi(0,x,y,z) s_{n_x}^{L_x}(x) s_{n_y}^{L_y}(y) s_{n_z}^{L_z}(z) \Big) \tag{3.97}$$

[28]The process of obtaining a general solution from the products of particular solutions in the different variables is described in more detail for the 2D membrane in 4.2.

Chapter 4

Vibrating membrane

4.1 The wave equation

An important differential equation is the previously mentioned *wave equation*, that describes the propagation of light or the propagation of a signal ("vibration") in a medium[1]

$$\partial_t^2 \Phi(t, \mathbf{x}) = c^2 \nabla^2 \Phi(t, \mathbf{x}) \tag{4.1}$$

4.1.1 A "deduction"

We now present an argument that should convince that eq. (4.1) correctly describes the basic features of the propagation of a vibration or signal in a medium, and that will help in understanding the basic features of wave dynamics.

Let us consider the dynamical system of Fig. 4.1. Here we have $n+1$ beads located at positions $x = 0, a, \ldots, ia, \ldots, na$, connected by springs and moving vertically on some frictionless poles. The vertical position of each bead as a function of time is given by $\Phi_i(t)$. Assuming all springs to have elastic constant k, the beads to have mass m, and springs to have 0 rest length, and recalling the Hooke law relating the recall force to the extension of a spring

$$m \frac{d^2 x(t)}{dt^2} = -kx(t) \tag{4.2}$$

[1]The wave equation has been developed initially to describe the propagation of a signal or vibration, and this led 19th century physicists to think about light as the vibration of some kind of medium, called aether. The position of modern physicists is basically the opposite, since nowadays we believe electromagnetic forces to be more fundamental than the vibration of any medium, being the cause of forces between atoms and molecules.

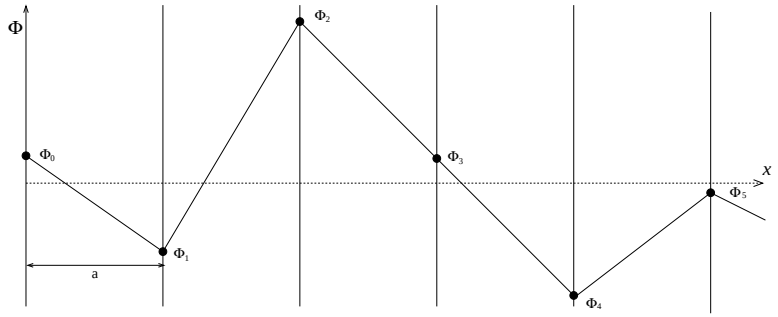

Figure 4.1: A system of beads as a model for a vibrating string.

we may write

$$\frac{d^2\Phi_i(t)}{dt^2} = -\frac{k}{m}\left[(\Phi_i(t) - \Phi_{i-1}(t)) + (\Phi_i(t) - \Phi_{i+1}(t))\right] \tag{4.3}$$

since the dynamics of $\Phi_i(t)$ will depend on the displacement with respect to its neighbours. We re-write it as

$$\frac{d^2\Phi_i(t)}{dt^2} = \frac{k}{m}\left(\Phi_{i+1}(t) - 2\Phi_i(t) + \Phi_{i-1}(t)\right) \tag{4.4}$$

Now, let us consider our system of beads and springs as the model for a continuous string. We send the distance $a \to 0$ and assume we may measure the vertical displacement as a continuous function of x. Namely, remembering that Φ_i corresponds to position ia we define

$$\Phi_i(t) = \Phi(t, ia) \to \Phi(t, x) \tag{4.5}$$

Before sending $a \to 0$, we re-write again our equation as

$$\frac{d^2\Phi(t, ia)}{dt^2} = \frac{k}{m}\left(\Phi(t, (i+1)a) - 2\Phi(t, ia) + \Phi(t, (i-1)a)\right) \tag{4.6}$$

We now use a Taylor expansion for the term in parentheses

$$\begin{aligned}
&\Phi(t, (i+1)a) - 2\Phi(t, ia) + \Phi(t, (i-1)a) = \\
&\Phi(t, ia) + a\partial_x\Phi(t, ia) + \frac{a^2}{2}\partial_x^2\Phi(t, ia) - 2\Phi(t, ia) + \Phi(t, ia) - a\partial_x\Phi(t, ia) + \frac{a^2}{2}\partial_x^2\Phi(t, ia) \\
&+ O(a^3) = a^2\partial_x^2\Phi(t, ia) + O(a^3)
\end{aligned} \tag{4.7}$$

If we now assume that the following quantity has a finite limit for $a \to 0$

$$\lim_{a\to 0}\frac{ka^2}{m} = c^2 \tag{4.8}$$

we obtain performing the limit

$$\partial_t^2 \Phi(t,x) = c\partial_x^2 \Phi(t,x) \tag{4.9}$$

A simple dimensional analysis shows that the expression in eq. (4.8) is indeed a squared velocity. From eq. (4.2) we have

$$[M][L][T]^{-2} = [k][L] \Rightarrow [k] = [M][T]^{-2} \tag{4.10}$$

and thus

$$[c] = [M][T]^{-2}[L]^2[M]^{-1} = [L]^2[T]^{-2} \tag{4.11}$$

Physical meaning

It should be very easy to understand why the second derivative emerges on the left side, by comparing the force acting on Φ_2 and Φ_3 in Fig. 4.1. In Φ_3 we have a high (negative) value of $\partial_x \Phi$, but this results in a balance in the force acting on the bead. On the other hand, in Φ_2 we have a change in the derivative, and a resulting force on the bead. It is in the positions in which the string is convex or concave (non zero second derivative) that we have a strong recall function.

Our simple model should also show clearly the nature of the wave (signal, vibration) propagation. We forced our beads not to move in the x direction, but the interaction between beads causes a signal (the displacement Φ) to propagate in x and t.

4.1.2 From string to membrane

It's not hard to generalise to a 2D membrane[2]. We start again with a grid of beads moving on frictionless poles. Now the vertical position of each bead is $\Phi_{i,j}(t)$. Each bead is connected to 4 other beads, its first neighbours in x and y (Fig. 4.2).

Now we get

$$\begin{aligned}\frac{d^2\Phi_{i,j}(t)}{dt^2} =& -\frac{k}{m}\Big[(\Phi_{i,j}(t) - \Phi_{i-1,j}(t)) + (\Phi_{i,j}(t) - \Phi_{i+1,j}(t)) \\ &+ (\Phi_{i,j}(t) - \Phi_{i,j-1}(t)) + (\Phi_{i,j}(t) - \Phi_{i,j+1}(t)) \Big] \\ =& \frac{ka^2}{m}\left[\frac{\Phi_{i+1,j}(t) - 2\Phi_{i,j}(t) + \Phi_{i-1,j}(t)}{a^2} + \frac{\Phi_{i,j+1}(t) - 2\Phi_{i,j}(t) + \Phi_{i,j-1}(t)}{a^2} \right]\end{aligned} \tag{4.12}$$

[2]The proposed models are extremely simplified but they are very easy to handle and describe the basic physics of the problem.

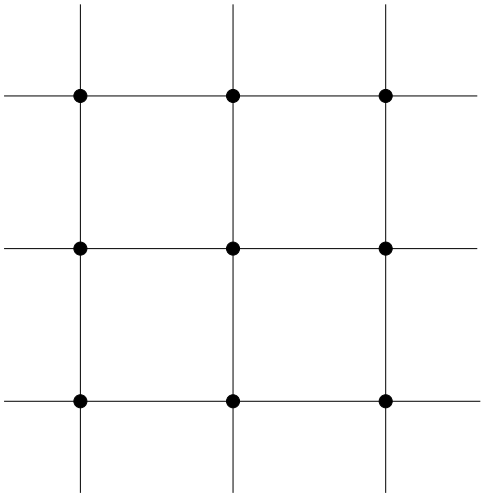

Figure 4.2: A system of beads as a model for a vibrating membrane.

and, in the $a \to 0$ limit

$$\partial_t^2 \Phi(t,x,y) = c^2 \left(\partial_x^2 \Phi(t,x,y) + \partial_y^2 \Phi(t,x,y) \right) \tag{4.13}$$

4.1.3 Getting rid of c

The velocity of light is the same in any inertial frame. Since nature provided us with such a universal constant, theoretical physicists like to measure their distances in seconds. For example, they would say that 1 meter is the distance that light travels in $(3 \cdot 10^8)^{-1}$ seconds.

Actually, you will never hear a theoretical physicists saying something like that. They will state that they use a system in which $c = 1$. Let us see why. Measuring distances as we just stated is equal to make a change of variables

$$\begin{aligned} x' = \frac{x}{c} \Rightarrow \partial_x \Phi = \frac{\partial \Phi}{\partial x} = \frac{\partial \Phi}{\partial x'} \frac{\partial x'}{\partial x} = \frac{1}{c} \partial_{x'} \Phi \\ \Rightarrow \partial_x^2 \Phi = \frac{1}{c} \partial_{x'} \left(\frac{1}{c} \partial_{x'} \Phi \right) \end{aligned} \tag{4.14}$$

so that in the new variables the wave equation becomes

$$\partial_t^2 \Phi(t,x) = \partial_x^2 \Phi(t,x) \tag{4.15}$$

The dimensional terms including c may be recovered at the end of computations with the same methods used for $\hbar$ in section 3.4.

Actually, in theoretical physics the change of variables

$$t' = ct, \tag{4.16}$$

(leaving $\mathbf{x}$ unchanged) is preferred. You may check that this change of variables removes c from eq. (4.1).

4.2 Separation of variables in the vibrating membrane problem

Let us suppose we have a vibrating membrane of size L_x, L_y, with the boundary conditions

$$\Phi(t, 0, y) = \Phi(t, L_x, y) = \Phi(t, x, 0) = \Phi(t, x, L_y) = 0 \tag{4.17}$$

namely the membrane is clamped on the boundary.

We proceed as usual, due to the linearity of the equation and the homogeneous conditions,

$$\Phi(t, x, y) = T(t)X(x)Y(y) \tag{4.18}$$

and obtain

$$c^2 \left(\frac{\partial_x^2 X(x)}{X(x)} + \frac{\partial_y^2 Y(y)}{Y(y)} \right) = K = \frac{\partial_t^2 T(t)}{T(t)} \tag{4.19}$$

Let us focus first on the left side, that we rewrite as

$$\frac{\partial_x^2 X(x)}{X(x)} = \frac{K}{c^2} - \frac{\partial_y^2 Y(y)}{Y(y)} \equiv K_x \tag{4.20}$$

The last step is obtained as usual noticing that we have an equality between functions of unrelated variables. We write also

$$\frac{\partial_y^2 Y(y)}{Y(y)} = \frac{K}{c^2} - K_x \equiv K_y \tag{4.21}$$

We should be familiar enough with these equations to write the conditions for K_x, K_y,

$$K_x = -\frac{n_x^2 \pi^2}{L_x^2}, \quad K_y = -\frac{n_y^2 \pi^2}{L_y^2}, \quad n_x, n_y \in \mathbb{N} \tag{4.22}$$

to which correspond the solutions

$$X_{n_x}(x) = A_{n_x} s_{n_x}^{L_x}(x), \qquad A_{n_y} Y_{n_y}(y) = s_{n_y}^{L_y}(y) \tag{4.23}$$

The product

$$A_{n_x} A_{n_y} s^{L_y}_{n_x}(x) s^{L_y}_{n_y}(y) \equiv \overline{A}_{n_x,n_y} s^{L_x}_{n_x}(x) s^{L_y}_{n_y}(y) \equiv \overline{A}_{n_x,n_y} s^{L_x,L_y}_{n_x,n_y}(x,y) \quad (4.24)$$

is thus a solution of eq. 4.19 with

$$K = -c^2 \left(\frac{n_x^2 \pi^2}{L_x^2} + \frac{n_y^2 \pi^2}{L_y^2} \right) = -\omega^2_{n_x,n_y} \quad (4.25)$$

The time equation becomes

$$\partial_t^2 T(t) = -\omega^2_{n_x,n_y} T(t) \quad (4.26)$$

Its (real) solutions are in the form

$$T_{n_x,n_y}(t) = A \sin(\omega_{n_x,n_y} t) + B \cos(\omega_{n_x,n_y} t) \quad (4.27)$$

By multiplying with eq. (4.24), and re-defining

$$A_{n_x,n_y} = A\overline{A}_{n_x,n_y}, \qquad B_{n_x,n_y} = B\overline{B}_{n_x,n_y} \quad (4.28)$$

we obtain the particular solution

$$A_{n_x,n_y} \sin(\omega_{n_x,n_y} t) s^{L_x,L_y}_{n_x,n_y}(x,y) + B_{n_x,n_y} \cos(\omega_{n_x,n_y} t) s^{L_x,L_y}_{n_x,n_y}(x,y) \quad (4.29)$$

where we should remember that ω is given by eq. (4.25). The general solution is thus

$$\Phi(t,x,y) = \sum_{n_x=1}^{\infty} \sum_{n_y=1}^{\infty} A_{n_x,n_y} \sin(\omega_{n_x,n_y} t) s^{L_x,L_y}_{n_x,n_y}(x,y) + B_{n_x,n_y} \cos(\omega_{n_x,n_y} t) s^{L_x,L_y}_{n_x,n_y}(x,y) \quad (4.30)$$

