Quantum Comeback ♡

Lecture 10–11 : Delta function potential, Griffiths 2·5

Lecture 12–13 : The finite square well & Tunelling. Griffiths 2·6 and Rae 2·5 – 2·6.

Lecture 14 & 15 ; Simple Harmonic Oscillator, Griffiths 2·3 & Rae 2·7.

Lecture 16 : Intro to Hilbert Space & Math formalism Griffiths 3·1

Lecture 17 : Observables & Hermitian operators (Griffiths 3·2, Rae 4·1 – 4·2)

Lecture 18 : Eigen functions & momentum space (Griffiths 3·3 & Rae 4·2 – 4·3)

(Quiz 2 portion Lec 10 to 18)

Simple Harmonic Oscillator

(Griffiths 2·3)

Hooke's law $\rightarrow$ $F = -kx = m\dfrac{d^2x}{dt^2}$

$x(t) = A\sin\omega t + B\cos\omega t$. and $\omega = \sqrt{\dfrac{k}{m}}$

$\therefore V(x) = \frac{1}{2}kx^2 \rightarrow$ Parabola.

This is for a perfect Harmonic Oscillator. But if you take any harmonic Oscillator, around the vicinity of a local minima, the graph of potential of an harmonic oscillator can be estimated to a parabola. → Taylor Series

$$V(x)\Big|_{x=x_0} = V(x_0) + V'(x_0)(x-x_0) + \frac{1}{2}V''(x_0)(x-x_0)^2 + \cdots$$

If $(x-x_0)$ is small [Vicinity of the local minima], higher order terms go to zero.

$\therefore$ We can consider till $(x-x_0)^2$.

And since it is a minima, $V'(x_0) = 0$

And $V(x_0)$ is going to be a constant, so will shift the graph only.

$$\therefore \; V(x) \approx V(x_0) + V''(x_0)\,\underline{(x-x_0)^2}$$

This describes simple harmonic oscillation about x_0, with an effective spring constant $k = V''(x_0)$.

This is why SHM is important. Any oscillatory motion is approx. SHM, as long as the amplitude is small.

The quantum problem, though, is:

Solving Schrödinger's eq^n

$$\omega = \sqrt{\frac{k}{m}}$$

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + \frac{1}{2}m\omega^2x^2\psi = E\psi \text{ , for potential } V(x) = \frac{1}{2}m\omega^2x^2.$$

There are 2 methods known to solve this eq^n for ψ:

a) The 'fun to do' algebraic method

b) The 'customary' Analytic method

It is very important to clearly understand both the methods.

A) THE Algebraic Method

$$\text{TISE: } \quad -\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + \frac{1}{2}m\omega^2x^2\psi = E\psi.$$

$$\Rightarrow \quad \frac{1}{2m}\left[\hat{p}^2 + m^2\omega^2x^2\right]\psi = E\psi.$$

And $\hat{H} = \frac{1}{\;}\left[\hat{p}^2 + (m\omega x)^2\right]$

If $\hat{p}$ and x were numbers, then this is pretty straightforward. But there are "Operators" – Ain't that easy.

If $\hat{p}$ and x were numbers, say, u and v,

$$u^2+v^2 = (iu+v)(-iu+v).$$

But we can use this though...

let $$\hat{a}_+ = \frac{1}{\sqrt{2\hbar m\omega}}\left(-i\hat{p}+m\omega\hat{x}\right)$$ and

$$\hat{a}_- = \frac{1}{\sqrt{2\hbar m\omega}}\left(+i\hat{p}+m\omega\hat{x}\right).$$

so, what is $\hat{a}_-\hat{a}_+$?

$$\hat{a}_-\hat{a}_+ = \frac{1}{2\hbar m\omega}(i\hat{p}+m\omega x)(-i\hat{p}+m\omega x)$$

Operators do not Commute : $AB \neq BA$ (Recall Matrices)

$$\therefore \hat{a}_-\hat{a}_+ = \frac{1}{2\hbar m\omega}\left[\hat{p}^2 + i\hat{p}\,m\omega x - im\omega\, x\hat{p} + (m\omega x)^2\right]$$

$$= \frac{1}{2\hbar m\omega}\left[\hat{p}^2 + (m\omega x)^2 - im\omega\,(x\hat{p}-\hat{p}x)\right]$$

There is an extra term... Hmm.

