Analysis $\underline{\overline{IV}}$

(for EL, GM, MX)

Week 14 - 26.05.25

Last week:

We solved the initial value problem for the heat and the wave equations, defined for $x \in \mathbb{R}$. We obtained a solution by applying the Fourier transform in the x variable and then solving the corresponding ODE in time.

Let's see one more example:

The Schrödinger equation:

Suppose that $u : \mathbb{R} \times (0, +\infty) \longrightarrow \mathbb{C}$ solves the following equation:

$$i\frac{\partial u}{\partial t}(x,t) + \frac{\partial^2 u}{\partial x^2}(x,t) - V(x,t)\cdot u(x,t) = 0 \qquad (1)$$

for $t>0$, $x \in \mathbb{R}$.

This is the Schrödinger equation with potential V.

- The potential is always assumed to be real valued (i.e. $V(x,t) \in \mathbb{R}$ $\forall x,t$)
- The solution u is necessarily complex valued, in view of the presence of i in the equation.

Physical interpretation: The above equation describes the evolution of a quantum particle moving under the influence of a (classical) potential $V(x,t)$.

The quantity $\int_a^b |u(x,t)|^2 \, dx$ is the probability that the particle at time t is in the interval $a \leq x \leq b$.

- In order for the above "probabilistic" interpretation to make sense, we must have $\int_{-\infty}^{+\infty} |u(x,t)|^2 \, dx = 1$ for all times.

In particular, $\int_{-\infty}^{+\infty} |u(x,t)|^2 \, dx$ must be constant in t for solutions u to (1)

Let's prove this conservation law:

Proof that $\int_{-\infty}^{+\infty} |u(x,t)|^2 \, dx$ is conserved if $u, \frac{\partial u}{\partial x} \to 0$ as $x \to \pm\infty$

$$\frac{\partial}{\partial t} \int_{-\infty}^{+\infty} |u(x,t)|^2 \, dx = \frac{\partial}{\partial t} \int_{-\infty}^{+\infty} u(x,t) \cdot \overline{u}(x,t) \, dx$$

$$= \int_{-\infty}^{+\infty} \left(\frac{\partial u}{\partial t} \cdot \overline{u} + u \cdot \overline{\frac{\partial u}{\partial t}} \right) dx$$

$$= \int_{-\infty}^{+\infty} 2 \cdot \mathrm{Re}\left\{ \frac{\partial u}{\partial t} \cdot \overline{u} \right\} dx$$

Equation:
$i \frac{\partial u}{\partial t} + \frac{\partial^2 u}{\partial x^2} - V \cdot u = 0$

$$= \int_{-\infty}^{+\infty} 2 \cdot \mathrm{Re}\left\{ \left(-\frac{1}{i} \frac{\partial^2 u}{\partial x^2} + \frac{1}{i} V \cdot u \right) \cdot \overline{u} \right\} dx$$

$$= \int_{-\infty}^{+\infty} 2 \cdot \mathrm{Re}\left\{ i \frac{\partial^2 u}{\partial x^2} \cdot \overline{u} - i V |u|^2 \right\} dx$$

A

Since $V(x,t)$ and $|u(x,t)|^2$ are real valued:
$i \cdot V(x,t) |u(x,t)|^2$ is purely imaginary, so

$$\mathrm{Re}\left\{ -i \cdot V \cdot |u|^2 \right\} = 0$$

Returing to A:

$$A = 2\int_{-\infty}^{+\infty} \mathrm{Re}\left\{i\frac{\partial^2 u}{\partial x^2}\cdot\bar{u}\right\}dx$$

integrate by parts

$$= 2\cdot\left(\left[\mathrm{Re}\left\{i\frac{\partial u}{\partial x}\cdot\bar{u}\right\}\right]_{x=-\infty}^{+\infty} - \int_{-\infty}^{+\infty}\mathrm{Re}\left\{i\frac{\partial u}{\partial x}\cdot\frac{\partial\bar{u}}{\partial x}\right\}dx\right).$$

