Mathematical basics

1 The Schrödinger Equation

In this course we're interested in describing the behaviour of quantum particles. We'll motivate this further later on, but for the moment all you need to know, is that any such system is determined by the Schrödinger equation:

$$i\hbar\frac{\partial}{\partial t}\Psi(t) = H\Psi(t) \tag{1}$$

The left side of the equation is the time evolution operator acting on the time dependent wave-function $\Psi(\mathrm{t})$, while the right hand side is the Hamiltonian acting on the time dependent wave function. In order to understand this equation, you're going to need to understand 3 mathematical concepts:

- Complex numbers

- Differentiation

- Matrices and vectors

In this document we'll give a brief introduction for each of these concepts, but don't worry if you haven't fully understood them by the end of it; Over the next two weeks everything you've learned here will be re-used and re-learned multiple times.

1.1 Mathematics: Complex numbers

The equation above contains the letter i, which some of you may have recognized as denoting an imaginary number. What are complex and imaginary numbers, and how do we work with them?

If we try to calculate the square root of a negative number $-x \in \mathbb{R}^-$, there is no solution among the real numbers:

$$\sqrt{-x} \notin \mathbb{R} \tag{2}$$

However, as it turns out, for many problems in mathematics it is a very useful concept to have solutions to such equations! We therefore define *imaginary* numbers using the square root of -1:

$$i = \sqrt{-1} \tag{3}$$

Any real number can be multiplied with i to get an imaginary number: For $r \in \mathbb{R}$, $i\,r \in \mathbb{I}$. The square root of any negative number $-x \in \mathbb{R}^-$ is therefore given by $\sqrt{-x} = \sqrt{-1}\,\sqrt{x} = i\sqrt{x}$. However, imaginary numbers alone are not that useful; We need to be able to combine them with real numbers. We therefore define *complex* numbers by adding real numbers and imaginary numbers together. For $r_1, r_2 \in \mathbb{R}$, $r_1 + i\,r_2 \in \mathbb{C}$ is a complex number.

A complex number $c = r_1 + i \cdot r_2$ has a real part $\mathrm{Re}(c) = r_1$, and it also has an imaginary part $\mathrm{Im}(c) = r_2$. Both the real and imaginary parts are themselves real numbers.

Question 1. Algebra with complex numbers

Bring the following expressions into the standard form $r_1, r_2 \in \mathbb{R}$, $r_1 + i r_2 \in \mathbb{C}$:

1. $(a + ib) + (c + id)$
2. $(a + ib)(c + id)$
3. $(a + ib) / (c + id)$

Once you have done this, verify by doing the same calculations in the Notebook

1.1.1 Complex conjugate and Norm

We define the conjugate of a complex number $c = r_1 + i r_2$ as the complex number where the imaginary part changes sign:

$$c^\star = r_1 - i r_2 \tag{4}$$

With this, we also define the *norm* of complex numbers. A norm is a general concept in mathematics, an example you are likely familiar with is taking the absolute value of a real number: $\|r\| = |r|$ for $r \in \mathbb{R}$. We want the corresponding operation for the complex numbers, that fulfills the following axioms (rules) for any $c_1, c_2 \in \mathbb{C}$:

1. **Definiteness**: If and only if $\|c_1\| = 0$, then $c_1 = 0$.
2. **Absolute Homogeneity**: For any $r \in \mathbb{R}$, $\|r c_1\| = |r| \, \|c_1\|$.
3. **Triangle inequality**: $\|c_1 + c_2\| \leqslant \|c_1\| + \|c_2\|$.

We define the norm for complex numbers $c \in \mathbb{C}$ as

$$\|c\| = \sqrt{c^\star c}. \tag{5}$$

Question 2. Check the axioms using Julia

Go to the Julia notebook and try out different values to see that the above definition of the norm fulfills all axioms.

Question 3. OPTIONAL: Prove the Axioms

Verify that the norm as defined in equation 5 fulfils the axioms 1-3 for any complex number.

Hint: You may assume that for any real number $r \in \mathbb{R}$ $\sqrt{r^2} = |r|$.

