FRIB-TA summer school

A practical walk through formal scattering theory

Kévin Fossez

MICHIGAN STATE UNIVERSITY

Argonne
NATIONAL LABORATORY

U.S. DEPARTMENT OF ENERGY | Office of Science

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Review of basic concepts (D1-M1, 1h)

- Hilbert space and quantum mechanics.

- Coordinate- vs. momentum-space representations.

- The Schrödinger equation and the two body problem.

- Inhomogeneous second order differential equation.

- Complex analysis.

Hilbert space and quantum mechanics

The concept of Hilbert space is used in quantum mechanics because, fundamentally, it corresponds with the way one thinks about quantum systems.

A Hilbert space is defined as:

A vectorial space with a scalar product and in which any Cauchy series (sequence) converges.

State of/information about a quantum system = vector $|\Psi\rangle$.

Amplitude of probability $\langle\Psi|\Phi\rangle$ instead of probability, norm $||\Psi||^2 = \langle\Psi|\Psi\rangle$.

Complete space = for a series $|\psi_l\rangle$ with $||\psi_l - \psi_m|| \to 0$ when $l, m \to \infty$, $\exists |\psi\rangle$ so that $||\psi_l - \psi|| \to 0$ when $l \to \infty$.

Allows superposition.

Interference experiments.

No "hole" in the space of quantum states.

Hilbert space and quantum mechanics

Postulates of quantum mechanics:

1) All the information on a physical system is contained in its state $|\Psi\rangle$ defined in a Hilbert space H, with $\langle\Psi|\Psi\rangle = 1$.

2) If $|\Psi\rangle$ and $|\Phi\rangle$ are states of a system, the amplitude of probability for the system to change from $|\Phi\rangle$ to $|\Psi\rangle$ is $a(\Phi \rightarrow \Psi) = \langle\Psi|\Phi\rangle$.

The probability is given by: $p(\Phi \rightarrow \Psi) = |a(\Phi \rightarrow \Psi)|^2 = \langle\Psi|\Phi\rangle^2$.

Hilbert space and quantum mechanics

Postulates of quantum mechanics:

3) For each (physical) property A of a system, it exists an Hermitian operator $\hat{A}$ ($\hat{A}^\dagger = \hat{A}$) acting on states of the system $\{|\Psi\rangle\} \in H$.

$$\hat{A}\,|\Psi_n\rangle = a_n\,|\Psi_n\rangle \quad \Rightarrow \quad \hat{A} = \sum_n a_n\,|\Psi_n\rangle\langle\Psi_n|$$

4) The time evolution of a closed quantum system is given by:

$$i\hbar\frac{d\,|\Psi(t)\rangle}{dt} = \hat{H}(t)\,|\Psi(t)\rangle$$

This is the Schrödinger equation. See also the evolution operator $\hat{U}(t, t')$ later.

Hilbert space and quantum mechanics

Some troubles:

1. In a scattering experiment, one might want to know something about the position $|\mathbf{r}\rangle$ or momentum $|\mathbf{p}\rangle$ of the particles, however $\langle \mathbf{r}'|\mathbf{r}\rangle = \delta(\mathbf{r} - \mathbf{r}') \neq 1$, which is zero everywhere except in $\mathbf{r} = \mathbf{r}'$ where it diverges…

   The ill formulation of QM in the Hilbert space was already known at its foundation (P. Dirac, J. von Neumann), see the concept of rigged Hilbert space (RHS) later.

2. In an open quantum system (OQS) i.e. a system coupled to an environment, the time evolution is not unitary anymore.

   This aspect is important when discussing decaying resonances (loss of particle).

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The r- and p- representations

In actual calculations, the abstract vectors (states) and operators acting in the Hilbert space are expressed in a given representation.

For example, one might want to know the probability $P(\psi, \mathbf{r})$ of finding a particle in a state $|\psi\rangle$ at the position $\mathbf{r}$. According to postulate 3) there should be an operator $\hat{P}_{\mathbf{r}}$ that projects the state $|\psi\rangle$ on the state $|\mathbf{r}\rangle$ associated with the position $\mathbf{r}$, since the position is a physical property.

$$\hat{P}_{\mathbf{r}}|\psi\rangle = a_{\mathbf{r}}|\mathbf{r}\rangle$$

Obviously, $\hat{P}_{\mathbf{r}} = |\mathbf{r}\rangle\langle\mathbf{r}|$ is a projector ($\hat{P}_{\mathbf{r}}^2 = \hat{P}_{\mathbf{r}}$), $a_{\mathbf{r}} = \langle\mathbf{r}|\psi\rangle = \psi(\mathbf{r})$ is the wave function, and $P(\psi, \mathbf{r}) = |\psi(\mathbf{r})|^2$.