We have

$$\Phi(0,x,y) = \sum_{n_x=1}^{\infty} \sum_{n_y=1}^{\infty} B_{n_x,n_y} s^{L_x,L_y}_{n_x,n_y}(x,y) \quad (4.31)$$

We will assume that this Fourier series may express any physical initial condition $\Phi_0(x,t)$. We notice that

$$\begin{aligned} &\int_0^{L_x} dx \int_0^{L_y} dx \left(s^{L_x,L_y}_{n_x,n_y}(x,y) s^{L_x,L_y}_{m_x,m_y}(x,y) \right) = \\ &\left(\int_0^{L_x} s^{L_x}_{n_x}(x) s^{L_x}_{m_x}(x) dx \right) \left(\int_0^{L_y} s^{L_x}_{n_y}(y) s^{L_x}_{m_x}(y) dy \right) \\ &= \delta_{n_x,m_x} \delta_{n_y,m_y} \end{aligned} \quad (4.32)$$

so that

$$B_{n_x,n_y} = \int_0^{L_x} dx \int_0^{L_y} dy \left(\Phi_0(x,t) s^{L_x,L_y}_{n_x,n_y}(x,y) \right) \quad (4.33)$$

These results tell us that the initial condition $\Phi_0(x,t)$ cannot completely specify the solution, since it provides no information on the constants A_{n_x,n_y}. Let us then compute

$$\partial_t\Phi(t,x,y) = \sum_{n_x=1}^{\infty}\sum_{n_y=1}^{\infty}\omega_{n_x,n_y}\left[A_{n_x,n_y}\cos(\omega_{n_x,n_y}t)s^{L_x,L_y}_{n_x,n_y}(x,y) - B_{n_x,n_y}\sin(\omega_{n_x,n_y}t)s^{L_x,L_y}_{n_x,n_y}(x,y)\right] \tag{4.34}$$

and

$$\partial_t\Phi(0,x,y) = \sum_{n_x=1}^{\infty}\sum_{n_y=1}^{\infty}\omega_{n_x,n_y}A_{n_x,n_y}s^{L_x,L_y}_{n_x,n_y}(x,y) \tag{4.35}$$

If now if we know also the initial time derivative $\partial_t\Phi(0,x,y) = \dot{\Phi}_0(x,t)$ we may obtain the constants A_{n_x,n_y} through

$$A_{n_x,n_y} = \frac{1}{\omega_{n_x,n_y}}\int_0^{L_x}dx\int_0^{L_y}dy\left(\dot{\Phi}_0(x,t)s^{L_x,L_y}_{n_x,n_y}(x,y)\right) \tag{4.36}$$

and completely specify the solution of our problem.

Chapter 5

Laplace equation

5.1 Introduction

When we consider the stationary, i.e. time independent, versions of the heat or wave equation, we obtain the Laplace equation

$$\nabla^2 \Phi = 0 \tag{5.1}$$

5.1.1 Electrostatics

This equation is extremely important in many physical problems, and in particular in electrostatics, i.e. in the study of electric fields produced by non moving[1] charges.

One of Maxwell equations of Electromagnetism reads as

$$\mathrm{div}\mathbf{E}(t, \mathbf{x}) = k_E \, \rho(t, \mathbf{x}) \tag{5.2}$$

where $\mathbf{E}$ is the electric field, ρ the electric charge, and k_E is a constant that *depends on the choice of the unit system.*

Furthermore, *for stationary electric and magnetic fields* it is possible to obtain the electric field from a potential[2]

$$\mathbf{E}(\mathbf{x}) = -\boldsymbol{\nabla}\Phi(\mathbf{x}) \tag{5.3}$$

[1] Also charges moving at constant velocities can be described using electrostatics, but they generate also a magnetic field.

[2] Maxwell equations relate magnetic and electric fields. Nevertheless, the the equations can be separated in equations for the electric field and equations for the magnetic field under stationary conditions, since the terms that couple the two fields involve time derivatives.

so that, putting the two equations together, we get

$$k_E\,\rho(\mathbf{x}) = \mathrm{div}\mathbf{E}(\mathbf{x}) = \mathrm{div}\,(-\boldsymbol{\nabla}\Phi(\mathbf{x})) = -\nabla^2\Phi(\mathbf{x}) \Rightarrow \nabla^2\Phi(\mathbf{x}) = -k_E\,\rho(\mathbf{x}) \tag{5.4}$$

Equation (5.4) is called the Poisson equation, and relates the difference between the average value of Φ in a small volume centred in $\mathbf{x}$ to the amount of charge in $\mathbf{x}$ (section 1.5.5)

$$\overline{\Phi}(\mathbf{x}) - \Phi(\mathbf{x}) \propto -\rho(\mathbf{x}) \tag{5.5}$$

In absence of charge (for example in vacuum) the Poisson equation turns into the Laplace one, eq. (5.1).

A "deduction" from Coulomb's law

The law for the force felt by a charge δq in presence of another charge q is, for static charges,

$$\mathbf{F} = \frac{k_E\,\delta q\,q}{4\pi r^2}\mathbf{e}_r \tag{5.6}$$

Different unit systems use different definitions of k_E. Theoreticians prefer to define k_E as a pure number (either 1 or 4 π) so that the dimensionality of q is given by

$$[M][L][T]^{-2} = [q]^2[L]^{-2} \Rightarrow [q] = [M]^{\frac{1}{2}}[L]^{\frac{3}{2}}[T]^{-1} \tag{5.7}$$

while in practical applications a specific dimension for charge is introduced and $k_E = 1/\epsilon_0$ is used.

We define the electric charge by considering δq small enough not to affect the surrounding charges, and by dividing the force by δq so that

$$\mathbf{E} = k_E\frac{q}{4\pi r^2}\mathbf{e}_r \tag{5.8}$$

Let us compute the flux of $\mathbf{E}$ on a surface

$$\int_{S_V}\mathbf{E}\cdot\mathbf{n}\,dS = \int_V \mathrm{div}\mathbf{E}\,dV \tag{5.9}$$

To compute the divergence it is useful to use eq. (1.74)

$$\mathrm{div}\boldsymbol{E}(r,\theta,\varphi) = \frac{k_E q}{4\pi}\frac{1}{r^2}\partial_r[r^2\frac{1}{r^2}] = 0 \tag{5.10}$$

This equation is computed using spherical coordinates and placing the origin of the coordinate system on the particle's position. Nevertheless, since we defined the divergence in a geometrical way, the result is valid regardless

of our choice of the coordinate system. As a result, the flux of the electric field is zero through every surface **that does not include the charged particle.**

The last remark is extremely important, since the spherical coordinate system fails on the origin (zero Jacobian) which is exactly the place where the field diverges, and thus the above computation does not apply there. How can we deal with surfaces that include the charge?

It is very easy to compute the flux on a spherical surface centred on the charge of radius R

$$\int_{S_V} \mathbf{E}\cdot\mathbf{n}\,dS = k_E \frac{q}{4\pi}\int_0^{\pi} d\theta \int_0^{2\pi} d\varphi\, R^2 \frac{1}{R^2} = k_E\, q \tag{5.11}$$

We may now compute the flux through any surface as the sum of the fluxes through two surfaces: a spherical one centred on the charge, plus the surface that limits a volume given by the original total volume *minus* the ball delimited by the spherical surface. The sum of these two fluxes gives the wanted results, since the terms on the spherical surface get opposite signs (Fig. 5.1).

$$\int_{S-\text{ball}} \mathbf{E}\cdot\mathbf{n}\,dS = \int_S \mathbf{E}\cdot\mathbf{n}\,dS + \int_{\text{ball}} \mathbf{E}\cdot(-\mathbf{e}_r)dS \Rightarrow \int_{S-\text{ball}} \mathbf{E}\cdot\mathbf{n}\,dS + \int_{\text{ball}} \mathbf{E}\cdot\mathbf{n}\,dS =$$
$$\int_S \mathbf{E}\cdot\mathbf{n}\,dS + \int_{\text{ball}} \mathbf{E}\cdot(\mathbf{e}_r)dS - \int_{\text{ball}} \mathbf{E}\cdot(\mathbf{e}_r)dS = \int_S \mathbf{E}\cdot\mathbf{n}\,dS \tag{5.12}$$

We may conclude that the flux through a surface is $k_E\, q$ if the surface includes the charge, and 0 if it does not.

An important principle of electrodynamics is that **the field generated by a system of charges is the sum of the fields generated by the single charges**. This, together with the linearity of integration, allows us to write for a system of charges

$$\int_{S_V} \mathbf{E}\cdot\mathbf{n}\,dS = \sum_{q_i \text{ in } V} k_E\, q_i \tag{5.13}$$

Let us now assume to have a continuous distribution of charges $\rho(\mathbf{x})$, so that

$$\sum_{q_i \text{ in } V} q_i = \int_V \rho(\mathbf{x})dV \tag{5.14}$$

Using Gauss theorem we get

$$\int_V \text{div}\mathbf{E}\,dV = \int_{S_V} \mathbf{E}\cdot\mathbf{n}\,dS = \sum_{q_i \text{ in } V} k_E\, q_i = \int_V \rho(\mathbf{x})dV \tag{5.15}$$

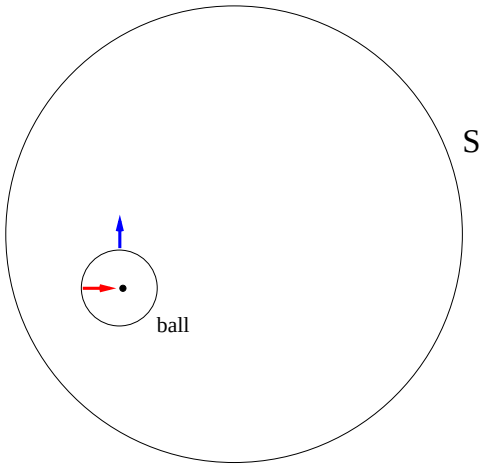

Figure 5.1: The flux through a surface as the sum of the flux on the ball centred on the charge, plus the flux on the surface of the volume excluding the ball. The red arrow shows the outgoing vector $\mathbf{n} = \mathbf{e}_r$ on the ball, while the blue arrow shows the outgoing vector for the surface of the volume excluding the ball, $\mathbf{n} = -\mathbf{e}_r$.

Since this result is true regardless of the choice of the volume, we obtain[3]

$$\text{div}\mathbf{E} = \rho(\mathbf{x}) \tag{5.16}$$

The relation

$$\mathbf{E} = -\boldsymbol{\nabla}\Phi \tag{5.17}$$

for a field in the form (5.6) may be verified by computing the gradient of

$$\Phi(\mathbf{x}) = \frac{k_E q}{4\pi r} \tag{5.18}$$

Substitution in eq. (1.42) gives the wanted result[4].

5.1.2 Unicity of solution for the Lapace equation

Eq. (5.5) becomes

$$\overline{\Phi}(\mathbf{x}) = \Phi(\mathbf{x}) \tag{5.19}$$

[3]Otherwise, we could integrate on a small volume centred in an area in which the equality does not hold.

[4]Electric fields and potentials for continuous charge distributions may be written by first writing sums over charges and then passing to the integral, as shown in any elementary or advance Electrodynamics text.

in absence of charges, i.e. when Lapace's equation holds. This clearly implies that Φ cannot assume a minimum or maximum in a charge free zone[5].

Let assume that we want to solve the Laplace equation in a volume V, and that we know the value of Φ on the boundary of such region. Then the solution is unique.

To show it, let us assume we have two solutions of the Laplace equation, Φ_1 and Φ_2, assuming the same value on the boundary. The function

$$\tilde{\Phi} \equiv \Phi_1 - \Phi_2 \tag{5.20}$$

is then zero on the boundary, and satisfies Laplace's equation

$$\nabla^2\tilde{\Phi} = \nabla^2(\Phi_1 - \Phi_2) = \nabla^2\Phi_1 - \nabla^2\Phi_2 = 0 \tag{5.21}$$

As a result, $\tilde{\Phi}$ cannot assume a maximum inside the volume. But since its value is zero on the boundary, we necessarily have

$$\tilde{\Phi} = 0 \Rightarrow \Phi_1 = \Phi_2 \tag{5.22}$$

and accordingly the solution is unique.

This argument can be used also for the Poisson equation, since the difference $\tilde{\Phi}$ satisfies Laplace equation even in presence of charges,

$$\nabla^2\tilde{\Phi} = \nabla^2(\Phi_1 - \Phi_2) = \nabla^2\Phi_1 + \nabla^2\Phi_2 = k_E\rho - k_E\rho = 0 \tag{5.23}$$

This result is extremely important in physics since it tells us that if we assign a given potential to a set of conductors delimiting a given volume, the value of the potential, and thus of the electric field, will be uniquely determined in the whole volume[6].

We may now proceed to study some solutions of the Laplace equation, using again the separation of variables method.

5.2 2D Laplace equation in a rectangular area

According to the discussion above, providing the value of Φ on the border of a rectangle

$$\begin{aligned} \Phi(0, y) &= f(y) \\ \Phi(L_x, y) &= g(y) \\ \Phi(x, 0) &= h(x) \\ \Phi(x, L_y) &= l(x) \end{aligned} \tag{5.24}$$

[5]If, for example, Φ assumed a maximum in $\mathbf{x}_0$, then there would be an area around such point in which $\Phi(\mathbf{x}) < \Phi(\mathbf{x}_0)\ \forall\mathbf{x}$, so that $\overline{\Phi}(\mathbf{x}) < \Phi(\mathbf{x})$, leading to a contradiction.