But this is familiar!

Oh yes! $x\hat{p}-\hat{p}x = [\hat{x},\hat{p}]$ = Commutator of 2 operators!

Commutator is a measure of how badly they fail to commute.

$\therefore$ If commutator is zero, then they "Commute"!

But, here, it is non-zero. How do we know? Well, we'll find it!

Operators are notorious: We need a test function to avoid mistakes.

$$\therefore \quad [x, \hat{p}] f(x) = \left(x \, \hat{p} f(x) - \hat{p} \, x f(x) \right)$$

$$= \left\{ x \cdot -i\hbar \frac{df(x)}{dx} - \left[-i\hbar \frac{d}{dx} [x f(x)] \right] \right\}$$

$$= -x \cancel{i\hbar \frac{df}{dx}} + i\hbar \left[\cancel{x \frac{df}{dx}} + f(x) \right]$$

Lonely you know?

$$= i\hbar f(x). \quad \Rightarrow \quad \boxed{[x, \hat{p}] = i\hbar.}$$

The above formula is known as the canonical commutation relation.

Now that we know $[x, \hat{p}]$, we plug it in the $\hat{a}_- \hat{a}_+$ eq^n [Remember, our goal was to solve the TISE for a $V(x)$ = parabola]

$$\left[V(x) = \frac{1}{2} m\omega^2 x^2 \right]$$

$$\hat{a}_- \hat{a}_+ = \frac{1}{2\hbar m\omega} \left[\hat{p} + (m\omega x)^2 - i m\omega (\hbar i) \right]$$

$$= \frac{1}{2\hbar m\omega} \left[\hat{p} + (m\omega x)^2 + m\omega\hbar \right]$$

$$= \frac{1}{\hbar\omega} \left[\frac{[\hat{p} + (m\omega x)^2]}{2m} \right] + \frac{1}{2} = \frac{\hat{H}}{\hbar\omega} + \frac{1}{2}.$$

$$\therefore \quad \hat{H} = \hbar\omega \left(\hat{a}_- \hat{a}_+ - \frac{1}{2} \right)$$

also, $\hat{a}_+ \hat{a}_- = \dfrac{\hat{H}}{\hbar\omega} - \dfrac{1}{2}$. and $\hat{H} = \hbar\omega \left(\hat{a}_+ \hat{a}_- + \dfrac{1}{2} \right)$

This gives, $[\hat{a}_-, \hat{a}_+] = 1.$

Now, the TISE for harmonic oscillator is:

$$\hbar\omega \left(\hat{a}_\pm \hat{a}_\mp \pm \frac{1}{2} \right) \psi = E\psi$$

If ψ satisfies the TISE with energy E ($\hat{H}\psi = E\psi$), then

$\hat{a}_+ \psi$ satisfies the TISE with energy $(E+\hbar\omega)$: $\hat{H}(\hat{a}_+\psi) = (E+\hbar\omega)(\hat{a}_+\psi)$ and

$\hat{a}_-\psi$ satisfies the TISE with energy $(E-\hbar\omega)$: $\hat{H}(\hat{a}_-\psi) = (E-\hbar\omega)(\hat{a}_-\psi)$.