The r- and p- representations

In more details, what is meant by $|\mathbf{r}\rangle$ is the tensor product of, for example, the vectors $|x\rangle$, $|y\rangle$, and $|z\rangle$ associated with the corresponding Cartesian coordinates. It can be useful to show that:

$$\int_{\mathbf{r}} d\mathbf{r} |\mathbf{r}\rangle\langle\mathbf{r}| = 1 \quad \Rightarrow \quad |\psi\rangle = \int_{\mathbf{r}} d\mathbf{r} |\mathbf{r}\rangle\langle\mathbf{r}|\psi\rangle$$

with $\langle\mathbf{r}|\mathbf{r}'\rangle = \delta^3(\mathbf{r} - \mathbf{r}')$ is the Dirac distribution.

However, in many spherical problems (e.g. scattering exp.), spherical coordinates $\mathbf{r} = (r, \theta, \phi)$ are preferred and instead the distance $r = |\mathbf{r}|$ is considered directly while the angular part is treated in the angular momentum representation using spherical harmonics $\langle\theta, \phi | l, m_l\rangle = Y_{l,m_l}(\theta, \phi)$:

$$\langle\mathbf{r}|\psi\rangle = \psi(\mathbf{r}) = R(r)Y_{l,m_l}(\theta, \phi)$$

The r- and p- representations

It is of course possible to follow the same reasoning using the momentum **p** of a particle. In this case, one can show that:

$$\int_{\mathbf{p}} d\mathbf{p} \, |\mathbf{p}\rangle\langle\mathbf{p}| = 1$$

We say that the $\{|\mathbf{r}\rangle\}$ and $\{|\mathbf{p}\rangle\}$ vectors form continuous bases. The important point here is that these are different representations of the same abstract objects and must be equivalent.

How we go from one representation to another depends on each case, but for these bases one has the Fourier transforms:

$$|\mathbf{p}\rangle = \frac{1}{(2\pi\hbar)^{3/2}} \int_{\mathbf{r}} = d^3\mathbf{r} \, |\mathbf{r}\rangle e^{+\frac{i}{\hbar}\mathbf{p}.\mathbf{r}} \qquad\qquad |\mathbf{r}\rangle = \frac{1}{(2\pi\hbar)^{3/2}} \int_{\mathbf{r}} = d^3\mathbf{p} \, |\mathbf{p}\rangle e^{-\frac{i}{\hbar}\mathbf{p}.\mathbf{r}}$$

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The Schrödinger eq. and the 2-body problem

We saw that the time evolution of a quantum system is given by the Schrödinger eq. (postulate 4). When considering stationary (= time independent) solutions, this equation becomes:

$$i\hbar\frac{d\,|\,\Psi(t)\rangle}{dt} = \hat{H}(t)\,|\,\Psi(t)\rangle \quad \Rightarrow \quad \hat{H}\,|\,\Psi\rangle = E\,|\,\Psi\rangle$$

where E is the energy of the system. We usually divide solutions into two groups: $E < 0$ (bound states), and $E > 0$ (scattering and resonant states). The special case of resonant states might seem odd as these are not stationary properly speaking (see quasi-stationary formalism later).

In nuclear physics, this separation gave rise to a "traditional" divide between the studies of nuclear structure and reactions. Their theoretical unification is a major goal in the field.

The Schrödinger eq. and the 2-body problem

If we want stationary solutions of the two-body problem in r- space using spherical coordinates, we need to solve:

$$(\hat{T} + \hat{V})|\Psi\rangle = E|\Psi\rangle$$

Where $\hat{T}$ is the kinetic energy of the system and $\hat{V}$ is the potential between the two particles.