[6]This is true also for a non-finite volume, provided that the behaviour at infinity is given as a further boundary condition, as we will see in some examples.

is given, the potential is uniquely determined inside the area.

This is clearly not a homogeneous boundary condition, but we will nevertheless be able to solve it with the separation of variables, though the definition of four sub-problems.

5.2.1 A simpler problem

Let us consider the following simpler problem, i.e. boundary conditions

$$\begin{aligned} &\Phi(0,y) = f(y) \\ &\Phi(L_x,y) = \Phi(x,0) = \Phi(x,L_y) = 0 \end{aligned} \tag{5.25}$$

The conditions are again not homogeneous at $x = 0$, but this is not a problem. As we could handle the initial condition at $t = 0$ through a Fourier series for the heat, wave and Schrödinger equations, we will be able to deal with the $x = 0$ condition in the Laplace problem.

Let us write

$$\Phi(x,y) = X(x)Y(x) \tag{5.26}$$

The Laplace equation implies

$$\frac{\partial_x^2 X(x)}{X(x)} = C = -\frac{\partial_x^2 X(x)}{X(x)} \tag{5.27}$$

We have

$$X(x)Y(0) = X(x)Y(L_y) = 0 \quad \forall x \Rightarrow Y(0) = Y(L_y) = 0 \tag{5.28}$$

from which we get, as usual

$$-C = -\frac{n^2\pi^2}{L_y 2}, \quad n \in \mathbb{N} \Rightarrow C = \frac{n^2\pi^2}{L_y 2} > 0 \tag{5.29}$$

to which corresponds the particular solution

$$Y_n(y) = A_n s_n^{L_y}(y) \tag{5.30}$$

Since C is positive let us define $C = \gamma^2$. We have, regarding the X equation

$$\partial_x^2 X(x) = \gamma^2 X(x) \tag{5.31}$$

whose general solution is

$$X(x) = A\text{sinh}\gamma x + B\text{cosh}\gamma x \tag{5.32}$$

We want $X(x)$ to be zero in $x = L_x$. It is thus easier to define

$$x' = L_x - x \tag{5.33}$$

so that

$$\partial_{x'}^2 X(x') = \gamma^2 X(x') \tag{5.34}$$

and

$$X(x') = A\sinh\gamma x' + B\cosh\gamma x' \tag{5.35}$$

Now we ask

$$X(x' = 0) = 0 \Rightarrow B = 0 \tag{5.36}$$

and obtain the solution

$$X(x') = A\sinh\gamma x' \tag{5.37}$$

or

$$X(x) = A\sinh(\gamma[L_x - x]) \tag{5.38}$$

The general solution of the Laplace equation that assumes 0 in $x = L_x$, $y = 0$, $y = L_y$ is thus

$$\Phi(x, y) = \sum_{n=1}^{\infty} A_n \sinh(\gamma[L_x - x]) s_n^{L_y}(y), \qquad \gamma = \frac{n\pi}{L_y} \tag{5.39}$$

from which we have

$$\Phi(0, y) = \sum_{n=1}^{\infty} A_n \sinh(\gamma L_x) s_n^{L_y}(y) = f(y) \tag{5.40}$$

and finally

$$A_n = \frac{1}{\sinh(\gamma L_x)} \int_0^{L_y} f(y) s_n^{L_y}(y) \tag{5.41}$$

5.2.2 Solution to the full problem

We may use the procedure above to solve the following four problems

$$\nabla^2\Phi_I = 0, \quad \Phi_I(0, y) = f(y), \quad \Phi_I(L_x, y) = \Phi_I(x, 0) = \Phi_I(x, L_y) = 0 \tag{5.42}$$

$$\nabla^2\Phi_{II} = 0, \quad \Phi_{II}(L_x, y) = g(y), \quad \Phi_{II}(0, y) = \Phi_{II}(x, 0) = \Phi_{II}(x, L_y) = 0 \tag{5.43}$$

$$\nabla^2\Phi_{III} = 0, \quad \Phi_{III}(x, 0) = h(x), \quad \Phi_{III}(0, y) = \Phi_{III}(L_x, y) = \Phi_{III}(x, L_y) = 0 \tag{5.44}$$

$$\nabla^2\Phi_{IV} = 0, \quad \Phi_{IV}(x, L_y) = l(x), \quad \Phi_{IV}(0, y) = \Phi_{IV}(L_x, y) = \Phi_{IV}(x, 0) = 0 \tag{5.45}$$

After we found the four solutions, we have obtained the solution to our problem in the form

$$\Phi = \Phi_I + \Phi_{II} + \Phi_{III} + \Phi_{IV} \tag{5.46}$$

Indeed

$$\nabla^2\Phi = \nabla^2\Phi_I + \nabla^2\Phi_{II} + \nabla^2\Phi_{III} + \nabla^2\Phi_{IV} = 0 \tag{5.47}$$

and

$$\begin{aligned}
\Phi(0,y) &= f(y) + 0 + 0 + 0 = f(y) \\
\Phi(L_x,y) &= 0 + g(y) + 0 + 0 = g(y) \\
\Phi(x,0) &= 0 + 0 + h(x) + 0 = h(x) \\
\Phi(x,L_y) &= 0 + 0 + 0 + l(x) = l(x)
\end{aligned} \tag{5.48}$$

5.3 Laplace equation in polar coordinates

Let us assume we want to know the solution of the 2D Laplace inside a circle of radius $\overline{r}$, given the boundary condition on the circle

$$\Phi(\overline{r},\theta) = h(\theta) \tag{5.49}$$

The symmetry of the problem suggests obviously the use of polar coordinates. We recall (eq. 1.82 at fixed z)

$$\nabla^2\Phi(r,\theta) = \frac{1}{r}\partial_r(r\partial_r\Phi(r,\theta)) + \frac{1}{r^2}\partial_\theta^2\Phi(r,\theta) = 0 \tag{5.50}$$

We try to solve the problem again with the method of separation of variables (it will be clear soon why it works) setting

$$\Phi(r,\theta) = \Theta(\theta)R(r) \tag{5.51}$$

We get

$$\Theta(\theta)\frac{1}{r}\partial_r(r\partial_r R(r)) + \frac{R(r)}{r^2}\partial_\theta^2\Theta(\theta) = 0 \tag{5.52}$$

Dividing by Φ we get

$$\frac{1}{rR(r)}\partial_r(r\partial_r R(r)) = -\frac{1}{\Theta(\theta)r^2}\partial_\theta^2\Theta(\theta) \tag{5.53}$$

The variable r still appears on the right, but if we multiply by r^2 we get

$$\frac{r}{R(r)}\partial_r(r\partial_r R(r)) = C = -\frac{1}{\Theta(\theta)}\partial_\theta^2\Theta(\theta) \tag{5.54}$$

The equation for Θ is easier and familiar

$$\partial_\theta^2\Theta(\theta) = -C\Theta(\theta) \tag{5.55}$$

When dealing with the angle θ, the boundary conditions are determined by the need to have

$$\Theta(\theta + 2n\pi) = \Theta(\theta) \tag{5.56}$$

We treated this problem in section 2.2. The particular solutions are

$$\Theta_0(\theta) = \overline{A}_0 c_0^p, \quad C = 0 \tag{5.57}$$

and

$$\Theta_n(\theta) = \overline{A}_n c_n^p(\theta) + \overline{B}_n s_n^p(\theta), \quad C = n^2 \tag{5.58}$$

For each value of n, the radial equation becomes

$$r\partial_r(r\partial_r R_n(r)) = n^2 R_n(r) \tag{5.59}$$

We guess a function in the form $R_n(r) = A' r^\alpha$. From

$$\begin{aligned} \partial_r r^\alpha &= \alpha r^{\alpha-1} \\ r\partial_r r^\alpha &= \alpha r^\alpha \\ \partial_r(r\partial_r r^\alpha) &= \alpha^2 r^{\alpha-1} \\ r\partial_r(r\partial_r r^\alpha) &= \alpha^2 r^\alpha \end{aligned} \tag{5.60}$$

we get

$$A'\alpha^2 r^\alpha = A' n^2 r^\alpha \tag{5.61}$$

so that we we have an identity for $\alpha = \pm n$. We are dealing with a second order differential equation in r, and for $n \neq 0$ we have found a solution depending on two constants

$$R_n(r) = A'_n r^n + B'_n r^{-n} \tag{5.62}$$

For $n = 0$ we found a single solution, $R_0 = A'_0$. Nevertheless, we have

$$r\partial_r\Big[r\partial_r R(r)\Big] = 0 \tag{5.63}$$

so that a solution may be found also by asking that the term in square parentheses is constant, so that

$$r\partial_r R(r) = \text{const} = B'_0 \Rightarrow \partial_r R(r) = \frac{B'_0}{r} \Rightarrow R(r) = B'_0 \ln r \tag{5.64}$$

We thus obtain, by redefining the constants (e.g. $A_n = \overline{A}_n A'_n$, $\tilde{A}_n = \overline{A}_n B'_n$, etc.) the general solution for the problem as

$$\Phi(r,\theta) = (A_0 + \tilde{A}_0 \ln r) c_0^p + \sum_{n=1}^{\infty} \Big(A_n c_n^p(\theta) r^n + \tilde{A}_n c_n^p(\theta) r^{-n} + B_n s_n^p(\theta) r^n + \tilde{B}_n c_n^p(\theta) r^{-n} \Big) \tag{5.65}$$

We obtain at $\overline{r}$

$$\Phi(\overline{r},\theta) = (A_0 + \tilde{A}_0 \ln \overline{r}) c_0^p + \sum_{n=1}^{\infty} \Big(A_n c_n^p(\theta) \overline{r}^n + \tilde{A}_n c_n^p(\theta) \overline{r}^{-n} + B_n s_n^p(\theta) \overline{r}^n + \tilde{B}_n c_n^p(\theta) \overline{r}^{-n} \Big) \tag{5.66}$$

We appear to have a problem, since the general expression for the function $h(\theta)$ giving the boundary condition at $\overline{r}$ is

$$h(\theta) = A_0 c_0^p + \sum_{n=1}^{\infty} \Big(A_n c_n^p(\theta) + B_n s_n^p(\theta) \Big) \tag{5.67}$$

so that the number of constants in eq. (5.66) doubles those of eq. (bcsingle).

This is due to the fact that when we specify the boundary condition for a problem that is defined on an area extending to infinite distance (in opposition to the limited area studied in section 5.2), we need to specify also the behaviour at infinity. Namely, in studying the solution outside the circle, we may ask the potential not to diverge when $r \to \infty$ [7].

Since

$$\lim_{r\to\infty} \ln r = \infty, \qquad \lim_{r\to\infty} r^n = \infty \tag{5.68}$$

we have

$$\tilde{A}_0 = A_n = B_n = 0 \tag{5.69}$$

The general solution outside the circle reads

$$\Phi(r,\theta) = A_0 c_0^p + \sum_{n=1}^{\infty} \Big(\tilde{A}_n c_n^p(\theta) r^{-n} + \tilde{B}_n c_n^p(\theta) r^{-n} \Big) \tag{5.70}$$

with

$$A_0 = \int_0^{2\pi} h(\theta) c_0^p d\theta, \quad \tilde{A}_n = \frac{\int_0^{2\pi} h(\theta) c_n^p(\theta) d\theta}{\overline{r}^{-n}}, \quad \tilde{B}_n = \frac{\int_0^{2\pi} h(\theta) s_n^p(\theta) d\theta}{\overline{r}^{-n}} \tag{5.71}$$

If you read carefully, you probably noticed that this is not the solution that we were seeking, because we wanted to find a solution *inside* the circle! But as we discussed before, the polar coordinate system fails at $r = 0$. This means that the $r = 0$ point has to be treated in a special way, since if we do not treat it carefully the solution would be ill defined in the origin.

To find a solution inside the circle, we ask the potential not to diverge in the origin, and since

$$\lim_{r\to 0} \ln r = -\infty, \qquad \lim_{r\to\infty} r^{-n} = \infty \tag{5.72}$$

we have

$$\tilde{A}_0 = \tilde{A}_n = \tilde{B}_n = 0 \tag{5.73}$$

[7] This is not the only possible condition. For example, a term growing like r in the potential can express a field that behaves as constant at infinity. Although a real physical field will never have this property, such a boundary condition may be useful in solving specific problems (e.g., when the field is constant at distances large when compared to the scale at which we study the problem).

The general solution inside the circle reads

$$\Phi(r,\theta) = A_0 c_0^p + \sum_{n=1}^{\infty} \left(A_n c_n^p(\theta) r^n + B_n c_n^p(\theta) r^n \right) \tag{5.74}$$

with

$$A_0 = \int_0^{2\pi} h(\theta) c_0^p d\theta, \quad A_n = \frac{\int_0^{2\pi} h(\theta) c_n^p(\theta) d\theta}{\overline{r}^n}, \quad B_n = \frac{\int_0^{2\pi} h(\theta) s_n^p(\theta) d\theta}{\overline{r}^n} \tag{5.75}$$

A general solution reads as eq. (5.70) for $r > \overline{r}$, and eq. (5.70) for $r < \overline{r}$. Continuity at $\overline{r}$ is obtained by construction, since both solutions are equal to $h(\theta)$ on the boundary.