If $u(x,t)$, $\frac{\partial u}{\partial x}(x,t) \longrightarrow 0$ as $x\to\pm\infty$ (reasonable assumption for a "localized" particle), then the above is

$$= -2\int_{-\infty}^{+\infty}\mathrm{Re}\left\{i\cdot\frac{\partial u}{\partial x}\cdot\frac{\partial\bar{u}}{\partial x}\right\}dx.$$

But $i\frac{\partial u}{\partial x}\cdot\frac{\partial\bar{u}}{\partial x} = i\left|\frac{\partial u}{\partial x}\right|^2$ is purely imaginary, so the above is

$$= 0$$

$\square$

Initial value problem for the (inhomogeneous) Schrödinger equation:

$$\begin{cases} i\dfrac{\partial u}{\partial t}(x,t) + \dfrac{\partial^2 u}{\partial x^2}(x,t) - V(x,t)\cdot u(x,t) = F(x,t) \\ u(x,0) = u_0(x) \end{cases}$$

for $t>0$, $x\in\mathbb{R}$

particle source

Uniqueness of solutions:

If u_1, u_2 are solutions, then $w = u_1 - u_2$ solves

$$\begin{cases} i\dfrac{\partial w}{\partial t} + \dfrac{\partial^2 w}{\partial x^2} - V\cdot w = 0 \\ w(x,0) = 0 \end{cases}$$

So by the conservation law we proved before:

$$\forall t>0: \int_{-\infty}^{+\infty} |w(x,t)|^2\,dx = \int_{-\infty}^{+\infty} |w(x,0)|^2\,dx = 0$$

So $w \equiv 0$ $\forall\, t>0$, $x\in\mathbb{R}$, so $u_1 = u_2$.

(so we have uniqueness in the class of solutions that decay as $x \to \pm\infty$, which are the physically relevant ones).

Remark:
Qualitatively, solutions to the Schrödinger equations behave in some sense like waves (but with unbounded speed of propagation).
The Schrödinger equation belongs to the class of dispersive equations.

Construction of a solution when $V(x,t) \equiv 0$:

$$\begin{cases} i \dfrac{\partial u}{\partial t}(x,t) + \dfrac{\partial^2 u}{\partial x^2}(x,t) = F(x,t), & x \in \mathbb{R},\ t > 0, \\ u(x,0) = u_0(x) \end{cases}$$

Fourier transform in x:

$$\hat{u}(a,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} e^{-iax} u(x,t)\, dx$$

$$\hat{F}(a,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} e^{-iax} F(x,t)\, dx$$

$$\hat{u}_0(a) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} e^{-iax} u_0(x)\, dx$$

Then $\hat{u}$ satisfies:

$$\begin{cases} i \dfrac{\partial \hat{u}}{\partial t}(a,t) - a^2 \cdot \hat{u}(a,t) = \hat{F}(a,t) \\[2ex] \hat{u}(a,0) = \hat{u}_0(a) \end{cases}$$

First order ODE in time: We have seen how to solve it (e.g. using the Laplace transform in the t variable): (Note the i factor in front of ∂/∂_t)

$$\hat{u}(a,t) = e^{-ia^2t}\,\hat{u}_0(a) - i\int_0^t e^{-ia^2(t-s)}\,\hat{F}(a,s)\,ds$$

Now we need to invert the Fourier transform.

Note: e^{-ita^2} looks like a Gaussian with a complex rescaling.