Hint: You may want to show the triangle inequality holds for the absolute value of real numbers before you attempt to show it for complex numbers.

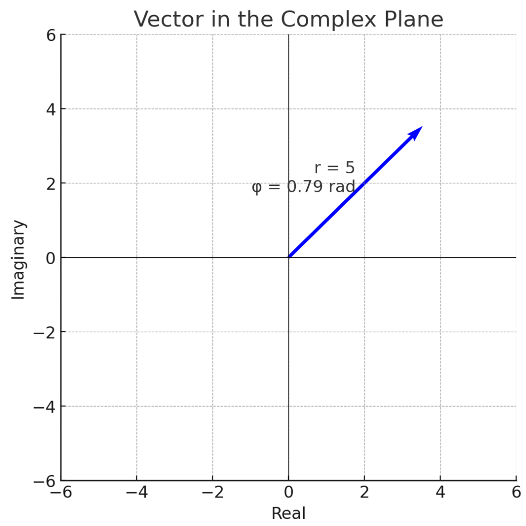

Figure 1. The complex plane

1.1.2 The complex plane

One useful concept for understanding complex numbers is the complex plane. We can imagine the real and imaginary parts of a complex number as two dimensions in a plane, with e.g. the x-axis corresponding to the real part, and the y-axis corresponding to the imaginary part, as seen in figure 1.

We can now try to understand the regular albebraic operations like addition, multiplication and division in the context of the complex plane.

Addition:

As we saw earlier, for addition (and thereby also subtraction), the real and imaginary parts can be treated independently. The resulting vector (or "arrow" in the plane) is therefore constructed by simply adding the two vectors together.

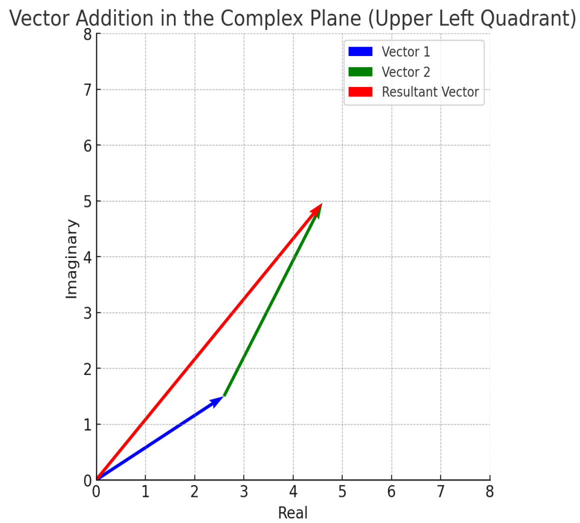

Figure 2.

Subtracting a complex number from another is done simply by adding the negative of the number. We can also see how to construct the real and imaginary parts of a complex number this way. For $c = r_1 + i r_2,\ r_1, r_2 \in \mathbb{R}$:

$$\mathrm{Re}(c) = \frac{1}{2}(c + c^\star) = r_1 \tag{6}$$

$$\mathrm{Im}(c) = \frac{1}{2i}(c - c^\star) = r_2 \tag{7}$$

Question 4. Addition in the complex plane

Draw the addition and subtraction for some vectors in the complex plane in the julia notebook or on paper. Convince yourself that the above definitions for the real and complex parts are true, and understand the geometric reasoning behind this.

Question 5. Multiplication in the complex plane

Before you read on, head to the Notebook, and play around with the multiplication of different complex numbers. Pay special attention to how the vectors rotate, and how they become longer or shorter when multiplied. Can you see how each of these is determined?

Multiplication in the complex plane

Multiplying complex numbers is a little less straightforward to understand. While writing complex numbers as the sum of real and imaginary parts has served us well so far, it is time to replace this representation with another. Looking at the vector in the complex plane it becomes clear that we can specify it by an angle of rotation and the length of the vector as seen in fig 1.