Chapter 6

A short introduction to function spaces and Dirac formalism

6.1 Introduction

We have often written the general solution of our partial differential equation as

$$\Phi(t,x) = \sum_{n=1}^{\infty} A_n f_n(t) s_n(x) \tag{6.1}$$

where the time dependent functions $f_n(t)$ are uniquely determined by n. The knowledge of the particular solution implies knowing the A_n, that we obtain from the initial condition $\Phi(0,x) = g(x)$ as

$$A_n = \int g(x) s_n(x)\, dx \tag{6.2}$$

through

$$\int s_m(x) s_n(x)\, dx = \delta_{n,m} \tag{6.3}$$

This procedure should recall us of another mathematical problem. Let us assume we have a symmetric n by n matrix[1], A, such that this matrix admits an orthonormal set of eigenvalues $\mathbf{v}_{\lambda_i}$ which is a basis for the vector

[1] A more general class of matrix, normal matrices, would still have the same properties.

space, i.e. vectors such that

$$\begin{aligned} &A\mathbf{v}_{\lambda_i} = \lambda_i \mathbf{v}_{\lambda_i} \\ &\mathbf{v}_{\lambda_i} \cdot \mathbf{v}_{\lambda_j} = \delta_{i,j} \\ &\mathbf{a} = \sum_{i=1}^{n} \alpha_i \mathbf{v}_{\lambda_i} \quad \forall\, \mathbf{a} \in \mathbb{R}^n \end{aligned} \tag{6.4}$$

A very straightforward way of computing $A\,\mathbf{a}$ is thus

$$A\,\mathbf{a} = A \sum_{i=1}^{n} \alpha_i \mathbf{v}_{\lambda_i} = \sum_{i=1}^{n} \alpha_i A \mathbf{v}_{\lambda_i} = \sum_{i=1}^{n} \alpha_i \lambda_i \mathbf{v}_{\lambda_i} \tag{6.5}$$

In order to know the coefficients α_i, we compute

$$\mathbf{v}_{\lambda_j} \cdot \mathbf{a} = \sum_{i=1}^{n} \alpha_i \mathbf{v}_{\lambda_i} \cdot \mathbf{v}_{\lambda_j} = \sum_{i=1}^{n} \alpha_i \delta_{i,j} = \alpha_j \tag{6.6}$$

The formal analogy should be clear. Both procedures use indeed the properties of vector spaces provided with a scalar product, the main difference being, as it will be clear soon, that in one case the vector space has finite dimension, while in the other case it has infinite dimension. Since this mathematical structure is extremely powerful, we will study its basic principles in this chapter, learning in the process an extremely useful formalism due to the British physicist and Nobel Prize Paul Dirac[2].

6.2 Vector spaces

6.2.1 Basic geometry and physics

Vectors are usually introduced in basic physics trough a graphic representation as arrows connecting two points in 3D space. They have magnitude and direction, may be summed through the parallelogram rule, and multiplied by a number, that scales their magnitude without changing their direction if positive, while scales the magnitude and reverses the orientation if negative.

[2]Whose many contributions include the development of a formalism from which Heisenberg's and Schrödinger's theories may be derived, an equation to describe the dynamics of a relativistic electron, the theoretical prediction of anti-matter, the statistical theory of many electrons (independently developed also by the Italian Fermi), the seminal works in the fields of Quantum Field Theory and Path Integral formulation of Quantum Mechanics, and the introduction of the Dirac delta function, based on previous works by Furier and Heaviside, an ill-defined mathematical concept that will be later formalised into distribution theory. A popular book about Dirac's life is entitled "The strangest man".

A scalar product is introduced as an operation that gives a number from two vectors

$$\mathbf{a} \cdot \mathbf{b} = a\, b\, \cos\theta \tag{6.7}$$

a and b being the magnitudes of the vectors and θ the angle between them.

Once we choose a Cartesian reference frame, the vector may represented by its 3 components

$$\mathbf{x} = (x, y, z) = (x_1, x_2, x_3) \tag{6.8}$$

vector sum by

$$\mathbf{x} + \mathbf{y} = (x_1 + y_1, x_2 + y_2, x_3 + y_3) \tag{6.9}$$

product by a scalar by

$$\alpha\mathbf{x} = (\alpha x_1, \alpha x_2, \alpha x_3) \tag{6.10}$$

and scalar product by

$$\mathbf{x} \cdot \mathbf{y} = x_1 y_1 + x_2 y_2 + x_3 y_3 \tag{6.11}$$

6.2.2 Generalisation

$\mathbb{R}^n$

We may easily generalise these concepts to the n dimensional case

$$\mathbf{x} = (x_1, \ldots, x_n) \tag{6.12}$$

$$(\mathbf{x} + \mathbf{y})_i = x_i + y_i \tag{6.13}$$

$$(\alpha\mathbf{x})_i = \alpha x_i \tag{6.14}$$

$$\mathbf{x} \cdot \mathbf{y} = \sum_i x_i y_i \tag{6.15}$$

Abstract vector space

But we can do better. Let us call a vector space V a set provided with the operations of sum and a product by a scalar, such that if $\mathbf{x}, \mathbf{y} \in V$ and α is a number, then

$$\mathbf{x} + \mathbf{y} = \mathbf{z} \in V, \qquad \alpha\,\mathbf{x} = \mathbf{w} \in V \tag{6.16}$$

We basically call vector space a set on which we may define a sum and product by a number is such a way that the result still belongs to the set. This is clearly related to the studies we have been performing up to now. Consider for example the set of periodic functions,

$$f(\theta + 2n\pi) = f(\theta) \tag{6.17}$$

If we define the sum of two functions f and g as the function that assumes in θ the value

$$(f+g)(\theta) = f(\theta) + g(\theta) \tag{6.18}$$

and as the product of f with the number α the function that assumes in θ the value

$$(\alpha f)(\theta) = \alpha f(\theta) \tag{6.19}$$

we may trivially verify that the resulting functions are still members of the set. Other examples of interest are functions that assume zero value on boundaries, functions that have zero derivative on the boundaries, and solutions of linear differential equations[3].

Complex numbers

Until now we have been talking of a product with "a number" α. This vague concept was used to hint that $\alpha \in \mathbb{R}$. [4] But we may actually be interested to generalise to $\alpha \in \mathbb{C}$. [5]

The main reason for using complex numbers is the *Fundamental theorem of algebra*, that states that any polynomial of degree $n > 0$ with complex coefficients has at least a complex root (and actually, if counted with multiplicity, exactly n roots). Namely, when we are dealing with complex polynomial equations, we may always find a solution, and actually all the solutions we need. Two examples will help us in understanding better this issue.

Let us consider the second order differential equation

$$\frac{d^2 f}{dx^2} = a\frac{df}{dx} + bf \tag{6.20}$$

If we guess a solution in the form $e^{\lambda x}$ we get

$$(\lambda^2 - a\lambda - b)e^{\lambda x} = 0 \tag{6.21}$$

A solution is then found by solving the algebraic equation

$$\lambda^2 - a\lambda - b = 0 \tag{6.22}$$

The equation above does not necessarily have real solutions, while it has exactly two complex solutions, providing the correct number of integration

[3] Examples of sets that are not vector spaces are functions assuming non zero value on boundaries, or solutions of non-linear differential equations.

[4] In such a case we say that V is a vector space on the real field.

[5] In such a case we say that V is a vector space on the complex field.

constants for a second order equation. For example, the most important version of this equation is probably the harmonic oscillator one, $a = 0$, $b = -1$, whose solutions are complex, $\lambda = \pm i$. By working with complex numbers we may obtain the solutions

$$e^{\pm ix} \tag{6.23}$$

and from their linear combination the real solutions $\sin x$ and $\cos x$.

The reader should be already familiar with the concept of eigenvectors and eigenvalues of a matrix (that will be reviewed soon and related to the problem of solving differential equations). Let us consider the simple matrix (rotation of $\pi/2$)

$$A = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \tag{6.24}$$

To find its eigenvalues, we compute

$$\det(A - \lambda \mathbb{1}) = \lambda^2 + 1 = 0 \tag{6.25}$$

There is no real solution, as understandable since no real vector is left unchanged by such a rotation. Nevertheless, as we have seen above (eq. 6.4), it is useful to operate on eigenvectors of the matrix, so it is important to know that to the complex eigenvalues $\pm i$ correspond the eigenvectors

$$\mathbf{v}_i = \begin{pmatrix} \alpha \\ i\alpha \end{pmatrix} \qquad \mathbf{v}_{-i} = \begin{pmatrix} \alpha \\ -i\alpha \end{pmatrix} \tag{6.26}$$

6.2.3 The scalar or inner product

A scalar or inner product on a Vector space is an operator that takes two vectors and gives a complex number

$$\langle \mathbf{x}, \mathbf{y} \rangle \in \mathbb{C} \tag{6.27}$$

withe the following properties

1. Complex conjugation under exchange:

$$\langle \mathbf{x}, \mathbf{y} \rangle = (\langle \mathbf{y}, \mathbf{x} \rangle)^* \tag{6.28}$$

2. Positive definiteness:

$$\langle \mathbf{x}, \mathbf{x} \rangle \geq 0, \qquad \langle \mathbf{x}, \mathbf{x} \rangle = 0 \text{ iff } \mathbf{x} = 0 \tag{6.29}$$

3. Linearity:

$$\langle \mathbf{x}, \alpha\mathbf{y} \rangle = \alpha \langle \mathbf{x}, \mathbf{y} \rangle , \qquad \langle \mathbf{x}, \mathbf{y} + \mathbf{z} \rangle = \langle \mathbf{x}, \mathbf{y} \rangle + \langle \mathbf{x}, \mathbf{z} \rangle \tag{6.30}$$

The definition eq. (6.15) satisfies the above conditions *when applied to real vectors*, but needs to be modified to

$$\mathbf{x} \cdot \mathbf{y} = \sum_i x_i^* y_i \tag{6.31}$$

to satisfy them in the complex case. One may wonder then why we asked the scalar product to satisfy eq. (6.28) in the first place. First of all, such a property automatically assures

$$\langle \mathbf{x}, \mathbf{x} \rangle \in \mathbb{R} \tag{6.32}$$

Furthermore, coupled with linearity, we have

$$\langle \alpha\mathbf{x}, \mathbf{y} \rangle = (\langle \mathbf{y}, \alpha\mathbf{x} \rangle)^* = (\alpha \langle \mathbf{y}, \mathbf{x} \rangle)^* = \alpha^* (\langle \mathbf{y}, \mathbf{x} \rangle)^* = \alpha^* \langle \mathbf{x}, \mathbf{y} \rangle \tag{6.33}$$

so that

$$\langle \alpha\mathbf{x}, \alpha\mathbf{x} \rangle = \alpha^* \alpha \langle \mathbf{x}, \mathbf{x} \rangle = |\alpha|^2 \langle \mathbf{x}, \mathbf{x} \rangle \tag{6.34}$$

so that the required property eq. (6.28) allows us to define a positive definite scalar product. Indeed, for the specific definition eq. (6.31) we have

$$\mathbf{x} \cdot \mathbf{x} = \sum_i |x_i|^2 \geq 0 \tag{6.35}$$

A positive definite scalar product allows us to use the scalar product to define a norm

$$\|\mathbf{x}\| = \sqrt{\langle \mathbf{x}, \mathbf{x} \rangle} \tag{6.36}$$

6.2.4 Linear independence, bases, dimension and the like

Linear independence

We say that a set of vectors of n vectors $\mathbf{v}_i \in V$ is linearly independent if

$$\sum_i c_i \mathbf{v}_i = 0 \Rightarrow c_i = 0 \, \forall \, i \tag{6.37}$$

(or, equivalently, if it is impossible to write one of them as a combination of some of the others).

Basis and dimension

Linear combinations of these vectors forms a subspace of V, i.e. a vector space $V' \subset V$. If $V' = V$, i.e. if any vector in V may be written as a linear combination of the $\mathbf{v}_i$, we say that the vectors for a *basis* of the vector space, and that the *dimension* of the vector space is n. It may indeed be shown that if the vector space has basis of size n, all its bases will necessarily have the same size[6].

Obviously, not all vector spaces admit a basis of dimension n. If they do, we say that the space is finite dimensional. Finite dimension spaces are "easier" and we will focus on them for a while.