In particular: the above looks like the solution of the heat equation, but with it in place of t:

Heat Solution:

$$\hat{u}(a,t) = e^{-a^2t}\,\hat{u}_0(a) + \int_0^t e^{-a^2(t-s)}\,\hat{F}(a,s)\,ds$$

For the heat equation:

$$\mathcal{F}^{-1}\left[e^{-a^2t}\cdot\hat{u}_0(a)\right] = \frac{1}{\sqrt{4\pi t}}\int_{-\infty}^{+\infty} e^{-\frac{(x-y)^2}{4t}}\,u_0(y)\,dy$$

In the Schrödinger case:

$$\mathcal{F}^{-1}\left[e^{-ia^2t}\cdot\hat{u}_0(a)\right] = \frac{1}{\sqrt{4\pi it}}\int_{-\infty}^{+\infty} e^{-\frac{(x-y)^2}{4it}}\,u_0(y_0)\,dy$$

In particular, the total solution takes the form:

$$u(x,t) = \frac{1}{\sqrt{4\pi i t}} \int_{-\infty}^{+\infty} e^{-\frac{(x-y)^2}{4it}} u_0(y)\, dy$$

$$- i \int_0^t \int_{-\infty}^{+\infty} \frac{1}{\sqrt{4\pi i (t-s)}} e^{-\frac{(x-y)^2}{4i(t-s)}} F(y,s)\, dy\, ds.$$

You can verify that the above is indeed a solution (and, thus, due to uniqueness, the unique solution), even though the method we used to derive it was not really rigorous.

But we can explicitly compute the inverse Fourier transform in special cases.

Example: If $F=0$, $u_0(x) = e^{-x^2/2}$

Then $\hat{u}_0(a) = e^{-a^2/2}$ (Fourier transform of Gaussian is Gaussian), then

$$\hat{u}(a,t) = e^{-ia^2t}\,\hat{u}_0(a) = e^{-ia^2t}\cdot e^{-a^2/2}$$

$$= e^{-(it+\frac{1}{2})a^2}$$

So $$u(x,t) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty} e^{+iax}\cdot e^{-(it+\frac{1}{2})a^2}\,da$$

$$= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty} e^{ixa-(it+\frac{1}{2})a^2}\,da. \quad B$$

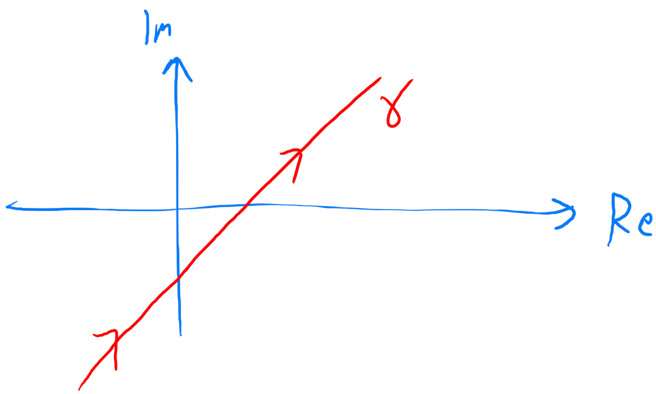
The above integral can be computed using the methods of complex integration:

Setting $z = \left(a - \frac{ix}{2it+1}\right)\cdot\sqrt{2it+1}$, we have $e^{ixa-(it+\frac{1}{2})a^2} = e^{-\frac{x^2}{4it+2}} \cdot e^{-z^2/2}$

and $da = \dfrac{dz}{\sqrt{2it+1}}$.

Note that when a goes from $-\infty$ to $+\infty$, $z = z(a)$ parametrizes the straight line

$$\gamma = \left\{ \left(a - \frac{ix}{2it+1}\right) \cdot \sqrt{2it+1} \; : \; a \in \mathbb{R} \right\}$$



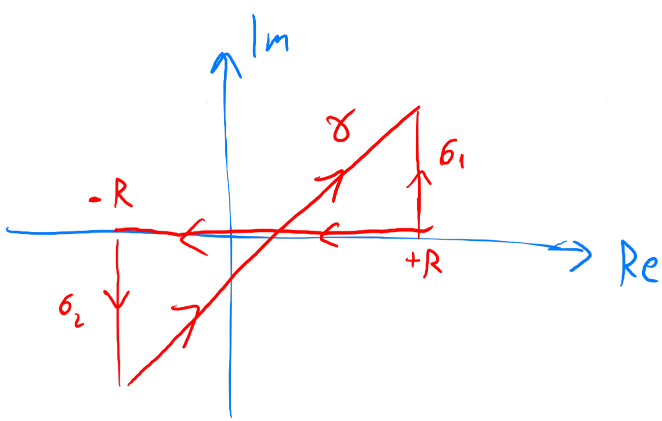
So, from B:

$$u(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} e^{ixa - (it+\frac{1}{2})a^2} \, da$$

$$= \frac{1}{\sqrt{2\pi}} \int_{\gamma} e^{-\frac{x^2}{4it+2}} \cdot e^{-z^2/2} \cdot \frac{dz}{\sqrt{2it+1}}$$

$$= \frac{1}{\sqrt{2\pi}} \cdot \frac{e^{-\frac{x^2}{4it+2}}}{\sqrt{2it+1}} \int_{\gamma} e^{-z^2/2} \, dz .$$

Using Cauchy's theorem, we can move the integration curve γ to $\mathbb{R}$:



$\int_{\sigma_1} e^{-z^2/2} dz$, $\int_{\sigma_2} e^{-z^2/2} dz \to 0$

as $R \to +\infty$

But $\int_{\mathbb{R}} e^{-z^2/2}\, dz = \sqrt{2\pi}$

So $u(x,t) = \dfrac{e^{-\frac{x^2}{4it+2}}}{\sqrt{2it+1}}$.

More remarks:

- If we wanted to solve the equation on $0 < x < L$, with (say) Dirichlet boundary conditions: $u|_{x=0} = 0$, $u|_{x=L} = 0$

(infinite-depth well problem)

We would proceed as in the case of the heat or the wave equation, i.e set

$$u(x,t) = \sum_{n=1}^{\infty} b_n(t) \cdot \sin\left(\frac{\pi n}{L} x\right)$$

and solve the (1^{st} order) ODE for $b_n(t)$.

But now: $\underline{b_n(t) \in \mathbb{C}}$

Thank you!

(and please complete the in-depth evaluations for the course)

Examples of exercises:

1) Compute the integral

$$\int_0^{2\pi} \frac{\cos\theta}{2+\cos\theta}\, d\theta$$

We will reformulate it as a complex integral over the unit circle:

If $z = e^{i\theta}$, $\theta \in [0, 2\pi]$,

so that $dz = ie^{i\theta} d\theta = iz\, d\theta$, we have: (set $\gamma = \{|z| = 1\}$, parametrized by $e^{i\theta}$)

$$\int_0^{2\pi} \frac{\cos\theta}{2+\cos\theta}\, d\theta = \int_0^{2\pi} \frac{\frac{1}{2}(e^{i\theta}+e^{-i\theta})}{2+\frac{1}{2}(e^{i\theta}+e^{-i\theta})}\, d\theta$$

$$= \int_\gamma \frac{\frac{1}{2}\left(z+\frac{1}{z}\right)}{2+\frac{1}{2}\left(z+\frac{1}{z}\right)} \cdot \frac{1}{iz}\, dz$$

$$= \int_\gamma \frac{z^2+1}{iz\left(z^2+4z+1\right)}\, dz \qquad \text{I}$$

If $F(z) = \dfrac{z^2+1}{iz\cdot\left(z^2+4z+1\right)} = \dfrac{(z+i)(z-i)}{iz\cdot\left(z+2+\sqrt{3}\right)\left(z+2-\sqrt{3}\right)}$

Then F has simple poles at $z=0$, $z=-2-\sqrt{3}$, $z=-2+\sqrt{3}$. Of those, only $z=0$ and $z=-2+\sqrt{3}$ are inside the unit disc.

