Chapter 2 – Intro to Math Techniques for Quantum Mechanics

Intro to differential equations

Function $y = y(x)$ is to satisfy a differential equation

$$\frac{d^2 y}{dx^2} - 5\frac{dy}{dx} + 6y = 0 \quad \forall x \quad (1)$$

For this ‘type’ of Differential equation (more later), try solution $y = e^{\lambda x}$

Then

$$\frac{dy}{dx} = \lambda e^{\lambda x}$$
$$\frac{d^2 y}{dx^2} = \lambda^2 e^{\lambda x}$$
$$\frac{d^n y}{dx^n} = \lambda^n e^{\lambda x}$$

Substitute into differential equation (1)

$$\lambda^2 e^{\lambda x} - 5\lambda e^{\lambda x} + 6e^{\lambda x} = 0 \quad \forall x$$

Or

$$\lambda^2 - 5\lambda + 6 = 0$$
$$(\lambda - 3)(\lambda - 2) = 0$$

$\Longrightarrow$ Solutions: $\lambda = 3, \lambda = 2$

$e^{3x}$:

$$9e^{3x} - 15e^{3x} + 6e^{3x} = 0$$

$e^{2x}$:

$$4e^{2x} - 10e^{2x} + 6e^{2x} = 0$$

But: any linear combination of solutions is also solution
\( y(x) = c_1 e^{3x} + c_2 e^{2x} \)

\[ \Rightarrow \quad 9c_1 e^{3x} + 4c_2 e^{2x} \left( \frac{d^2 y}{dx^2} \right) \]
\[ -15c_1 e^{3x} - 10c_2 e^{2x} \left( -5 \frac{dy}{dx} \right) \]
\[ 6c_1 e^{3x} + 6c_2 e^{2x} \left( 6y \right) \]

Let us try another one

\[ \frac{d^2 y}{dx^2} + y = 0 \quad \forall x \]

\[ \lambda^2 e^{\lambda x} + e^{\lambda x} = 0 \]

\[ \lambda^2 + 1 = 0 \quad \Rightarrow \quad \lambda = \pm i \]

General Solution: \( c_1 e^{ix} + c_2 e^{-ix} \)

Alternative way to write:

\[ e^{ix} = \cos x + i \sin x \]

\[ e^{-ix} = \cos x + i \sin(-x) = \cos x - i \sin x \]

\[ \Rightarrow \quad y(x) = (c_1 + c_2) \cos x + i(c_1 - c_2) \sin x \]
\[ = d_1 \cos x + d_2 \sin x \]

define \( d_1 = c_1 + c_2, \quad d_2 = i(c_1 - c_2) \)

\( \Rightarrow \) choose \( d_1, \ d_2 \) ‘real’

Verify:

\[ \frac{d^2 \cos x}{dx^2} = \frac{d}{dx}(-\sin x) = -\cos x \]

\[ \frac{d^2 \sin x}{dx^2} = \frac{d}{dx}(\cos x) = -\sin x \]

\[ \Rightarrow \quad \frac{d^2 y}{dx^2} + y = 0, \quad \text{as expected} \]

Type of solutions \( e^{\lambda x}, \ e^{-\lambda x}, \ \cos \lambda x, \ \sin \lambda x, \ \lambda \) real, \( \lambda > 0 \)
When does this work?

\[ 0 = c_0 y + c_1 \frac{dy}{dx} + c_2 \frac{d^2 y}{dx^2} + c_3 \frac{d^3 y}{dx^3} + \ldots \]

(1) Constant coefficients in front of \( y \) and its derivatives

→ not: \( \frac{d^2 y}{dx^2} + x^2 y = 0 \)

(2) Linear in function \( y \)

→ not: \( \frac{d^2 y}{dx^2} + y \frac{dy}{dx} = 0 \)

(3) Homogeneous equation

→ not: \( c_2 \frac{\partial^2 y}{\partial x^2} + c_1 \frac{\partial y}{\partial x} + c_2 y = f(x) \)

For inhomogeneous differential equation (last case 3):

→ Find particular solution \( y = P(x) \) add to this the general solution of inhomogeneous equation.