6.2.5 Orthonormalisation

If a (non-zero) vector $\mathbf{v}_1$ is given, it is trivial to obtain a *normalised* vector from it, i.e.

$$\mathbf{e}_1 = \frac{1}{\sqrt{\langle \mathbf{v}_1, \mathbf{v}_1 \rangle}} \mathbf{v}_1 \tag{6.38}$$

so that

$$\langle \mathbf{e}_1, \mathbf{e}_1 \rangle = \frac{1}{\sqrt{\langle \mathbf{v}_1, \mathbf{v}_1 \rangle}} \langle \mathbf{v}_1, \mathbf{v}_1 \rangle = 1 \tag{6.39}$$

Let us now consider a second vector $\mathbf{v}_2$, and assume $\mathbf{v}_1$ and $\mathbf{v}_2$ to be linearly independent. We now compute

$$\mathbf{v}_2' = \mathbf{v}_2 - \langle \mathbf{e}_1, \mathbf{v}_2 \rangle \, \mathbf{e}_1 \neq 0 \tag{6.40}$$

The result is necessarily non-zero, otherwise it would mean that $\mathbf{v}_2$ may be written as a linear combination of $\mathbf{v}_1$. We may now compute

$$\left\langle \mathbf{e}_1, \mathbf{v}_2' \right\rangle = \langle \mathbf{e}_1, \mathbf{v}_2 \rangle - \langle \mathbf{e}_1, \mathbf{v}_2 \rangle \, \langle \mathbf{e}_1, \mathbf{e}_1 \rangle = \langle \mathbf{e}_1, \mathbf{v}_2 \rangle - \langle \mathbf{e}_1, \mathbf{v}_2 \rangle = 0 \tag{6.41}$$

We may now define

$$\mathbf{e}_2 = \frac{1}{\sqrt{\langle \mathbf{v}_2', \mathbf{v}_2' \rangle}} \mathbf{v}_2' \tag{6.42}$$

so that

$$\langle \mathbf{e}_1, \mathbf{e}_1 \rangle = \langle \mathbf{e}_2, \mathbf{e}_2 \rangle = 1, \quad \langle \mathbf{e}_1, \mathbf{e}_2 \rangle = 0 \tag{6.43}$$

[6]The logic behind the proof is the following. Assume you have a basis $\mathbf{x}_i$ of size n, and a basis $\mathbf{y}_i$ of size $m > n$. You can write $\mathbf{y}_1$ as a combination of the $\mathbf{x}_i$, and use the obtained formula to express one of the $\mathbf{x}_i$, let us call it $\mathbf{x}_1$ (a re-ordering may be necessary), as a combination of $\mathbf{y}_1$, $\mathbf{x}_i$, $i > 1$. This set of n vectors is thus a basis, that we use to express $\mathbf{y}_2$. By repeating the process, you finally obtain that the first n $\mathbf{y}_i$ are a basis, in contradiction with the hypothesis.

If now a third vector $\mathbf{v}_3$, forming a linearly independent set with $\mathbf{v}_1$ and $\mathbf{v}_2$, is given, we define

$$\mathbf{v}_3' = \mathbf{v}_3 - \langle \mathbf{e}_1, \mathbf{v}_3 \rangle \, \mathbf{e}_1 - \langle \mathbf{e}_2, \mathbf{v}_3 \rangle \, \mathbf{e}_2 \neq 0 \tag{6.44}$$

This vector is again non-zero, since $\mathbf{e}_1$ and $\mathbf{e}_2$ are linear combinations of $\mathbf{v}_1$ and $\mathbf{v}_2$, and thus if we had a zero we could write

$$\mathbf{v}_3 = \langle \mathbf{e}_1, \mathbf{v}_3 \rangle \, \mathbf{e}_1 - \langle \mathbf{e}_2, \mathbf{v}_3 \rangle \, \mathbf{e}_2 = c_1 \mathbf{v}_1 + c_2 \mathbf{v}_2 \tag{6.45}$$

in contradiction with the hypothesis. Now we have

$$\begin{aligned} &\left\langle \mathbf{e}_1, \mathbf{v}_3' \right\rangle = \langle \mathbf{e}_1, \mathbf{v}_3 \rangle - \langle \mathbf{e}_1, \mathbf{v}_3 \rangle \, \langle \mathbf{e}_1, \mathbf{e}_1 \rangle - \langle \mathbf{e}_2, \mathbf{v}_3 \rangle \, \langle \mathbf{e}_1, \mathbf{e}_2 \rangle = \\ &\langle \mathbf{e}_1, \mathbf{v}_3 \rangle - \langle \mathbf{e}_1, \mathbf{v}_3 \rangle - 0 = 0 \end{aligned} \tag{6.46}$$

and

$$\left\langle \mathbf{e}_2, \mathbf{v}_3' \right\rangle = \langle \mathbf{e}_2, \mathbf{v}_3 \rangle - \langle \mathbf{e}_1, \mathbf{v}_3 \rangle \, \langle \mathbf{e}_2, \mathbf{e}_1 \rangle - \langle \mathbf{e}_2, \mathbf{v}_3 \rangle \, \langle \mathbf{e}_2, \mathbf{e}_2 \rangle = 0 \tag{6.47}$$

By defining

$$\mathbf{e}_3 = \frac{1}{\sqrt{\langle \mathbf{v}_3', \mathbf{v}_3' \rangle}} \mathbf{v}_3' \tag{6.48}$$

we get

$$\langle \mathbf{e}_i, \mathbf{e}_j \rangle = \delta_{i,j}, \;\; i, j = 1, 2, 3 \tag{6.49}$$

The generalisation

$$\mathbf{v}_k' = \mathbf{v}_k - \sum_{i=1}^{k-1} \langle \mathbf{e}_i, \mathbf{v}_k \rangle \, \mathbf{e}_i \neq 0 \tag{6.50}$$

$$\mathbf{e}_k = \frac{1}{\sqrt{\langle \mathbf{v}_k', \mathbf{v}_k' \rangle}} \mathbf{v}_k' \tag{6.51}$$

leads clearly to the construction of a orthonormal basis

$$\langle \mathbf{e}_i, \mathbf{e}_j \rangle = \delta_{i,j} \tag{6.52}$$

starting from any given basis.

6.2.6 Scalar product and orthonormal bases

Given vectors $\mathbf{x}$, $\mathbf{y}$ in a finite dimensional vector space V, we have, as shown above,

$$\mathbf{x} = \sum_i x_i \mathbf{e}_i, \qquad \mathbf{y} = \sum_i y_i \mathbf{e}_i \tag{6.53}$$

where the x_i and y_i are the coefficients that give the vectors as linear combination of the vectors in the basis (the components in that basis), and the basis has been chosen to be orthonormal with respect to the scalar product of the vector space.

We then have

$$\langle \mathbf{x}, \mathbf{y} \rangle = \left\langle \sum_i x_i \mathbf{e}_i, \sum_j y_j \mathbf{e}_j \right\rangle = \sum_j y_j \left(\left\langle \sum_i x_i \mathbf{e}_i, \mathbf{e}_j \right\rangle \right) = \sum_j y_j \left(\sum_i \langle x_i \mathbf{e}_i, \mathbf{e}_j \rangle \right) =$$
$$\sum_j y_j \left(\sum_i x_i^* \langle \mathbf{e}_i, \mathbf{e}_j \rangle \right) = \sum_j y_j \left(\sum_i x_i^* \delta_{i,j} \right) = \sum_j x_j^* y_j \tag{6.54}$$

We thus see that once we assign a orthonormal basis to a vector space of dimension n, we may establish (eq. 6.53) a one-to-one correspondence with the space $\mathbb{C}^n$, that preserves (eq. 6.54) the form of the scalar product eq. (6.31).

We may also show that if we have, in a space of dimension n, n orthonormal vectors, they are independent, and thus a base. Indeed, if we assume

$$\mathbf{e}_i = \sum_{j \neq i} c_j \mathbf{e}_j \tag{6.55}$$

we get the contradiction that all c_j are zero

$$0 = \langle \mathbf{e}_k, \mathbf{e}_i \rangle = \sum_{j \neq i} c_j \langle \mathbf{e}_k, \mathbf{e}_j \rangle = c_k \tag{6.56}$$

6.3 Linear operators

6.3.1 Definition

Let us consider an *linear operator* A from V to V, i.e. and operator such that, if $\mathbf{x}$, $\mathbf{v}$ are in V then we have

$$A\mathbf{x} = \mathbf{z} \in V \tag{6.57}$$

$$A(\alpha \mathbf{x}) = \alpha A \mathbf{x} \tag{6.58}$$

$$A(\mathbf{x} + \mathbf{y}) = A\mathbf{x} + A\mathbf{y} \tag{6.59}$$

6.3.2 Linear operators on a finite dimensional space

Let us consider a finite dimensional space with orthonormal basis $\mathbf{e}_i$. When a linear operator A acts on a member of the basis $\mathbf{e}_i$, it produces a vector in V, that may again be written as a linear combination of the members of the basis

$$A\mathbf{e}_i = \mathbf{z} = \sum_{j=1}^{n} z_j \mathbf{e}_j \tag{6.60}$$

Now, since the z_j are determined by A and $\mathbf{e}_i$ we may call them A_{ji}. Let us now have A to act on a generic vector $\mathbf{x}$

$$\begin{aligned} A\mathbf{x} &= A\left(\sum_i x_i \mathbf{e}_i\right) = \sum_i x_i A\mathbf{e}_i = \sum_i x_i \sum_j A_{j,i}\mathbf{e}_j = \sum_j \left(\sum_i A_{j,i}x_i\right)\mathbf{e}_j \\ &= \mathbf{z} = \sum_j z_j \mathbf{e}_j \end{aligned} \tag{6.61}$$

The action of the linear operator is thus to take a vector with components x_i and to generate a vector with components $\sum_i A_{j,i}x_i$. We have thus created a correspondence between linear operators and matrices acting on $\mathbb{R}^n$.

What is exactly $A_{j,i}$? We can see it easily by computing

$$\langle \mathbf{e}_j, A\mathbf{e}_i \rangle = \left\langle \mathbf{e}_j, \sum_k A_{k,i}\mathbf{e}_k \right\rangle = \sum_k A_{k,i} \langle \mathbf{e}_j, \mathbf{e}_k \rangle = \sum_k A_{k,i}\delta_{j,k} = A_{j,i} \tag{6.62}$$

What happens when a linear operator acts on the result of another linear operator?

$$\begin{aligned} BA\mathbf{x} = B(A\mathbf{x}) = B\left(\sum_j \left(\sum_i A_{j,i}x_i\right)\mathbf{e}_j\right) = \sum_j B\left(\left(\sum_i A_{j,i}x_i\right)\mathbf{e}_j\right) = \\ \sum_j \left(\sum_i A_{j,i}x_i \left(B\mathbf{e}_j\right)\right) = \sum_j \left(\sum_i A_{j,i}x_i \left(\sum_k B_{k,j}\mathbf{e}_k\right)\right) = \sum_k \left(\sum_j \sum_k B_{k,j}A_{j,i}x_i\right)\mathbf{e}_k \end{aligned} \tag{6.63}$$

The components of the new vector are given by $\sum_j \sum_k B_{k,j}A_{j,i}x_i$ so that also the rule of matrix product is obtained for operators on general vector spaces. This means that

$$\langle \mathbf{e}_k, BA\mathbf{e}_i \rangle = \sum_j \langle \mathbf{e}_k, B\mathbf{e}_j \rangle \langle \mathbf{e}_j, A\mathbf{e}_i \rangle \tag{6.64}$$

a formula that will result trivial once we introduce the Dirac formalism.

6.3.3 Eigenvalues and eigenvectors

In general, the action of a linear operator on a vector is more complex than a simple multiplication by a complex number

$$A\mathbf{x} \neq \alpha\mathbf{x} \tag{6.65}$$

and indeed an operator for which the above equation would hold *for all* $\mathbf{x}$ would be just a multiple of the identity operator $\mathbb{1}$.

Nevertheless, for each operator A, there may be some *eigenvalues* λ and *eigenvectors* $\mathbf{v}_\lambda$ such that

$$A\mathbf{v}_\lambda = \lambda\mathbf{v}_\lambda \tag{6.66}$$

The knowledge of such eigenvalues and eigenvectors is extremely important, as already discussed above (eq. 6.6). In order to explicitly compute the eigenvalues and eigenvectors, the matrix representation of linear operators is extremely valuable. Let us first rewrite eq. (6.66) as

$$(A - \lambda\mathbb{1})\mathbf{v}_\lambda = 0 \tag{6.67}$$

Using an explicit basis, we get

$$\sum_j (A - \lambda\mathbb{1})_{i,j}(\mathbf{v}_\lambda)_j = 0 \tag{6.68}$$

From the theory of linear equations, we know that this is possible only if

$$\det(A - \lambda\mathbb{1})_{i,j} = \det(A_{i,j} - \lambda\delta_{i,j}) = 0 \tag{6.69}$$

The above equation is a polynomial of order n in λ, and its solution gives (since we are working with complex numbers) n roots λ_i, (possibly some of them being equal, i.e. of multiplicity larger than one). The solution of the linear equations

$$\sum_j A_{k,j}(\mathbf{v}_{\lambda_i})_j = \lambda_i(\mathbf{v}_{\lambda_i})_k \tag{6.70}$$

will provide the explicit form of the eigenvector $\mathbf{v}_{\lambda_i}$. Obviously, the solution of eq. (6.70) is *not* unique. We know this both from the theory of linear equations (since $\det(A - \lambda_i\mathbb{1}) = 0$) and from general theory of linear operators

$$A\mathbf{v} = \lambda\mathbf{v} \Rightarrow A(\alpha\mathbf{v}) = \alpha A\mathbf{v} = \lambda(\alpha\mathbf{v}) \tag{6.71}$$

so that if $\mathbf{v}$ is an eigenvector, also $\alpha\mathbf{v}$ is an eigenvector with the same eigenvalue.