If we denote the positions (momenta) of the two particles $\mathbf{r}_1$ and $\mathbf{r}_2$ ($\mathbf{p}_1$ and $\mathbf{p}_2$), and their masses m_1 and m_2, we can express the position and momentum of the center-of-mass (COM) of the system as:

$$\mathbf{R} = \frac{m_1\mathbf{r}_1 + m_2\mathbf{r}_2}{m_1 + m_2} \qquad\qquad \mathbf{P} = \mathbf{p}_1 + \mathbf{p}_2$$

The Schrödinger eq. and the 2-body problem

Similarly, one can define the relative motion and momentum of the two particles:

$$\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2 \qquad\qquad \mathbf{p} = \frac{m_2 \mathbf{p}_1 - m_1 \mathbf{p}_2}{m_1 + m_2}$$

The interest of this change of coordinates is that while the Hilbert space $\mathscr{E}^{(\mathbf{r}_1)} \otimes \mathscr{E}^{(\mathbf{r}_2)}$ cannot be factorized, the perfectly equivalent Hilbert space $\mathscr{E}^{(\mathbf{r})} \otimes \mathscr{E}^{(\mathbf{R})}$ can, and the COM part has no effect on the properties of the system!

We can rewrite the Hamiltonian as:

$$H = \frac{\mathbf{P}^2}{2(m_1 + m_2)} + \frac{\mathbf{p}^2}{2\mu} + V(r)$$

where $\mu = m_1 m_2 / (m_1 + m_2)$ is the reduced mass.

We assume a spherical potential.

The Schrödinger eq. and the 2-body problem

Since we can neglect the COM contribution, the two-body Hamiltonian to consider is just:

$$H = \frac{\mathbf{p}^2}{2\mu} + V(r)$$

The first term is the relative kinetic energy, which in r- space writes:

$$\frac{\mathbf{p}^2}{2\mu} = -\frac{\hbar^2}{2\mu}\Delta_{\mathbf{r}}$$

In spherical coordinates, the Laplacian operator writes:

$$\Delta_{\mathbf{r}} = \frac{1}{r}\frac{d^2}{dr^2}(r\cdot) + \frac{1}{r^2 \sin\theta}\frac{d}{d\theta}(\sin\theta\frac{d}{d\theta}) + \frac{1}{\sin^2\theta}\frac{d^2}{d\phi^2}$$

$$\frac{1}{r}\frac{d^2}{dr^2}(r\cdot) = \frac{d}{dr}(r^2\frac{d\cdot}{dr})$$

The Schrödinger eq. and the 2-body problem

It is then possible to show that:

$$L^2 = -\hbar^2 \left(\frac{1}{r^2 \sin\theta} \frac{d}{d\theta} (\sin\theta \frac{d}{d\theta}) + \frac{1}{\sin^2\theta} \frac{d^2}{d\phi^2} \right)$$

where L is the orbital angular momentum operator associated with $\mathbf{L} = \mathbf{r} \wedge \mathbf{p}$. We can write:

$$H = -\frac{\hbar^2}{2\mu} \frac{1}{r} \frac{d^2}{dr^2}(r\cdot) + \frac{L^2}{2\mu} + V(r)$$

Using the fact that the eigenvectors of the $\hat{L}^2$ operator commute with $\hat{H}$, the solutions must be eigenvectors of both, and thus on can assume:

$$\Psi(r, \theta, \phi) = R_{n,l,m}(r) Y_{l,m}(\theta, \phi)$$

The Schrödinger eq. and the 2-body problem

Finally, by defining the reduced radial wave function $u_{n,l}(r) = rR_{n,l}(r) = rR_{n,l,m}(r)$ and treating the angular part separately (it is independent), one obtains the standard radial stationary Schrödinger equation:

$$\left(-\frac{\hbar^2}{2\mu}\frac{d^2}{dr^2} + \frac{\hbar^2 l(l+1)}{2\mu r^2} + V(r) \right) u_{n,l}(r) = E_{n,l} u_{n,l}(r)$$

This is the equation that one needs to solve to find the radial wave functions of bound (E<0) and scattering states (E>0), but also for resonances modulo some tricks and limitations.

Because it is a differential equation (inhomogeneous, 2nd order), the only thing missing are the boundary conditions in $r = 0$ and $r \to \infty$. In the integral formulation (Lippmann-Suchwinger) those are already included (see later).

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- **Inhomogeneous second order differential equation.**

- Complex analysis.

Inhomogeneous 2nd order differential eq.

There are a few "methods" to solve the following type of equation and find $y(x)$:

$$y''(x) + b(x)y'(x) + c(x)y(x) = f(x)$$

Typically, the "variation of parameters" method, also sometimes called the "constant variable" method (bad name), is the most reliable approach. Essentially, it reduces a second order differential equation into a system of two first order differential equations.