For more complicated differential equations (ie. Not homogeneous DE with constant coefficients) solutions are often hard to find

- Many tricks of the trade
- Use symbolic math program (it knows many of the tricks)
- Numerical approaches (often work very easily → picture of solution)
Boundary Conditions

Let us consider our original differential equation.

\[
\frac{d^2 y}{dx^2} - 5 \frac{dy}{dx} + y = 0
\]

\[y(x) = c_1 e^{3x} + c_2 e^{2x}\]

Now impose further conditions. Eg:

\[y(0) = 0 \quad \Rightarrow \quad c_1 + c_2 = 0\]

\[\left( \frac{dy}{dx} \right)_{x=0} = 1 \quad \Rightarrow \quad 3c_1 + 2c_2 = 1\]

\[c_2 = -c_1\]

\[\Rightarrow 3c_1 - 2c_1 = 1 \quad \Rightarrow \quad c_1 = 1 \quad \Rightarrow \quad c_2 = -1\]

\[y(x) = e^{3x} - e^{2x}\]

Satisfies both DE and boundary conditions

Solution is completely specified if one supplies as many conditions as one has free coefficients \(c_1, c_2, \ldots\) in the solution

\[\Rightarrow \text{always linear set of equations}\]

So recipe is very simple

Try \(y(x) = e^{3x}\) and work it out!

Partial differential equations and separation of variables

Consider problem of vibrating string (eg. guitar, violin)

\[u(x,t)\]
We want to describe the amplitude $u(x,t)$

Differential Equation with partial derivatives:

$$\frac{\partial^2 u}{\partial x^2}(x,t) = \frac{1}{v^2} \frac{\partial^2 u}{\partial t^2}(x,t)$$

$v$: Velocity of wave propagation in string, related to spring constant, (as sound of the string)

Boundary Condition:

$$u(0,t) = u(a,t) = 0 \quad \forall t$$

$u(x,t)$: function of 2 variables → use partial derivatives $\left(\frac{\partial u}{\partial x}\right)$

In math we typically do not write is kept constant
(in contrast to thermodynamics)

How to solve PDE (partial differential equation)?

**Try** solution $u(x,t) = X(x)T(t)$

Simple product of a function of $x$ and a function of $t$

Boundary Condition: $X(0) = X(a) = 0$

Substitute trial function into PDE

$$\frac{d^2 X(x)}{dx^2} T(t) = \frac{1}{v^2} \frac{d^2 T}{dt^2} X(x)$$

Divide both sides by $X(x)T(t)$:

$$\frac{1}{X(x)} \frac{d^2 X(x)}{dx^2} = \frac{1}{v^2} \frac{1}{T(t)} \frac{d^2 T}{dt^2}$$

only depends on $x$ only depends on $t$

Like $f(x) = g(t)$. It is clear that this should be true for all $x$, $t$

$$f(x) = g(t_0) \quad \rightarrow \quad f(x) \text{ is constant}$$

$$= g(t_1) \quad \rightarrow \quad f(x) \text{ is constant, should be same}$$

$$g(t) = f(x_0) \quad \rightarrow \quad g(t) \text{ is constant}$$

$$= f(x_1)$$
\[ f(x) = g(t) \quad \forall x, t \]

Can only be true if both functions are constant! I.e. The same constant

Let us call this constant, the separation constant \(-k^2\) (for later simplicity)

\[
\frac{d^2 X}{dx^2} = -k^2 X(x) \quad X(0) = X(a) = 0 \\
\frac{1}{v^2} \frac{d^2 T}{dt^2} = -k^2 T(t) \quad \text{no boundary conditions}
\]

Now we can use techniques discussed before \((k\) is constant)

\[ \text{Try } X(x) = e^{\lambda x} \]
\[ \lambda^2 e^{\lambda x} = -k^2 e^{\lambda x} \]

\[ \lambda = ik, \quad \lambda = -ik \]

\[ X(x) = c_1 e^{ikx} + c_2 e^{-ikx} \]