6.3.4 Inverse operator

Let us consider an operator A such that each $\mathbf{y}$ in V may be written as

$$\mathbf{y} = A\mathbf{x} \tag{6.72}$$

We define the operator A^{-1} as the operator

$$A^{-1}A = \mathbb{1} \Rightarrow A^{-1}\mathbf{y} = \mathbf{x} \tag{6.73}$$

We may easy verify that

$$AA^{-1} = \mathbb{1} \tag{6.74}$$

Indeed

$$AA^{-1}\mathbf{y} = AA^{-1}(A\mathbf{x}) = A(A^{-1}A\mathbf{x}) = A\mathbf{x} = \mathbf{y} \tag{6.75}$$

In matrix representation we have

$$\delta_{i,j} = \langle \mathbf{e}_i, \mathbb{1}\mathbf{e}_j \rangle = \left\langle \mathbf{e}_i, A^{-1}A\mathbf{e}_j \right\rangle = \sum_k A^{-1}_{i,k} A_{k,j} \tag{6.76}$$

6.3.5 Adjoint operator

Definition

Given the linear operator A, we define its adjoint $A^\dagger$ by asking

$$\langle \mathbf{x}, A\mathbf{y} \rangle = \left\langle A^\dagger \mathbf{x}, \mathbf{y} \right\rangle, \ \forall\, \mathbf{x}, \mathbf{y} \tag{6.77}$$

Let us first notice that, once we assign an orthonormal basis $\mathbf{e}_i$ we have

$$\begin{aligned} \langle \mathbf{x}, A\mathbf{y} \rangle &= \sum_i x_i^* \langle \mathbf{e}_i, A\mathbf{y} \rangle = \sum_i x_i^* \left\langle \mathbf{e}_i, \sum_j \sum_k A_{j,k} y_k \mathbf{e}_j \right\rangle \\ &= \sum_i \sum_j \sum_k x_j^* A_{j,k} y_k \langle \mathbf{e}_i, \mathbf{e}_j \rangle = \sum_i \sum_j \sum_k x_j^* A_{j,k} y_k \delta_{i,j} = \sum_j \sum_k x_j^* A_{j,k} y_k \end{aligned} \tag{6.78}$$

and

$$\left\langle A^\dagger \mathbf{x}, \mathbf{y} \right\rangle = \left(\left\langle \mathbf{y}, A^\dagger \mathbf{x} \right\rangle \right)^* = \left(\sum_j \sum_k y_k^* A^\dagger_{k,j} x_j \right)^* = \sum_j \sum_k x_j^* \left(A^\dagger_{k,j} \right)^* y_k \tag{6.79}$$

so that, since the relation has to be true for each $\mathbf{x}$ and $\mathbf{y}$, the adjoint operator's matrix representation is given by the the complex conjugate of the transpose

$$\left(A^\dagger_{k,j} \right)^* = A_{j,k} \Rightarrow A^\dagger_{k,j} = (A_{j,k})^* \tag{6.80}$$

We may easily verify that

$$(AB)^\dagger = B^\dagger A^\dagger \tag{6.81}$$

Indeed

$$\langle \mathbf{x}, AB\mathbf{y}\rangle = \left\langle A^\dagger \mathbf{x}, B\mathbf{y}\right\rangle = \left\langle B^\dagger A^\dagger \mathbf{x}, \mathbf{y}\right\rangle \tag{6.82}$$

Self adjoint operators

We say that an operator is self-adjoint if, for any $\mathbf{x}$, $\mathbf{y}$, the following holds

$$\langle \mathbf{x}, A\mathbf{y}\rangle = \langle A\mathbf{x}, \mathbf{y}\rangle \tag{6.83}$$

Namely the operator is self-adjoint if we can move it on the other side of the scalar product without changing it.

According to the theory developed above, a linear operator on a finite dimensional vector space is self-adjoint if its matrix representation satisfies

$$A_{k,j} = (A_{j,k})^* \tag{6.84}$$

Eigenvalues and eigenvectors of a self-adjoint operator

Self-adjoint operators (symmetric operators in the real case) have properties that make them extremely important. First of all, their eigenvalues λ such that

$$A\mathbf{v}_\lambda = \lambda \mathbf{v}_\lambda \tag{6.85}$$

are real, $\lambda \in \mathbb{R}$. Indeed

$$\begin{aligned} &\lambda \langle \mathbf{v}, \mathbf{v}\rangle = \langle \mathbf{v}, \lambda\mathbf{v}\rangle = \langle \mathbf{v}, A\mathbf{v}\rangle = \left\langle A^\dagger \mathbf{v}, \mathbf{v}\right\rangle = \langle A\mathbf{v}, \mathbf{v}\rangle = \langle \lambda\mathbf{v}, \mathbf{v}\rangle = \\ &\lambda^* \langle \mathbf{v}, \mathbf{v}\rangle \Rightarrow \lambda = \lambda^* \end{aligned} \tag{6.86}$$

Furthermore, two eigenvalues corresponding two different eigenvectors of a self-adjoint operator are orthogonal. Indeed if

$$A\mathbf{v}_{\lambda_1} = \lambda_1 \mathbf{v}_{\lambda_1}, \qquad A\mathbf{v}_{\lambda_2} = \lambda_2 \mathbf{v}_{\lambda_2}, \qquad \lambda_1 \neq \lambda_2 \tag{6.87}$$

we have, using $A = A^\dagger$ and $\lambda = \lambda^*$,

$$\begin{aligned} &\lambda_1 \langle \mathbf{v}_{\lambda_1}, \mathbf{v}_{\lambda_2}\rangle = \langle A\mathbf{v}_{\lambda_1}, \mathbf{v}_{\lambda_2}\rangle = \langle \mathbf{v}_{\lambda_1}, A\mathbf{v}_{\lambda_2}\rangle = \lambda_2 \langle \mathbf{v}_{\lambda_1}, \mathbf{v}_{\lambda_2}\rangle \\ &\Rightarrow (\lambda_1 - \lambda_2) \langle \mathbf{v}_{\lambda_1}, \mathbf{v}_{\lambda_2}\rangle \Rightarrow \langle \mathbf{v}_{\lambda_1}, \mathbf{v}_{\lambda_2}\rangle = 0 \end{aligned} \tag{6.88}$$

This is not enough to assure that A has n orthogonal eigenvectors, since the multiplicity of some eigenvalues may be higher than one (the sub-space corresponding to some eigenvalue λ is more than one.). Nevertheless, it is

possible to show that a self-adjoint A has an orthonormal basis of eigenvectors.

We can show it using the principle of induction. For $n = 1$ it is clear that any operator (simply the multiplication by a number) has any vector as an eigenvector, and such vector may be normalised and be, by itself, a basis for the vector space. Let us assume that on any space of dimension $n-1$ a self-adjoint operator A admits an orthonormal basis. For a n dimensional space, we start by finding an eigenvector $\mathbf{v}_1$, since we may always do that, as shown above, due to the fundamental theorem of algebra. Let us call the corresponding eigenvalue λ_1. This vector may be normalised as

$$\mathbf{e}_1 = \frac{1}{\sqrt{\langle \mathbf{v}_1, \mathbf{v}_1 \rangle}} \mathbf{v}_1 \tag{6.89}$$

We may always now find $n-1$ vectors $\mathbf{v}_i$, $i > 1$ that form a basis together with $\mathbf{e}_1$. We may orthonormalise them in the basis $\{\mathbf{e}_1, \overline{\mathbf{e}}_i\}$. The linear combinations of the $\overline{\mathbf{e}}_i$ form obviously a subspace of vectors orthogonal to $\mathbf{e}_1$. The important point, in which the fact that A is self-adjoint is crucial, is that the action of A on vectors in the subspace, stays in the subspace, since $A\,\overline{\mathbf{e}}_i$ is orthogonal to $\mathbf{e}_1$

$$\langle A\,\overline{\mathbf{e}}_i, \mathbf{e}_1 \rangle = \langle \overline{\mathbf{e}}_i, A\,\mathbf{e}_1 \rangle = \lambda_1 \langle \overline{\mathbf{e}}_i, \mathbf{e}_1 \rangle = 0 \tag{6.90}$$

Now we can use the induction hypothesis, and find $n-1$ orthonormal eigenvectors on the $n-1$ space orthogonal to $\mathbf{e}_1$, that we may call $\mathbf{e}_i$ and that, being in a subspace orthogonal to $\mathbf{e}_1$, form with it an orthonormal basis.

Symmetric real matrices

$$A_{i,j} = A_{j,i} \tag{6.91}$$

are clearly self-adjoint and thus admit a orthonormal basis of eigenvectures with real eigenvalues.

Anti-adjoint operator

It is interesting to check what happens to an anti-adjoint operator

$$A^\dagger = -A \tag{6.92}$$

Their eigenvalues λ such that

$$A\mathbf{v}_\lambda = \lambda \mathbf{v}_\lambda \tag{6.93}$$

are *purely imaginary*. Indeed

$$\lambda \langle \mathbf{v}, \mathbf{v} \rangle = \langle \mathbf{v}, \lambda \mathbf{v} \rangle = \langle \mathbf{v}, A\mathbf{v} \rangle = \left\langle A^\dagger \mathbf{v}, \mathbf{v} \right\rangle = \langle -A\mathbf{v}, \mathbf{v} \rangle = \langle -\lambda \mathbf{v}, \mathbf{v} \rangle = \\ -\lambda^* \langle \mathbf{v}, \mathbf{v} \rangle \Rightarrow \lambda = -\lambda^* \tag{6.94}$$

Furthermore, two eigenvalues corresponding two different eigenvectors are orthogonal. Indeed if

$$A\mathbf{v}_{\lambda_1} = \lambda_1 \mathbf{v}_{\lambda_1}, \qquad A\mathbf{v}_{\lambda_2} = \lambda_2 \mathbf{v}_{\lambda_2}, \qquad \lambda_1 \neq \lambda_2 \tag{6.95}$$

we have, using $A^\dagger = -A$ and $\lambda^* = -\lambda$,

$$\lambda_1 \langle \mathbf{v}_{\lambda_1}, \mathbf{v}_{\lambda_2} \rangle = \langle -\lambda_1 \mathbf{v}_{\lambda_1}, \mathbf{v}_{\lambda_2} \rangle \langle -A\mathbf{v}_{\lambda_1}, \mathbf{v}_{\lambda_2} \rangle = \langle \mathbf{v}_{\lambda_1}, A\mathbf{v}_{\lambda_2} \rangle = \lambda_2 \langle \mathbf{v}_{\lambda_1}, \mathbf{v}_{\lambda_2} \rangle \\ \Rightarrow (\lambda_1 - \lambda_2) \langle \mathbf{v}_{\lambda_1}, \mathbf{v}_{\lambda_2} \rangle \Rightarrow \langle \mathbf{v}_{\lambda_1}, \mathbf{v}_{\lambda_2} \rangle = 0 \tag{6.96}$$

To show that these operators admit a basis of orthonormal eiegnvectors, we just need to repeat the proof above using this time

$$\langle A\,\overline{\mathbf{e}}_i, \mathbf{e}_1 \rangle = \langle \overline{\mathbf{e}}_i, -A\mathbf{e}_1 \rangle = -\lambda_1 \langle \overline{\mathbf{e}}_i, \mathbf{e}_1 \rangle = 0 \tag{6.97}$$

Purely imaginary symmetric matrices are anti-adjoint, so that they share these properties.

6.3.6 Commuting operators

In general, linear operators on a vector space *do not commute*. Let us consider for example a $n = 2$ space with an orthonormal basis $\mathbf{e}_1$, $\mathbf{e}_2$. Let us consider the operator A such that

$$A\,\mathbf{e}_1 = \mathbf{e}_2, \qquad A\,\mathbf{e}_2 = 0 \tag{6.98}$$

whose matrix representation is

$$A = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \tag{6.99}$$

and the operator B such that

$$B\,\mathbf{e}_1 = 0, \qquad B\,\mathbf{e}_2 = \mathbf{e}_1 \tag{6.100}$$

whose matrix representation is

$$B = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \tag{6.101}$$

Both by considering their action on the basis, or by matrix multiplication, we have

$$AB = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}, \qquad BA = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \tag{6.102}$$

namely AB leaves $\mathbf{e}_1$ in itself and deletes $\mathbf{e}_2$, while BA has the opposite effect.

We may define the *commutator*

$$[A, B] = AB - BA = -[B, A] \tag{6.103}$$

and we will have in general $[A, B] \neq 0$. We will study later the properties of the commutator, when we will study the solution of the Laplace equation in spherical coordinates and its relation to Quantum Mechanics. In the meanwhile, we study some properties of self-adjoint and anti-adjoint commuting operators, i.e. such that

$$[A, B] = 0 \tag{6.104}$$

Let us assume A and B admit a orthonormal basis of eigenvectors, as for example self-adjoint and anti-adjoint operators (or, more in general, normal operators, as we will show later) do, and that they commute $AB = BA$. If $\mathbf{v}_\lambda$ is an eigenvector of A with eigenvalue λ, we have

$$A(B\mathbf{v}_\lambda) = AB\mathbf{v}_\lambda = BA\mathbf{v}_\lambda = \lambda(B\mathbf{v}_\lambda) \tag{6.105}$$

This equation tells us that $B\mathbf{v}_\lambda$ is an eigenvector of A, with eigenvalue λ, i.e. the subspace generated by the linear combinations of all the eigenvectors corresponding to the eigenvalue λ is left invariant by the action of B. Since B is self-adjoint (or anti-adjoint), we may diagonalise it on the subspace, i.e. find an orthonormal basis of eigenvectors of B in the subspace. Each of these eigenvectors will be at the same time an eigenvector of A (with eigenvalue λ, since it is a vector of the subspace) and of B. We may do that for all the eigenvalues λ_i of A and obtain a *common basis of eigenvectors* of A and B. These vectors form a orthonormal basis

$$\begin{aligned} &\mathbf{e}_{\lambda_i,\gamma_j}, \quad A\mathbf{e}_{\lambda_i,\gamma_j} = \lambda_i \mathbf{e}_{\lambda_i,\gamma_j}, \quad B\mathbf{e}_{\lambda_i,\gamma_j} = \gamma_j \mathbf{e}_{\lambda_i,\gamma_j} \\ &\left\langle \mathbf{e}_{\lambda_i,\gamma_j}, \mathbf{e}_{\lambda_k,\gamma_l} \right\rangle = \delta_{i,k}\delta_{j,l} \end{aligned} \tag{6.106}$$

Since in general to the eigenvalues of a (self-adjoint) operator may correspond a subspace with dimension larger than one, although it is possible to find a orthonormal basis of eigenvalues corresponding to it, it is not possible to identify in a unique way all the vector of the basis through the eigenvalue. By using enough commuting operators, it is possible to identify all vectors

in the basis through a set of eigenvalues corresponding to each operator, a process which is extremely useful in Quantum Mechanics (as we will see in our analysis of the Hydrogen atom).