Another way to think about this method is to say rather loosely that the general solution is the sum of the solution $y_0(x)$ to the associated homogeneous equation (i.e. $f(x) = 0$) and a particular solution $y_p(x)$ to the inhomogeneous equation.

It is thus clear that this method only works if one can get our hands on $y_0(x)$ at the very least. All other approaches involve some form of guessing.

Inhomogeneous 2nd order differential eq.

The first step is to write the general solution for both the inhomogeneous and homogeneous equations:

$$y_0(x) = c_1 y_1(x) + c_2 y_2(x)$$

$$y(x) = c_1(x)y_1(x) + c_2(x)y_2(x)$$

where in the first eq. $c_{1,2}$ are constants, while in the second case they are functions. There are two components $y_{1,2}(x)$ because it is a second order equation.

Inhomogeneous 2nd order differential eq.

Then, one looks at the first derivatives:

$$y_0'(x) = c_1 y_1'(x) + c_2 y_2'(x)$$

$$y'(x) = c_1'(x)y_1(x) + c_1(x)y_1'(x) + c_2'(x)y_2(x) + c_2(x)y_2'(x)$$

Since in the limit $f(x) \to 0$ one must have $y'(x) \to y_0'(x)$, it is easy to see that one must have:

$$c_1'(x)y_1(x) + c_2'(x)y_2(x) = 0$$

This condition can be seen as a continuity condition.

Inhomogeneous 2nd order differential eq.

Then, one looks at the second derivative:

$$y''(x) = c_1'(x)y_1'(x) + c_1(x)y_1''(x) + c_2'(x)y_2'(x) + c_2(x)y_2''(x)$$

The inhomogeneous equation then writes:

$$c_1'(x)y_1'(x) + c_1(x)y_1''(x) + c_2'(x)y_2'(x) + c_2(x)y_2''(x)$$
$$+b(x)[c_1(x)y_1'(x) + c_2(x)y_2'(x)]$$
$$+c(x)[c_1(x)y_1(x) + c_2(x)y_2(x)] = f(x)$$

Inhomogeneous 2nd order differential eq.

It can be rearranged into:

$$c_1'(x)y_1'(x) + c_2'(x)y_2'(x)$$

$$+c_1(x)[y_1''(x) + b(x)y_1'(x) + c(x)y_1(x)]$$

$$+c_2(x)[y_2''(x) + b(x)y_2'(x) + c(x)y_2(x)] = f(x)$$

but since $y_{1,2}(x)$ are solutions of the homogeneous equation, one is left with:

$$c_1'(x)y_1'(x) + c_2'(x)y_2'(x) = f(x)$$

This gives the second condition to solve an inhomogeneous second order differential equation.

Inhomogeneous 2nd order differential eq.

We can thus say that solving:

$$y''(x) + b(x)y'(x) + c(x)y(x) = f(x)$$

Is the same as solving:

$$y(x) = c_1(x)y_1(x) + c_2(x)y_2(x)$$

$$c_1'(x)y_1(x) + c_2'(x)y_2(x) = 0$$

$$c_1'(x)y_1'(x) + c_2'(x)y_2'(x) = f(x)$$

We will use this method to solve the Schrödinger equation for the two-body problem for any potential and at any energy. The functions $c_{1,2}(x)$ will be the Jost functions.

Inhomogeneous 2nd order differential eq.

Warm-up analytical example:
$$y'' - 5y' + 4y = e^{4x}$$

- Roots of the associated polynom:

$$r_{1,2} = \frac{-(-5) \pm \sqrt{(-5)^2 - 4 \times 1 \times 4}}{2 \times 1} = 4,1$$

- Solution of the form:

$$y(x) = C_1(x)e^{4x} + C_2(x)e^x$$

- Conditions:

$$C_1'(x)e^{4x} + C_2'(x)e^x = 0$$
$$C_1'(x)(e^{4x})' + C_2'(x)(e^x)' = e^{4x}$$

$\longrightarrow$

$$C_2'(x) = 0$$
$$C_1'(x) = \frac{1}{3}$$

$\longrightarrow$

$$C_2(x) = C_2$$
$$C_1(x) = \frac{x}{3} + a$$

Finally:
$$y(x) = \left(\frac{x}{3} + a\right)e^{4x} + C_2 e^x$$

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Complex analysis

It is not a secret that quantum mechanics makes use of complex numbers, but scattering theory in particular uses a fair amount of complex analysis.