To swap between the two representations we need a way to calculate the real and imaginary parts of the complex number from the angle and the length of the vector. For this, we dust off our old knowledge from geometry, and remember that for a vector in two dimensions the x-component is given by

$$x = r\cos(\phi) \tag{8}$$

and the y-component is given by

$$y = r\sin(\phi). \tag{9}$$

Here $r \in \mathbb{R}^{+,0}$ is the length of the vector, and ϕ is the angle it encloses with the x-axis. We arbitrarily choose the x-axis for this, since we identified the real part with the x-axis, and an angle of 0 corresponding to real numbers makes a lot of equations look nicer. With this in mind, we can rewrite any complex number as

$$c = r(\cos(\phi) + i\sin(\phi)) \tag{10}$$

NOTE: On specifying angles

You may be used to thinking about angles in terms of degrees, from 0 to 360. We will use the more natural definition, as it arises from the connection to the unit circle, and specify angles as real numbers from 0 to 2π.

Question 6. Complex algebra in polar coordinates

Bring the following expression into the standard form $r \in \mathbb{R}^{+,0}$, $\phi \in [0,\, 2\pi]$, $r(\cos(\phi) + i\sin(\phi)) \in \mathbb{C}$:

$$r_1(\cos(\phi_1) + i\sin(\phi_1))\, r_2(\cos(\phi_2) + i\sin(\phi_2)) \tag{11}$$

Hint: In order to do this, you will need these trigonometric identities:

$$\sin(\phi_1)\sin(\phi_2) = \frac{1}{2}(\cos(\phi_1 - \phi_2) - \cos(\phi_1 + \phi_2)) \tag{12}$$

$$\cos(\phi_1)\cos(\phi_2) = \frac{1}{2}(\cos(\phi_1 - \phi_2) + \cos(\phi_1 + \phi_2)) \tag{13}$$

1.2 Mathematics: Differential equations

We define the derivative of a function $f: \mathbb{R} \to \mathbb{R}$ as

$$\frac{\partial f(x)}{\partial x} = \lim_{\Delta x \to 0} \frac{f(x + \Delta x) - f(x)}{\Delta x} \tag{14}$$

This can be understood as the slope of the function at point x. The symbol $\lim_{x \to 0}$ denotes the *limit* of Δx going to zero. Limits are an entire field in mathematics by themselves, but for our purposes it is sufficient to think of this as meaning that Δx is very, very small. The smaller Δx is, the more accurate the expression becomes.

Question 7. Verify the derivative of a linear function

Verify that the derivative of the linear function $f: \mathbb{R} \to \mathbb{R}$, $f(x) = ax + b$ is equal to the slope a.

OPTIONAL: Calculate the general form for the derivative of a polynomial x^n.

Equation 14 is only an exact equality if Δx truly goes to zero. However, it is still approximately true, even if Δx is only very small, not zero. In this case, we can rephrase the equation as

$$f(x + \Delta x) \approx f(x) + \Delta x \frac{\partial f(x)}{\partial x} \tag{15}$$

This lets us interpret the derivative of a function as the linear approximation around x. As long as Δx is small, this is the linear function in Δx which makes the smallest error compared to the true function $f(x)$.

Question 8. Operations with the derivative

1. Show that taking the derivative is a linear operation:

$$\frac{\partial (f + g)(x)}{\partial x} = \frac{\partial f(x)}{\partial x} + \frac{\partial g(x)}{\partial x} \tag{16}$$

2. Based on the linearity of the derivative, consider how it may be generalized to complex valued functions $f: \mathbb{R} \to \mathbb{C}$ by treating the real and imaginary parts seperately.

3. Show that the second derivative $\frac{\partial^2 f(x)}{\partial x^2}$ (applying the derivative twice) can be written as

$$\frac{\partial^2 f(x)}{\partial x^2} = \lim_{\Delta x \to 0} \frac{f(x + \Delta x) - 2f(x) + f(x - \Delta x)}{\Delta x} \tag{17}$$

Hint: You can shift the argument x by Δx without changing the expression, since Δx is supposed to go to zero.