6.3.7 Normal operators

The most general class of operators that admits an orthonormal basis of eigenvectors is that of normal operators

$$[A, A^\dagger] = 0 \tag{6.107}$$

To prove it, we first see that *any operator* A may be written as the sum of a self-adjoint and anti-adjoint operator

$$A = A_{SA} + A_{AA} = \frac{1}{2}[(A + A^\dagger) + (A - A^\dagger)] \tag{6.108}$$

since

$$(A_{SA})^\dagger = \frac{1}{2}(A + A^\dagger)^\dagger = \frac{1}{2}(A^\dagger + A) = A_{SA} \tag{6.109}$$

and

$$(A_{AA})^\dagger = \frac{1}{2}(A - A^\dagger)^\dagger = \frac{1}{2}(A^\dagger - A) = -A_{SA} \tag{6.110}$$

Now, if A is normal, we have

$$\begin{aligned} A_{SA}A_{AA} &= \frac{1}{4}(A^2 - (A^\dagger)^2 - AA^\dagger + A^\dagger A) = \frac{1}{4}(A^2 - (A^\dagger)^2) \\ &= \frac{1}{4}(A^2 - (A^\dagger)^2 - A^\dagger A + AA^\dagger) = A_{AA}A_{SA} \end{aligned} \tag{6.111}$$

Since A_{SA} and A_{AA} admit an orthonormal basis of eigenvalues (one being self-adjoint, and the other one being anti-adjoint), and commute, they admit a *common* orthonormal basis of eigenvalues

$$\begin{aligned} &\mathbf{e}_{\lambda_i,\gamma_j}, \quad A_{SA}\mathbf{e}_{\lambda_i,\gamma_j} = \lambda_i \mathbf{e}_{\lambda_i,\gamma_j}, \quad A_{AA}\mathbf{e}_{\lambda_i,\gamma_j} = \gamma_j \mathbf{e}_{\lambda_i,\gamma_j} \\ &\left\langle \mathbf{e}_{\lambda_i,\gamma_j}, \mathbf{e}_{\lambda_k,\gamma_l} \right\rangle = \delta_{i,k}\delta_{j,l} \end{aligned} \tag{6.112}$$

so that these vectors are an orthonormal basis of eigenvalues of A

$$A\mathbf{e}_{\lambda_i,\gamma_j} = (A_{SA} + A_{AA})\mathbf{e}_{\lambda_i,\gamma_j} = (\lambda_i + \gamma_j)\mathbf{e}_{\lambda_i,\gamma_j} \tag{6.113}$$

Since the λ are real, and the γ are imaginary, in general the eigenvalues of a normal operator are complex.

6.3.8 Unitary operator

An important class of normal operators are the Unitary operators U such that

$$U^\dagger = U^{-1} \Rightarrow U^\dagger U = UU^\dagger = \mathbb{1} \tag{6.114}$$

The have the property that

$$\langle \mathbf{x}, \mathbf{y} \rangle = \left\langle \mathbf{x}, U^\dagger U \mathbf{y} \right\rangle = \langle U\mathbf{x}, U\mathbf{y} \rangle \tag{6.115}$$

namely U conserves the scalar product.

By being normal, U assumes a basis of eigenvectors. Its eigenvalues λ are such that

$$\langle \mathbf{v}_\lambda, \mathbf{v}_\lambda \rangle = \langle U\mathbf{v}_\lambda, U\mathbf{v}_\lambda \rangle = \langle \lambda \mathbf{v}_\lambda, \lambda \mathbf{v}_\lambda \rangle = \lambda^* \lambda \langle \mathbf{v}_\lambda, \mathbf{v}_\lambda \rangle \tag{6.116}$$

So that $|\lambda| = 1$, or $\lambda = e^{i\theta}$.

Let us consider an orthonormal basis $\mathbf{e}_i$, and a unitary operator U. If we define

$$\tilde{\mathbf{e}}_i = U\mathbf{e}_i \tag{6.117}$$

we see that the $\tilde{\mathbf{e}}_i$ are a new orthonormal basis

$$\langle \tilde{\mathbf{e}}_i, \tilde{\mathbf{e}}_j \rangle = \langle \mathbf{e}_i, \mathbf{e}_j \rangle = \delta_{i,j} \tag{6.118}$$

On the other end, let us assume we know two different orthonormal bases, $\mathbf{e}_i$ and $\mathbf{u}_i$. For example, the $\mathbf{u}_i$ may be eigenvectors of A, a normal operator. Each $\mathbf{u}$ is obviously possible to write as a combination of the $\mathbf{e}_i$

$$\mathbf{u}_i = \sum_j u_{i,j} \mathbf{e}_j \tag{6.119}$$

The operator whose matrix representation is $u_{i,j}$ is, by construction the operator that generates $\mathbf{u}_i$ when acting on $\mathbf{e}_i$. We may show that this operator is unitary. Indeed, calling U the operator, we have

$$(UU^\dagger)_{i,j} = \sum_k U_{i,k} (U^\dagger)_{k,j} = \sum_k u_{i,k} u^*_{j,k} = \langle \mathbf{u}_i, \mathbf{u}_j \rangle = \delta_{i,j} \tag{6.120}$$

It is also trivial to show that, if as stated above the $\mathbf{u}_i$ are the eigenvectors of the normal operator A, $U^\dagger AU$ is diagonal in the original basis

$$\begin{aligned} (U^\dagger AU)_{i,j} = \left\langle \mathbf{e}_i, U^\dagger AU \mathbf{e}_j \right\rangle = \langle U\mathbf{e}_i, AU\mathbf{e}_j \rangle = \\ \langle \mathbf{u}_i, A\mathbf{u}_j \rangle = \langle \mathbf{u}_i, \lambda_j \mathbf{u}_j \rangle = \lambda_j \langle \mathbf{u}_i, \mathbf{u}_j \rangle = \lambda_j \delta_{i,j} \end{aligned} \tag{6.121}$$

6.4 Dirac notation

6.4.1 Bras, kets, and scalar products

After this quick revision of (finite dimensional) vector spaces, we are ready to learn Dirac's notation and how it simplifies computations.

We defined the scalar product as an operator that takes two vectors and gives a number

$$\langle *, * \rangle \to \mathbb{C} \tag{6.122}$$

where the $*$ represent slots that may be filled with any vector.

We may also decide to fill the first slot with a vector,

$$\langle \mathbf{v}, * \rangle \to \mathbb{C} \tag{6.123}$$

and obtain an operator that associates to each vector $*$ a complex number. We will have an operator *for each* $\mathbf{v}$. Dirac notation is based on providing a different name and symbol for the vectors and for their version as operators that give numbers when applied on vectors, and to express all mathematical expressions in vector spaces through a combination of such symbols[7].

Let us denote the vectors in the space through a symbol called *ket*, i.e. the vector $\mathbf{v}$ is represented by

$$|v\rangle \tag{6.124}$$

The corresponding operator $\langle \mathbf{v}, * \rangle$ is represented through a symbol named *bra*[8]

$$\langle v| \tag{6.125}$$

The scalar product between $\mathbf{x}$ and $\mathbf{y}$, $\langle \mathbf{x}, \mathbf{y} \rangle$ is a *braket*

$$\langle x|y\rangle \tag{6.126}$$

We may write the product of a ket by a complex number α eqivalently as[9]

$$\alpha|v\rangle = |\alpha v\rangle \tag{6.127}$$

The linear combination of two kets may be written as

$$\alpha|v\rangle + \beta|u\rangle = |\alpha v\rangle + |\beta u\rangle = |\alpha v + \beta u\rangle \tag{6.128}$$

[7] Although in eq. (6.123) we defined the operator through the scalar product, in Dirac's notations such operators are more fundamental than the scalar product and define it.

[8] At a dinner with other acdemics in Cambridge that were discussing about who between them introduced new words in the English language, Dirac told them that he invented the word "bra". He never explained to the unbelieving colleagues that he did not refer to lingerie.

[9] We will use Greek letters for complex numbers and Latin letters for bras and kets.

Bras are obviously linear

$$\langle x|(\alpha|v\rangle + \beta|u\rangle) = \alpha\langle x|v\rangle + \beta\langle x|u\rangle \tag{6.129}$$

The bra corresponding to $|\alpha u\rangle$ is

$$\langle \alpha u| = \alpha^*\langle u| \tag{6.130}$$

6.4.2 Ketbras, projectors and representations of unity

Ketbra

What happens if we write a *ketbra*?

$$|v\rangle\langle u| \tag{6.131}$$

Is it a meaningful symbol? It is, and it represents an linear operator on the vector space. Let us apply it on a ket (vector)

$$(|v\rangle\langle u|)|x\rangle = |v\rangle(\langle u|x\rangle) = (\langle u|x\rangle)|v\rangle \tag{6.132}$$

The braket $\langle u|x\rangle$ is just a number, so we moved it on the front, just to show that the effect of the operator is to produce a ket (vector) parallel to $|v\rangle$ but multiplied by the scalar $\langle u|x\rangle$.

Since a ketbra is an operator, we may wonder how to write its adjoint. We may show that if $A = |x\rangle\langle y|$ then

$$(|x\rangle\langle y|)^\dagger = |y\rangle\langle x| \tag{6.133}$$

Indeed (see eq. 6.144 above for the Dirac operator notation)

$$\begin{aligned} &(\langle v|y\rangle\langle x|u\rangle)^* = \langle u|x\rangle\langle y|v\rangle = \langle u|Av\rangle = \langle A^\dagger u|v\rangle = \left(\langle v|A^\dagger u\rangle\right)^* \\ &\Rightarrow \langle v|y\rangle\langle x|u\rangle = \langle v|A^\dagger u\rangle \end{aligned} \tag{6.134}$$

projector

A very important case is when $|v\rangle$ is normalised, and we consider the *projector*

$$|v\rangle\langle v| \tag{6.135}$$

that projects a vector along $|v\rangle$, i.e.

$$|v\rangle\langle v|u\rangle = (\langle v|u\rangle)|v\rangle \tag{6.136}$$

It is easier to understand its meaning by taking $|v\rangle$ corresponding to $\mathbf{e}_i$, and

$$\mathbf{u} = \sum_j u_j \mathbf{e}_j \tag{6.137}$$

so that the action of the projector is

$$\langle i|u\rangle = \langle \mathbf{e}_i, \mathbf{u}\rangle \mathbf{e}_i = u_i \mathbf{e}_i \tag{6.138}$$

If we consider a few orthonormal vectors (not necessarily a basis for the whole space) $|i\rangle$ (representing $\mathbf{e}_i$), then

$$\sum_i |i\rangle\langle i| \tag{6.139}$$

is a projector on the the subspace generated by the linear combinations of the $\mathbf{e}_i$ (by being the sum of the projectors corresponding to each basis vector).

Representations of identity

If we take the sum over all the basis, we get a projector on the whole space, which is just the identity!

$$\sum_{i=1}^{n} |i\rangle\langle i| = \mathbb{1} \tag{6.140}$$

To see it in explicit terms let us remember

$$\mathbf{u} = \sum_i u_i \mathbf{e}_i, \qquad u_i = \langle \mathbf{e}_i, \mathbf{u}\rangle \tag{6.141}$$

Written in bra-ket notation, the latter reads

$$|u\rangle = \sum_i \langle i|u\rangle |i\rangle = \left(\sum_i |i\rangle\langle i|\right) |u\rangle \tag{6.142}$$

This is true for each $|u\rangle$, provided that the $|i\rangle$ are a basis, so that eq. (6.140) follows.

6.4.3 Operators

General notation

The action of operator A on ket $|v\rangle$ is

$$|Av\rangle = A|v\rangle \tag{6.143}$$

while the scalar product $\langle \mathbf{x}, A\mathbf{y} \rangle$ may be written as

$$\langle x|Ay\rangle = \langle x|A|y\rangle \tag{6.144}$$

the latter notation being more used. The Dirac notation is asymmetric in its treatment on operators on the two sides of the scalar product, since we have for $\langle A\mathbf{x}, \mathbf{y} \rangle$ only

$$\langle Ax|y\rangle \tag{6.145}$$

This asymmetry may be the only unpleasant feature of the notation. I like to write

$$\langle Ax|y\rangle = \langle x|A\|y\rangle \tag{6.146}$$

but it is only a personal notation.