As a reminder, the complex plane is traditionally divided into four quadrants:
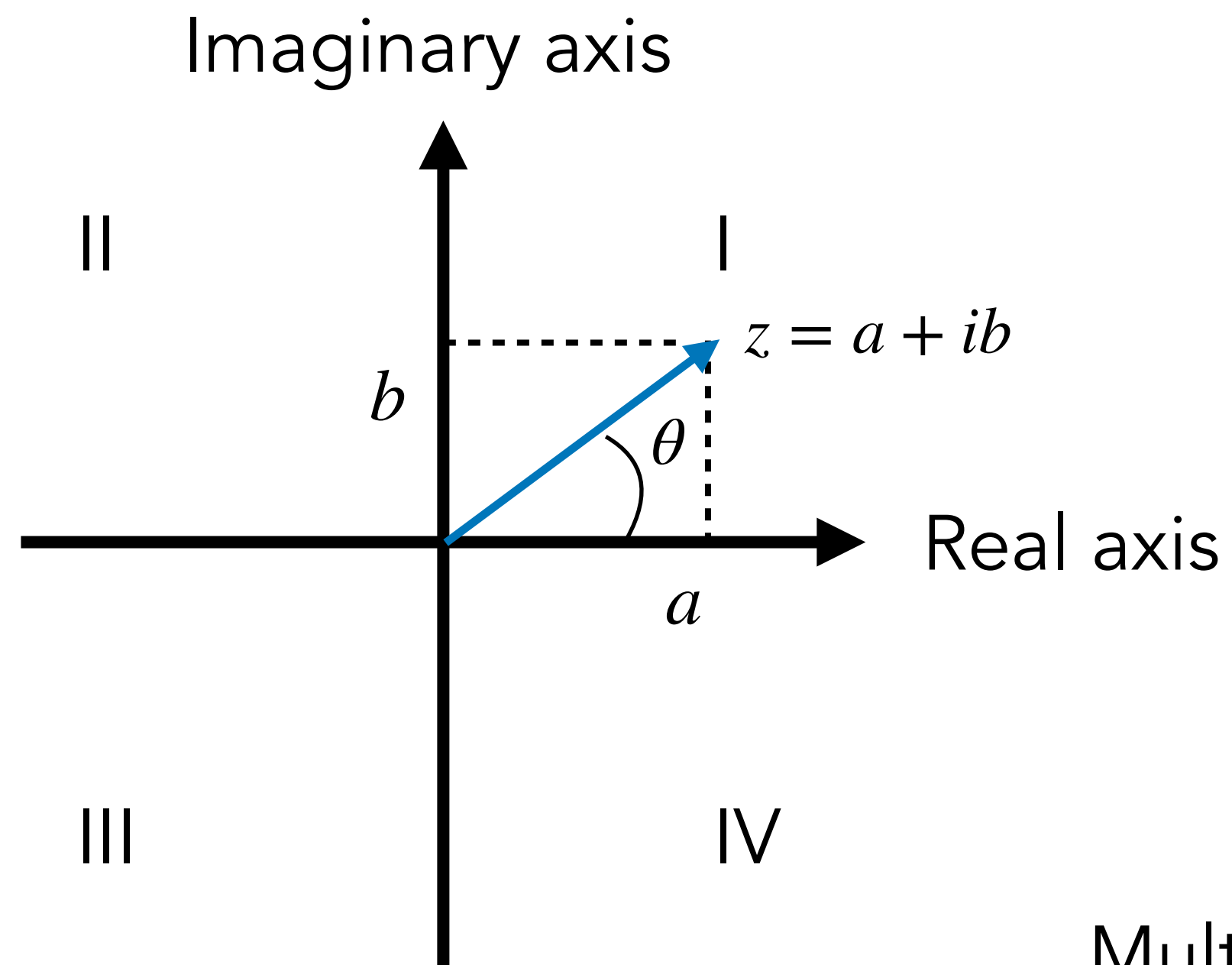
Complex numbers are written:
$z = a + ib$ with $i^2 = -1$ and a, b real, or $z = |z| e^{i\theta}$ with θ real in polar coordinates.