1.2.1 The Euler equation

Now that we have an understanding of what the derivative is, and how to evaluate it, it is time to look at differential equations. A differential equation is any equation which contains derivatives of a function with respect to one or more of its variables; However, for the moment, we are only interested in the Euler equation with $c \in \mathbb{C}$, $t \in \mathbb{R}$, $f: \mathbb{R} \to \mathbb{C}$.

$$\frac{\partial f(t)}{\partial t} = c f(t), f(0) = f_0 \tag{18}$$

In order to solve this, we insert the definition for the derivative which we saw earlier:

$$\lim_{\Delta t \to 0} \frac{f(t + \Delta t) - f(t)}{\Delta t} = c f(t). \tag{19}$$

We will ignore the limit of $\Delta t \to 0$ for now, and treat Δt as being merely a small real number. Doing this allows us to phrase t as $t = n\Delta t$, with $n \in \mathbb{N}$. We then rephrase the equation above as

$$f((n+1)\Delta t) = c f(n\Delta t)\Delta t + f(n\Delta t). \tag{20}$$

In the following we will adopt index-notation to make the formulas easier to grasp, so

$$f(n\Delta t) := f_n. \tag{21}$$

We can then write equation 20 as

$$f_{n+1} = (c\Delta t + 1) f_n. \tag{22}$$

We can now solve the discretized differential equation. We have assumed that at time $t = 0$, we have some value for the function $f(0) = f_0$. This is called the initial condition, and it is necessary to define the solution of the differential equation. This is because the differential equation only specifies the rate of change, so the value at every point in time depends on that previously - There needs to be a starting point, which we define to be $t = 0$.

The solution is then given by

$$f_n = (c\Delta t + 1)^n f_0. \tag{23}$$

It is possible to see this by looking at equation 22: If we multiply by a factor of $(c\Delta t + 1)$ at every time step, then after n steps, we will have multiplied n times. Repeated multiplication is exponentiation, so we get an exponent of n.

We can now go back to our initial way of looking at the equation, and rewrite it as:

$$f(t) = (c\Delta t + 1)^{t/\Delta t} f(0). \tag{24}$$

If we execute the limit, that we had ignored at the very beginning, this is a definition of the exponential function:

$$e^{ct} = \lim_{\Delta t \to 0} (c\Delta t + 1)^{t/\Delta t} \tag{25}$$

Going back to complex numbers, we can now create a correspondence between the solution to our differential equation e^{ct} and the general way to write complex numbers. For this, we use the Euler-equality, which states

$$e^{i\phi} = \cos(\phi) + i\sin(\phi)$$

for any $\phi \in \mathbb{R}$. With this, we can rewrite our solution as

$$f(t) = e^{\mathrm{Re}(c)\,t}(\cos(\mathrm{Im}(c)\,t) + i\sin(\mathrm{Re}(c)\,t)).$$

Provided the real part of c is zero, the solution to the differential equation therefore corresponds exactly to a rotation in the complex plane. On the other hand, if the imaginary part of c is zero, the solution corresponds to exponential growth or decrease.

Question 9. Visualize the solution

Go to the Julia Notebook in chapter INSERT HERE and do the exercises for visualizing the solution to the Euler equation.

1. Plot e^{ct} for real, imaginary and complex c. What do you observe?

2. Plot the solution as calculated by iteratively applying the rule

$$f_n = (c\Delta t + 1)^n f_0.$$

   Vary Δt and n, and observe how the solution differs from the exact solution.

Question 10. OPTIONAL: Fun with the exponential function

There are 3 ways to define the exponential function e^x:

1. $\frac{\partial}{\partial x} e^x = e^x$ and $e^0 = 1$

2. $e^x = \sum_{n=0}^{\infty} \frac{x^n}{n!}$

3. $e^n = \lim_{n\to\infty} (x/n + 1)^n$

Show that these definitions are equivalent. Then show that from (one of) these definitions follows that

$$e^x = (e^1)^x$$

with the usual definition of exponentiation ($a^y \cdot a^x = a^{x+y}$).

Question 11. Rephrasing the Schrödinger equation

The Schrödinger equation for a 1-D particle in a potential well (in natural units, so $\hbar = 1$ and mass is 1) is

$$i\frac{\partial}{\partial t}\Psi(x,t) = H\Psi(x,t) = \frac{1}{2}\frac{\partial^2}{\partial x^2}\Psi(x,t) + V(x)\Psi(x,t)$$

Rephrase this equation as a finite difference equation in both time and space.