The matrix representation of A in the $|i\rangle$ basis is clearly given by

$$A_{i,j} = \langle i|A|j\rangle \tag{6.147}$$

We are now ready to see how the Dirac formalism make some computations trivial. The matrix representation of BA is

$$\langle i|BA|j\rangle \tag{6.148}$$

We may insert an identity operator where ever we want and easily obtain eq. (6.64)

$$\langle i|B\mathbb{1}A|j\rangle = \langle i|B|\sum_k |k\rangle\langle k|A|j\rangle = \sum_k \langle i|B|k\rangle\langle k|A|j\rangle = \sum_k B_{i,k}A_{k,j} \tag{6.149}$$

It is a useful exercise to rewrite all the equations above using the new formalism, for example

$$A^\dagger_{i,j} = \langle i|A^\dagger|j\rangle = \langle i|A\|j\rangle = (\langle j|A|i\rangle)^* = (A_{j,i})^* \tag{6.150}$$

Normal operators

A normal operator admits an orthonormal basis of eigenvectors. We may enumerate them $i = 1, \ldots, n$, and call the eigenvalues λ_i (we may have degeneracy, $\lambda_i = \lambda_j$ for $i \neq j$). Then the normal operator may be written as

$$A = \sum_i \lambda_i |i\rangle\langle i| \tag{6.151}$$

Indeed, in the basis of its eiegnvectors, the matrix representation is

$$A_{i,j} = \sum_k \lambda_k \langle i|k\rangle\langle k|j\rangle = \sum_k \lambda_k \delta_{i,k}\delta_{k,j} = \lambda_i \delta_{i,j} \tag{6.152}$$

or, in an equivalent way

$$A|i\rangle = \sum_j \lambda_j |j\rangle\langle j|i\rangle = \sum_j \lambda_j |j\rangle \delta_{i,j} = \lambda_i |i\rangle \tag{6.153}$$

When defined on a basis, A is uniquely defined on the whole space, so that eq. (6.151) gives the wanted operator.

Unitary operators

A unitary operator brings an orthonormal basis $|i\rangle$ in another orthonormal basis $|i'\rangle$, so that it is by construction

$$U = \sum_i |i'\rangle\langle i| \tag{6.154}$$

where the prime in i' shows a change in the vector, not in the indexes, i.e. we may write

$$\langle i'|j'\rangle = \delta_{i,j} \tag{6.155}$$

and

$$U|j\rangle = \sum_i |i'\rangle\langle i|j\rangle = \sum_i |i'\rangle \delta_{i,j} = |j'\rangle \tag{6.156}$$

as wanted. We have

$$U^\dagger = \sum_i |i\rangle\langle i'| \tag{6.157}$$

and

$$U^\dagger U = \sum_j |j\rangle\langle j'| \sum_i |i'\rangle\langle i| = \sum_i \sum_j |j\rangle\langle j'|i'\rangle\langle i| = \sum_i \sum_j \delta_{i,j} |j\rangle\langle i| = \sum_i |i\rangle\langle i| = \mathbb{1} \tag{6.158}$$

The matrix representation of U is

$$U_{i,j} = \sum_k \langle i|k'\rangle\langle k|j\rangle = \sum_k \delta_{k,j}\langle i|k'\rangle = \langle i|j'\rangle \tag{6.159}$$

The matrix representation of an operator A in the basis $|i'\rangle$ is

$$A'_{i,j} = \langle i'|A|j'\rangle = \sum_{k,l} \langle i'|k\rangle\langle k|A|l\rangle\langle l|j'\rangle = U^\dagger_{i,k} A_{k,l} U_{l,j} \tag{6.160}$$

6.5 Function spaces

6.5.1 Introduction

We have seen that the concept of vector space may be applied also to functions, as for example by defining a vector space of periodic functions, or a vector space of solutions of a differential equations. Furthermore, a differential operators, as for example ∂_t, ∂_t^2, or ∇^2, are linear operators on such vector spaces, since

$$\nabla^2(\alpha f(\mathbf{x}) + \beta g(\mathbf{x})) = \alpha\nabla^2 f(\mathbf{x}) + \beta\nabla^2 g(\mathbf{x}) \tag{6.161}$$

It is thus clear that we are interested in developing the theory of these *functional vector spaces* as part of our theory of partial differential equations. Nevertheless, as hinted by the fact that our general solutions in the form of Fourier series included in general *infinite terms*, these spaces are not finite dimensional. The theory of functional analysis, dealing with these vector spaces, is not trivial and goes beyond the limits of this course. Nevertheless, we may learn the basic tools and methods of the theory, that we will develop, without proofs, using Dirac's notation and in analogy with the finite dimensional case.

If $f(x)$ is a function in our vector space, for example a periodic function between 0 and L, we may denote the corresponding ket as $|f\rangle$. We may formally define the sum and product by a complex number, and we identify

$$|\alpha f + \beta g\rangle \tag{6.162}$$

as the function

$$\alpha f(x) + \beta g(x) \tag{6.163}$$

We may also formally define the bra

$$\langle f| \tag{6.164}$$

and ask it to satisfy the formal properties that define

$$\langle f|g\rangle \tag{6.165}$$

as a scalar product. But it is clear that if we want out theory to be of any practical value, we need to find a way to express this braket in a explicit way.

6.5.2 Continuum limit

Let us first deal with some partial information. We may compute the value of the function in $i = 1, \ldots, n$ points,

$$f_i = f(x_i), \qquad x_i = -\frac{\Delta x}{2} + i\Delta x, \qquad \Delta x = \frac{L}{n} \tag{6.166}$$

This is just a n dimensional vector, so that we may treat it with the usual methods

$$f_i = f(x_i) = \langle x_i | f \rangle \tag{6.167}$$

$$\langle x_i | x_j \rangle = \delta_{i,j} \tag{6.168}$$

$$\sum_i |x_i\rangle\langle x_i| = \mathbb{1} \tag{6.169}$$

and

$$\langle f | g \rangle = \sum_i \langle f | x_i \rangle \langle x_i | g \rangle = \sum_i \left(f(x_i)\right)^* g(x_i) \tag{6.170}$$

This description works at fixed n, but for finite n we may have only an approximate information, and eventually we want to perform the continuum limit, $n \to \infty$ and $\Delta x \to 0$. But if we perform the limit with this naive approach, we soon meet a problem.

Let us consider a constant function $f(x) = C$. We have

$$\langle f | f \rangle = nC \tag{6.171}$$

a result that would diverge as $n \to \infty$. Let us then define

$$\sum_i |x_i\rangle\langle x_i| \Delta x = \mathbb{1} \tag{6.172}$$

so that the scalar product is

$$\langle f | g \rangle = \sum_i \langle f | x_i \rangle \langle x_i | g \rangle \Delta x = \sum_i \left(f(x_i)\right)^* g(x_i) \Delta x \tag{6.173}$$

Now the scalar product of the constant function is

$$\langle f | f \rangle = nC\Delta x = nC\frac{L}{n} = CL \tag{6.174}$$

a n independent result. We may now easily see that a candidate for the eigen-kets $|x_i\rangle$ are functions

$$\delta_i(x) = \begin{cases} \frac{1}{\sqrt{\Delta x}} \text{ for } x \in [(i-1)\Delta x, i\Delta x) \\ 0 \text{ elsewhere} \end{cases} \tag{6.175}$$

We finally send n to infinity. The kets $|x\rangle$ now represent an infinitely narrow and high function, a *Dirac delta function*[10]. The representation of the identity is

$$\int_0^L |x\rangle\langle x| dx = \mathbb{1} \tag{6.176}$$

so that

$$\langle x|y\rangle = \delta(x-y) \tag{6.177}$$

$$f(x) = \langle x|f\rangle \tag{6.178}$$

and

$$\langle f|g\rangle = \int_0^L \langle f|x\rangle\langle x|g\rangle dx = \int_0^L (f(x))^* g(x) dx \tag{6.179}$$

The scalar product between f and g becomes thus an integral of the product of the complex conjugate of f and g.

What is the meaning of the Dirac delta function? It may be defined by the following expression

$$f(x) = \langle x|f\rangle = \int_0^L \langle x|y\rangle\langle y|f\rangle dy = \int_0^L \delta(x-y) f(y) dy \tag{6.180}$$

When we integrate the product of a function $f(y)$ and the delta function $\delta(x-y)$, the result is the value of f in x (if $x \in [0, L]$). We will study these functions in deeper later.

6.5.3 Adjoint operator

An adjoint operator is defined by

$$\langle f, Ag\rangle = \left\langle A^\dagger f, g\right\rangle \tag{6.181}$$

for finite or infinite dimension spaces.

Let us consider the operator $D = \frac{d}{dx}$ *on the space of periodic functions.* We have

$$\begin{aligned}\langle f, Dg\rangle &= \int_0^L (f(x))^* \left(\frac{d}{dx} g(x)\right) dx = \int_0^L \frac{d}{dx}\left((f(x))^* g(x)\right) dx + \int_0^L \left(-\frac{d}{dx}(f(x))^*\right) g(x) dx \\ &= [(f(x))^* g(x)]_0^L + \int_0^L \left(-\frac{d}{dx} f(x)\right)^* g(x) dx \Rightarrow D^\dagger = -\frac{d}{dx} = -D\end{aligned} \tag{6.182}$$

where we performed an integration by part and used the fact that the functions are periodic to delete the total derivative term.

[10] As stated above, this is an ill defined function, but a formal definition may be provided as part of the theory of distributions.

We may now consider the operator $P = -i\frac{d}{dx}$, again *on the space of periodic functions*. We have

$$\begin{aligned}\langle f, Pg\rangle &= \int_0^L (f(x))^* \left(-i\frac{d}{dx}g(x)\right) dx = \\ &- i\int_0^L \frac{d}{dx}\left((f(x))^* g(x)\right) dx + i\int_0^L \left(\frac{d}{dx}(f(x))^*\right) g(x)dx \\ &= -i\left[(f(x))^* g(x)\right]_0^L + \int_0^L \left(-i\frac{d}{dx}f(x)\right)^* g(x)dx \Rightarrow P^\dagger = P\end{aligned} \tag{6.183}$$

The i in front of the operator changes sign with conjugation, and allows the operator to be self adjoint. In both cases, the operator's adjoint had a simple form because we had the correct boundary conditions, that thus have a very important role in infinite dimensional vector spaces.

Since

$$\frac{d^2}{dx^2} \equiv D^2 = -P^2 \Rightarrow (D^2)^\dagger = D^\dagger D^\dagger = (-)^2 D^2 \tag{6.184}$$

the second derivative operator is self-adjoint. This has an important effect on the possible eigenvalues of the operator ∇^2.

6.5.4 Enumerable basis

We have seen that the operator $P = -i\frac{d}{dx}$ is self-adjoint. In the finite dimensional case, a self-adjoint operator has a orthonormal basis of eigenvectors with real eigenvalues. You can easily check that in the proof regarding the eigenvalue being real we did not use the fact that the space was finite or not, so that a self-adjoint operator *always* has real eigenvalues[11].

What is an eigenvalue of a linear operator like P? It is the solution of the differential equation

$$P|\alpha\rangle = \alpha|\alpha\rangle \tag{6.185}$$

We already know that a solution is given by the a ket such that

$$\langle x|n\rangle = \sqrt{\frac{1}{L}} e^{i\frac{2\pi n}{L}x} \tag{6.186}$$

the eigenvalue being

$$\frac{2\pi n}{L}, \qquad n \in \mathbb{Z} \tag{6.187}$$

[11] In quantum mechanics, these eigenvalues play the role of the values assumed by physical observables, and for this reason only self-adjoint operators may be used to build physical observables. This is the reason the momentum operator in Schrödinger's equation includes the i term.

We have already shown that

$$\frac{1}{L}\int_0^L e^{-i\frac{2\pi m}{L}} e^{i\frac{2\pi n}{L}} dx = \langle m|n\rangle = \delta_{m,n} \tag{6.188}$$

This is an enumerable basis for the functional vector space, since each function that is smooth enough may be written as

$$|f\rangle = \sum_n |n\rangle\langle n|f\rangle \tag{6.189}$$

The coefficients of the Fourier expansion are the

$$|f\rangle = \langle n|f\rangle = \sqrt{\frac{1}{L}}\int_0^L e^{i\frac{2\pi n}{L}} f(x)dx \tag{6.190}$$

The Dirac notations helps us in derive, remember and manipulate these relations. We may, for example, remember that the functions

$$s_{n_x}^{L_x}(x)s_{n_y}^{L_y}(y)s_{n_z}^{L_z}(z) = \langle x, y, z|n_x, n_y, n_z\rangle \tag{6.191}$$

are the eigenkets of the the operator ∇^2 with zero boundary conditions (the quantum particle in the box). As a result

$$\sum_{n_x=1}^{\infty}\sum_{n_y=1}^{\infty}\sum_{n_z=1}^{\infty} |n_x, n_y, n_z\rangle\langle n_x, n_y, n_z| = \mathbb{1} \tag{6.192}$$

so that

$$|f\rangle = \sum_{n_x=1}^{\infty}\sum_{n_y=1}^{\infty}\sum_{n_z=1}^{\infty} |n_x, n_y, n_z\rangle\langle n_x, n_y, n_z|f\rangle \tag{6.193}$$

You may compare this to eqs. (3.96,3.97).

Bibliography