Also: $e^{i\theta} = \cos\theta + i\sin\theta$

Multiplying by a complex number = rotation + elongation.
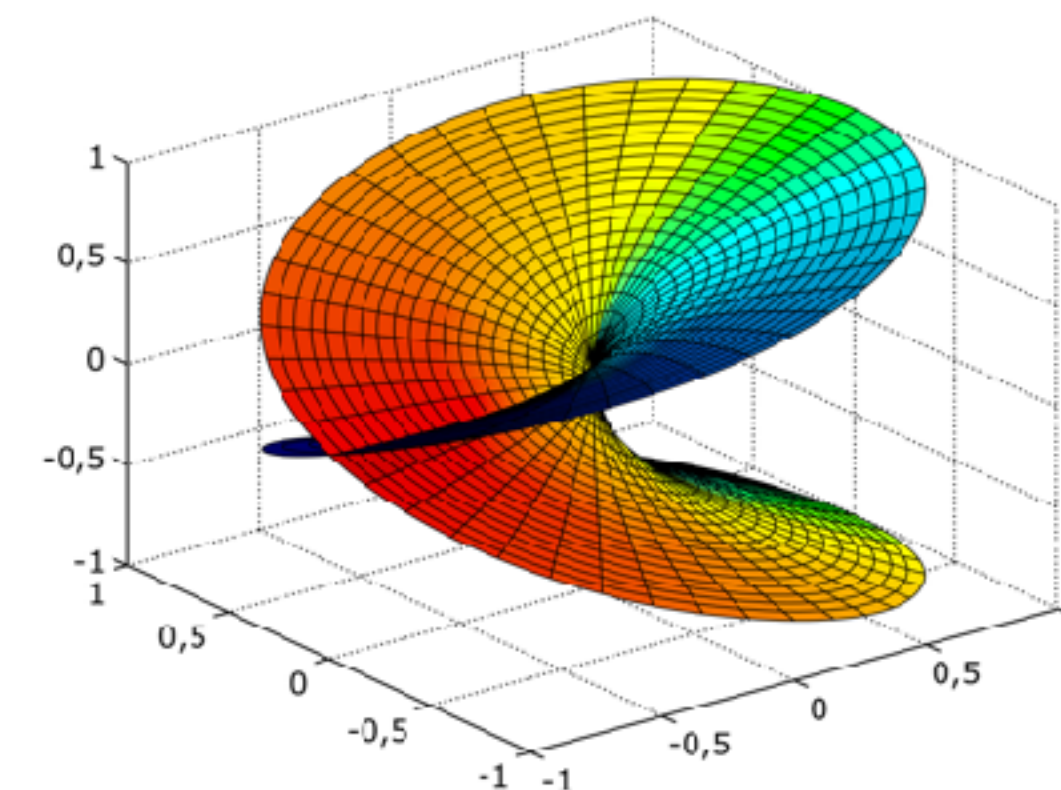
Complex analysis

The analytical continuation of a real fonction in the complex plane is, loosely speaking, the extension of the domain of the fonction to complex numbers, sometimes by redefining the function a little bit.

The typical (easy) example is the exponential e^x defined on the whole real axis. By using its expression as a series:

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

and by replacing x by a complex number z, one can evaluate the exponential function in the complex plane. In practice, it is not always that simple.

The "result" of a complex function can also be represented by a Riemann surface. Example: $f(z) = \sqrt{z}$.

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Complex analysis

A **pole** of order n of an analytical function $f(z)$ is an isolated point z_0 where the function is singular and behaves as $1/z^n$ with n positive.

One can show that around a pole, an analytical function $f(z)$ can be written uniquely as a Laurent series:

$$f(z) = \sum_{n=1}^{\infty} \frac{b_n}{(z - z_0)^n} + \sum_{n=0}^{\infty} a_n(z - z_0)^n$$

The **residue** of $f(z)$ at the pole z_0 is simply b_1.

$$\mathbf{Res}_{z=z_0}(f) = b_1$$

Complex analysis

Cauchy's integral theorem. If a function $f(z)$ is analytical on and inside a closed contour γ:

$$\oint_\gamma f(z)dz = 0$$

However, if the function has n poles z_k inside the contour, **Cauchy's residue theorem** gives for γ counter-clockwise:

$$\oint_\gamma f(z)dz = 2\pi i \sum_{k=1}^{n} \operatorname*{Res}_{z=z_k}(f) \qquad \operatorname*{Res}_{z=z_k}(f) = \frac{1}{2\pi i} \oint_{\gamma_k} f(z)dz$$

Sometimes residues can be calculated like this.

where γ_k is a contour around z_k only. For a simple pole (order 1) z_k :

$$\operatorname*{Res}_{z=z_k}(f) = \lim_{z \to z_k} (z - z_k)f(z)$$