So: Since these are simple poles,

$$\operatorname*{Res}_{z=0}(F(z)) = \lim_{z\to 0}\left(z\cdot F(z)\right) =$$

$$= \lim_{z\to 0}\left(\frac{z^2+1}{i(z^2+4z+1)}\right) = \frac{1}{i}$$

and $$\operatorname*{Res}_{z=-2+\sqrt{3}}(F(z)) = \lim_{z\to -2+\sqrt{3}}\left((z+2-\sqrt{3})F(z)\right)$$

$$= \lim_{z\to -2+\sqrt{3}}\left(\frac{z^2+1}{iz(z+2+\sqrt{3})}\right)$$

$$= \frac{8-4\sqrt{3}}{6-4\sqrt{3}}\cdot\frac{1}{i}.$$

So, by the residue theorem:

$$I = 2\pi i\left(\operatorname*{Res}_{z=0}(F) + \operatorname*{Res}_{z=-2+\sqrt{3}}(F)\right)$$

$$= 2\pi \left(1 + \frac{8-4\sqrt{3}}{6-4\sqrt{3}}\right)$$

$$= \pi \cdot \frac{14-8\sqrt{3}}{3-2\sqrt{3}}.$$

2) Solve the following initial value problem:

$$\begin{cases} y'''(t) + y(t) = 1, & t>0 \\ y(0)=0, \; y'(0)=0, \; y''(0)=1. \end{cases}$$

Applying a Laplace transform:
(setting $Y(z) = \mathcal{L}[y](z)$):

$$z^3 Y(z) - y''(0) - z \cdot y'(0) - z^2 y(0) + Y(z) = \frac{1}{z}$$

Given the in. data
$$\Longrightarrow \quad z^3 \cdot Y(z) - 1 + Y(z) = \frac{1}{z}$$

$$\Rightarrow \quad Y(z) = \frac{z+1}{z \cdot (z^3+1)} = \frac{1}{z \cdot (z^2 - z + 1)}$$

We now have to invert the Laplace transform.

Method 1: Decompose in simpler, recognizable functions

Since $$\frac{1}{z \cdot (z^2 - z + 1)} = \frac{A}{z} + \frac{B}{z^2 - z + 1} + \frac{Cz}{z^2 - z + 1}$$

$$\xrightarrow{\text{Mult. with } z \cdot (z^2 - z + 1)} \quad A = 1, \; B = 1, \; C = -1$$

So $$\frac{1}{z\cdot(z^2-z+1)} = \frac{1}{z} + \frac{1}{z^2-z+1} - \frac{z}{z^2-z+1}.$$

In order to find the inverse Laplace transform of these expressions:

Recall: $\mathcal{L}[\cos(\omega t)] = \frac{z}{z^2+\omega^2}$, $\mathcal{L}[\sin(\omega t)] = \frac{\omega}{z^2+\omega^2}$

So $$\frac{1}{z^2-z+1} = \frac{1}{(z-\frac{1}{2})^2+\frac{3}{4}} = \frac{1}{(z-\frac{1}{2})^2+\left(\frac{\sqrt{3}}{2}\right)^2}$$

$$= \frac{2}{\sqrt{3}} \cdot \frac{\frac{\sqrt{3}}{2}}{(z-\frac{1}{2})^2+\left(\frac{\sqrt{3}}{2}\right)^2}$$

$$= \frac{2}{\sqrt{3}} \mathcal{L}\left[\sin\left(\frac{\sqrt{3}}{2}t\right)\cdot e^{t/2}\right]$$

And $$\frac{z}{z^2-z+1} = \frac{z-\frac{1}{2}+\frac{1}{2}}{\left(z-\frac{1}{2}\right)^2+\left(\frac{\sqrt{3}}{2}\right)^2} =$$

$$= \frac{z-\frac{1}{2}}{\left(z-\frac{1}{2}\right)^2+\left(\frac{\sqrt{3}}{2}\right)^2} + \frac{1}{\sqrt{3}} \frac{\frac{\sqrt{3}}{2}}{\left(z-\frac{1}{2}\right)^2+\left(\frac{\sqrt{3}}{2}\right)^2}$$

$$= \mathcal{L}\left[\cos\left(\frac{\sqrt{3}}{2}t\right)e^{t/2}\right] + \frac{1}{\sqrt{3}}\mathcal{L}\left[\sin\left(\frac{\sqrt{3}}{2}t\right)e^{\frac{t}{2}}\right]$$