Note: \(k\) could be imaginary \(im\)

\[ -k^2 = -(im)^2 = +m^2 > 0 \]

However we know that the string will oscillate, and hence can anticipate \(e^{ikx}\), with \(k\) real

Using what we did before

\[ c_1 e^{ikx} + c_2 e^{ikx} = (c_1 + c_2) \cos kx + i(c_1 - c_2) \sin kx \]

\[ = d_1 \cos kx + d_2 \sin kx \]

\[ \text{This is general solution. Now consider boundary conditions.} \]

\[ x = 0: \quad d_1 \cos 0 + d_2 \sin 0 \]

\[ d_1 1 + d_2 0 = 0 \quad \Rightarrow [d_1 = 0] \]

\[ x = a: \quad d_2 \sin(ka) = 0 \]

\[ \Rightarrow d_2 = 0 \text{ (flat string possibility)} \quad \text{or} \quad \sin(ka) = 0 \]

When is \(\sin(x) = 0\)? \(x = \pm 0, \pm \pi, \pm 2\pi, \pm 3\pi\ldots\)

\[ x \to ka = n\pi \quad \Rightarrow \quad k = \frac{n\pi}{a} \]

General solution: \(X(x) = d_n \sin\left(\frac{n\pi x}{a}\right)\)

\[ -k_n^2 = -\frac{n^2 \pi^2}{a^2} \]
This is solution for $x$ at particular value for $k_n = \frac{n\pi}{a}$

Now consider corresponding solution for $T(t)$

$$\frac{1}{v^2} \frac{d^2 T}{dt^2} = -\left(\frac{n\pi}{a}\right)^2 T(t)$$

$$\frac{d^2 T}{dt^2} = -\omega_n^2 T(t) \quad \omega_n = \frac{n\pi v}{a}$$

Similar equation as before:

$$T(t) = c_1 \sin (\omega_n t) + c_2 \cos (\omega_n t)$$

If we combine this with $X$ we get

$$u(x,t) = A_n \sin \left(\frac{n\pi x}{a}\right) \sin \left(\frac{n\pi vt}{a}\right) + B_n \sin \left(\frac{n\pi x}{a}\right) \cos \left(\frac{n\pi vt}{a}\right)$$

This is a solution for any value of $A_n, B_n$ and any value of $n = 0, \pm 1, \pm 2, \pm 3$

Most general solution (we can restrict to non-negative n):

$$u(x,t) = \sum_{n=0,1,2,3,\ldots} \sin \left(\frac{n\pi x}{a}\right) \left[ A_n \sin (\omega_n t) + B_n \cos (\omega_n t) \right]$$

You can verify that this indeed satisfies PDE (quite some work).

How can we interpret this?

$$\sin \frac{n\pi x}{a}$$
\[
\sin \left( \frac{-n\pi x}{a} \right) = -\sin \left( \frac{n\pi x}{a} \right) :
\]

Same solution, restrict \( n = 0, 1, 2, 3 \)
\( (n < 0, \text{nothing extra}) \)

So a string vibrates as a linear combination of modes, each of the modes oscillates in time at a different frequency.

\[
\sin \left( \frac{n\pi x}{a} \right) \rightarrow \omega_n = \frac{n\pi v}{a} = n\omega_0
\]

All multiples of fundamental frequency \( \frac{\pi v}{a} = \omega_0 \)

This defines the pitch of the sound \( \rightarrow \omega_0 \)
The other modes are called overtones

\( \rightarrow \) Meaning of coefficients \( A_n, B_n \)?

\[
t = 0 \quad B_n \cos \left( \frac{n\pi v}{a} t \right)_{t=0} = B_n \rightarrow u(x,t=0) = \sum_n B_n \sin \left( \frac{n\pi x}{a} \right)
\]

\( \rightarrow \) The initial shape of function
\[
du \rightarrow A_n \left( \cos \frac{n\pi vt}{a} \right) \quad \frac{du(x,t)}{dt} \bigg|_{t=0} = \sum_n A_n \sin \left( \frac{n\pi x}{a} \right)
\]

The initial velocity of the string.