1.3 Matrices and Vector spaces

Space - the 3 dimensional space that we live in - is one example of a *vector space*. Every point in space can be labelled with a single vector, in our case with 3 components:

$$\vec{x} = \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix}$$

In general, a vector can be N-dimensional, so it will have N components. We can add and subtract vectors, and calculate their length via the norm. For a N-dimensional vector with entries $x_i, i \in \{1, \ldots, \mathrm{N}\}$ the norm is given by summing the squares of all components and taking the square root

$$\|\vec{x}\| = \sqrt{\sum_{i=1}^{N} x_i^2}.$$

1.3.1 Linear Transformations

We can act on vectors with linear transformations. One example would be a rotation. Given a vector in the 2D plane $\vec{x} = \left(\begin{smallmatrix} 1 \\ 0 \end{smallmatrix}\right)$, we can rotate it by 90° to get $\vec{x} = \left(\begin{smallmatrix} 0 \\ 1 \end{smallmatrix}\right)$. This rotation corresponds to a 2x2 *matrix*. In this case the rotation matrix is given by

$$A = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}.$$

In order to apply a matrix to a vector (and thereby transform the vector) the matrix and vector are multiplied:

$$A\,\vec{x} = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

For a general 2x2 matrix the multiplication works like this:

$$\begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} a_{11}\,x_1 + a_{12}x_2 \\ a_{21}x_1 + a_{22}x_2 \end{pmatrix}$$

The general rule is that the first entry in the new vector contains the element-wise product of the first row of the matrix with the vector. The second entry in the new vector is the element-wise product of the second row of the matrix with the vector, and so forth.

We can denote the elements of a matrix A as a_{ij}, where i denotes the row of the element, and j the column. Then matrix-0vector multiplication is written as

$$(A\vec{x})_i = \sum_{j=1}^{N} a_{ij} x_j. \tag{26}$$

Question 12. Matrix-vector multiplication

Calculate the matrix-vector product $\left(\begin{smallmatrix} 2 & -3 \\ 5 & 1 \end{smallmatrix}\right)\left(\begin{smallmatrix} 1 \\ 5 \end{smallmatrix}\right)$

Question 13. Show that the matrix-vector product is linear

Show that $A(\,\vec{x} + \vec{y}) = A\vec{x} + A\vec{y}$

Hint: Use equation 26

1.3.2 Eigenvectors and Eigenvalues

An *eigenvector* $\vec{x}_{\mathrm{eig}}$ of a matrix is a vector which is simply rescaled by the matrix, without changing its direction. The factor by which it is rescaled, $\epsilon \in \mathbb{C}$, is called an *eigenvalue*.

$$A\,\vec{x}_{\mathrm{eig}} = \epsilon\,\vec{x}_{\mathrm{eig}}$$

A *hermitian* NxN matrix has entries for which $a_{ij} = a^{\star}_{ji}$ is true. It always has exactly N eigenvalues, which are all real.

An example is the matrix $\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$. It has the eigenvectors $\vec{x}_1 = \begin{pmatrix} 1 \\ -1 \end{pmatrix}$ with eigenvalue $\epsilon_1 = -1$ and $\vec{x}_2 = \begin{pmatrix} 1 \\ 1 \end{pmatrix}$ with eigenvalue $\epsilon_2 = 1$.

Question 14. Find Eigenvalues

1. Find the eigenvectors and eigenvalues for the matrix $\begin{pmatrix} -2 & 0 \\ 0 & 1 \end{pmatrix}$ by hand

2. Go to the julia notebook, and numerically calculate the eigenvectors and eigenvalues for the matrix

$$A = \begin{pmatrix} -2 & 0 & 0 \\ 0 & 3 & 1 \\ 0 & 1 & 3 \end{pmatrix}$$

   Verify the results by doing the matrix-vector multiplication for each eigenvector by hand.

   Hint: The correct result has eigenvectors and eigenvalues with integer entries.