Overall

$$y(t) = \mathcal{L}^{-1}\left[\frac{1}{z(z^2-z+1)}\right] = \mathcal{L}^{-1}\left[\frac{1}{z}+\frac{1}{z^2-z+1}-\frac{z}{z^2-z+1}\right]$$

$$= 1 + \frac{2}{\sqrt{3}}\sin\left(\frac{\sqrt{3}}{2}t\right)e^{t/2} - \left(\cos\left(\frac{\sqrt{3}}{2}t\right)e^{t/2} + \frac{1}{\sqrt{3}}\sin\left(\frac{\sqrt{3}}{2}t\right)e^{t/2}\right)$$

$$= 1 + \frac{1}{\sqrt{3}}\sin\left(\frac{\sqrt{3}}{2}t\right)e^{t/2} - \cos\left(\frac{\sqrt{3}}{2}t\right)e^{t/2}$$

Method 2: Use the formula for the inverse Laplace transform:

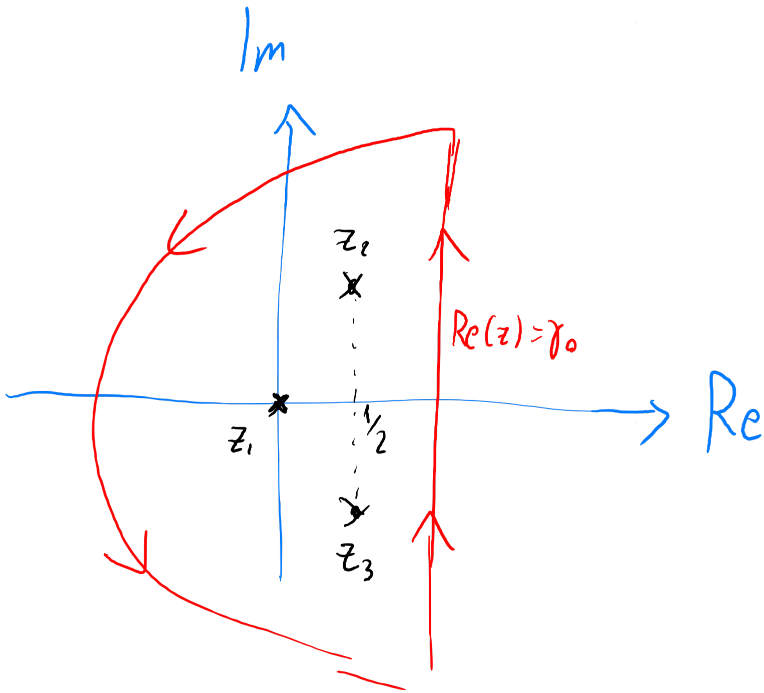
The singularities of

$$Y(z) = \frac{1}{z \cdot (z^2 - z + 1)}$$ are at

$$z_1 = 0, \quad z_2 = \frac{1}{2} + \frac{\sqrt{3}}{2} i, \quad z_3 = \frac{1}{2} - \frac{\sqrt{3}}{2} i$$

So for any $\gamma_0 > \frac{1}{2}$ (so that all the poles are to the left of the line $Re(z) = \gamma_0$), we have

$$y(t) = \frac{1}{2\pi i} \int_{\gamma_0 - i\infty}^{\gamma_0 + i\infty} e^{zt}\, Y(z)\, dz$$



Computing the integral by closing the loop to the left (and sending the radius to infinity), we get: (by applying the residue theorem):

$$y(t) = \frac{1}{\cancel{2\pi i}} \cdot \cancel{2\pi i} \cdot \sum_{k=1}^{3} \operatorname{Res}_{z=z_k} \left(\frac{e^{tz}}{z \cdot (z^2 - z + 1)} \right)$$

Calculating the residues, we obtain the same result as before.