Different instruments, guitars, violins, cello
→ different \( A_n \), \( B_n \)

How you attack the string determines the initial shape/velocity
→ compare Chinese zither: hit the snare in different spots or twang the string

None of this affects the pitch → \( \omega_0 \) the general harmonic

- Period \( \sin(\omega t) = \sin \omega(t + T) \)
- \( \sin(\omega t + 2\pi) \rightarrow \sin(\omega t) \)
- \( 2\pi = \omega T \)
- \( T = \frac{2\pi}{\omega} \); \( \omega = \frac{2\pi}{T} \) angular frequency

**Introduction to Statistics**

We will see that quantum mechanics is essentially a statistical theory. We can predict the results and their distribution from a large number of repeated experiments only. We cannot predict (even in principle) the outcome of an individual experiment.

Let us therefore talk about statistics using a simple example: the dice

If you throw the dice, each throw will yield the result 1, 2, 3, 4, 5 or 6.

<p>| | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1010</td>
</tr>
<tr>
<td>2</td>
<td>980</td>
</tr>
</tbody>
</table>
If you throw the dice many times, say 6000 times, we might get

<p>| | |</p>
<table>
<thead>
<tr>
<th></th>
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</thead>
<tbody>
<tr>
<td>3</td>
<td>995</td>
</tr>
<tr>
<td>4</td>
<td>1025</td>
</tr>
<tr>
<td>5</td>
<td>1030</td>
</tr>
<tr>
<td>6</td>
<td>960</td>
</tr>
<tr>
<td>Total</td>
<td>6000</td>
</tr>
</tbody>
</table>

For a fair dice, each number has equal chance, and so we say the probability to throw for example a ‘3’ is \( \frac{1}{6} \). This is reflected by the actual numbers we got in the example.

\[
\frac{n_i}{6000} \approx \frac{1000}{6000} = \frac{1}{6} = P_i
\]

In the limit that we throw a very large (infinite) times, we get closer and closer to \( \frac{1}{6} \)

\[
P_i = \frac{n_i}{N_{total}} \text{ only has meaning for many repeated experiments}
\]

\[
\sum P_i = 1
\]

We might call \( a_i \) the actual outcome of experiment, here \( a_i = 1, 2, 3, 4, 5, 6 \)

The average is given by

\[
\frac{1}{N_{tot}} \sum n_i a_i \rightarrow \sum P_i a_i
\]

For dice:

\[
\frac{1}{6} (1 + 2 + 3 + 4 + 5 + 6) = \frac{21}{6} = 3 \frac{1}{2}
\]

The average value does not need to be a possible outcome of an individual throw.

We are also interested in the variance of the results. We call the average \( \overline{A} \) or \( \langle A \rangle \). (both are used)

Then the variance is given by:

\[
\sigma_A^2 = \sum P_i (a_i - \overline{A})^2 \geq 0
\]

Let us take a dice with 5 sides to make the numbers easier

\( a_i = 1, 2, 3, 4, 5 \), \( P_i = \frac{1}{5} \)
\[ \bar{A} = 3 \]

\[ \sigma_A^2 = \frac{1}{5} [(1 - 3)^2 + (2 - 3)^2 + (3 - 3)^2 + (4 - 3)^2 + (5 - 3)^2] \]

\[ = \frac{1}{5} [4 + 1 + 0 + 1 + 4] = 2 \]

Standard Deviation \( \sigma_A = \sqrt{2} \)
I can write the variance differently as

\[
\sum P_i(a_i - \bar{A})^2 = \sum_i P_i(a_i^2 - 2a_i \bar{A} + \bar{A}^2) = \sum_i P_i a_i^2 - 2\bar{A} \sum_i P_i a_i + \bar{A}^2 \sum_i P_i = \langle A^2 \rangle - 2\bar{A}\bar{A} + \bar{A}\bar{A} = \langle A^2 \rangle - \langle A \rangle^2 = \sigma^2
\]

Let us check for the 5 face dice:

\[
\langle A^2 \rangle = \frac{1}{5} (1^2 + 2^2 + 3^2 + 4^2 + 5^2) = \frac{1}{5} (1 + 4 + 9 + 16 + 25) = \frac{1}{5} (55) = 11
\]

\[
\langle A \rangle^2 = 3 \cdot 3 = 9
\]

\[
\langle A^2 \rangle - \langle A \rangle^2 = 2 = \sigma^2
\]

Of course: We proved this is true mathematically!

This concludes (for now) discussion of discrete statistics.

Now consider the case of a continuous distribution. For example a density distribution.

\[
\rho(x)dx = dm
\]

= the mass between \( x \) and \( x + dx \) (in 1 dimension)

\[
\int_{-\infty}^{\infty} \rho(x)dx = M \quad \text{total mass}
\]

Also \( \int_{a}^{b} \rho(x)dx \) = mass between points \( a \) and \( b \)

If we normalize

\[
P(x)dx = \frac{1}{M} \rho(x)dx
\]

probability to find a fraction of the total mass between \( x \) and \( x + dx \)

We can define average position
\[
\langle x \rangle = \int_{-\infty}^{\infty} xP(x)\,dx \\
\langle x^2 \rangle = \int_{-\infty}^{\infty} x^2P(x)\,dx \\
\sigma_x^2 = \langle x^2 \rangle - \langle x \rangle^2
\]

Example: take a box between 0 and a

\[
P(x) = \begin{cases} 
\frac{1}{a} & 0 < x < a \\
0 & \text{elsewhere}
\end{cases}
\]

1) \[\int_{-\infty}^{\infty} P(x)\,dx = \int_{0}^{a} \frac{1}{a}\,dx = \frac{x}{a}\bigg|_{0}^{a} = 1\] “normalized”

2) \[\int_{-\infty}^{\infty} xP(x)\,dx = \int_{0}^{a} \frac{1}{a}x\,dx = \frac{x^2}{2a}\bigg|_{0}^{a} = \frac{a}{2}\]

3) \[\int_{-\infty}^{\infty} x^2P(x)\,dx = \int_{0}^{a} \frac{1}{a}x^2\,dx = \frac{x^3}{3a}\bigg|_{0}^{a} = \frac{1}{3}a^2\]

4) \[\sigma_x^2 = \langle x^2 \rangle - \langle x \rangle^2 = \frac{1}{3}a^2 - \left(\frac{1}{2}a\right)^2 = \frac{a^2}{12} \geq 0 \text{ Always}\]

More complicated distributions are possible of course

Famous is the Gaussian distribution

\[P(x) = ce^{-\frac{x^2}{2a^2}}\] ‘\(a\)’ parameter (will be \(\sigma_x\))

\(c\) : normalization constant

\[\int_{-\infty}^{\infty} P(x) = 1 \quad \rightarrow \quad c = \frac{1}{\sqrt{2\pi a^2}}\]

Then \(\langle x \rangle = \frac{1}{a\sqrt{2\pi}} \int_{-\infty}^{\infty} xe^{-\frac{x^2}{2a^2}} = 0\) Odd function \(f(-x) = -f(x)\)
\[
\langle x^2 \rangle = \frac{1}{a\sqrt{2\pi}} \int_{-\infty}^{\infty} x^2 e^{-\frac{x^2}{2a^2}} dx
\]

\[
= \frac{1}{a\sqrt{2\pi}} \cdot \frac{a^2 \sqrt{2\pi} a^2}{2} \cdot 2 = a^2
\]

\[
\Rightarrow \sigma_x = a \quad \text{as advertised}
\]

(this was the reason to define the Gaussian like this)

See book for discussion integrals