Proof:

$$H(\hat{a}_+\psi) = \hbar\omega\left(\hat{a}_+\hat{a}_- + \frac{1}{2}\right)(\hat{a}_+\psi) = \hbar\omega\left(a_+a_-a_+ + \frac{1}{2}a_+\right)\psi$$

$$= \hbar\omega\,\hat{a}_+\left(a_-a_+ + \frac{1}{2}\right)\psi = \hat{a}_+\left[\hbar\omega\left(\hat{a}_-\hat{a}_+ + \frac{1}{2}\right)\psi\right]$$

$$= \hat{a}_+\left[\hbar\omega\left(\hat{a}_+\hat{a}_- + 1 + \frac{1}{2}\right)\right]\psi = \hat{a}_+\left[\hat{H} + \hbar\omega\right]\psi$$

$[a_-a_+] = 1$

$$= \hat{a}_+\left[E + \hbar\omega\right]\psi = (E+\hbar\omega)(\hat{a}_+\psi)$$

$|||^{ly}$,

$$\hat{H}(\hat{a}_-\psi) = \hbar\omega\left(\hat{a}_-\hat{a}_+ - \frac{1}{2}\right)(\hat{a}_-\psi) = \hbar\omega\left(\hat{a}_-\hat{a}_+\hat{a}_- - \frac{1}{2}\hat{a}_-\right)\psi$$

$$= \hbar\omega\,\hat{a}_-\left(\hat{a}_+\hat{a}_- - \frac{1}{2}\right) = \hbar\omega\,\hat{a}_-\left(\hat{a}_-\hat{a}_+ - 1 - \frac{1}{2}\right)\psi$$

$$= \hat{a}_-\left[\hbar\omega\left(\hat{a}_-\hat{a}_+ - \frac{1}{2}\right) - \hbar\omega\right]\psi = \hat{a}_-\left[\hat{H} - \hbar\omega\right]\psi$$

$$= \hat{a}_-\left(E - \hbar\omega\right)\psi = (E-\hbar\omega)(\hat{a}_-\psi)$$

We call $\hat{a}_\pm$ as the ladder operators : $\hat{a}_+$: raising operator and $\hat{a}_-$: lowering operator.

There is a lowest rung on this ladder : $\hat{a}_-\psi_0 = 0$.

$$\psi_0(x) = \frac{1}{\sqrt{2\hbar m\omega}}\left(\hbar\frac{d}{dx} + m\omega x\right)\psi_0 = 0.$$

$$\frac{d}{dx}\psi_0 = -\frac{m\omega}{\hbar}x\psi_0$$

$$\int \frac{d\psi_0}{\psi_0} = \int -\frac{m\omega}{\hbar}\, x\, dx$$

$$\ln \psi_0 = -\frac{m\omega}{2\hbar} x^2 + c.$$

$$\therefore\ \psi_0(x) = A e^{-\frac{m\omega}{2\hbar} x^2}, \text{ where } A = e^c.$$

and normalising it:

$$1 = |A|^2 \int_{-\infty}^{\infty} \left(e^{-m\omega x^2/2\hbar}\right)^2 dx$$

$$= \int_{-\infty}^{\infty} e^{-m\omega x^2/\hbar}\, dx = \frac{1}{|A|^2}$$

$$= \int_{-\infty}^{\infty} e^{-x^2/[\sqrt{\hbar/m\omega}]^2} \cdot x^{2(0)}\, dx$$ Gaussian integral

$$\int_0^{\infty} x^{2n} e^{-x^2/a^2} dx = \sqrt{\pi}\, \frac{(2n)!}{n!} \left(\frac{a}{2}\right)^{2n+1}$$

$$2\int_0^{\infty} e^{-x^2/[\hbar/m\omega]} dx = \cancel{2} \cdot \sqrt{\pi} \left(\frac{\sqrt{\hbar/m\omega}}{\cancel{2}}\right)$$

$$= \sqrt{\frac{\pi\hbar}{m\omega}}.$$

$$\therefore\ 1 = |A|^2 \sqrt{\frac{\pi\hbar}{m\omega}}\ ;\quad |A| = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4}.$$

$$\therefore\ \psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} e^{-(m\omega/2\hbar)x^2}.$$

We now simply apply the raising operator (repeatedly) to the $\psi_0(x) \longrightarrow$ the ground state to generate excited states.

$\therefore\ \psi_1(x) = A_1 \hat{a}_+ \psi_0$, where A_1 is the normalisation const. for $\psi_1(x)$.

$\psi_2(x) = A_2(\hat{a}_+)^2 \psi_0$
$\psi_3(x) = A_3(\hat{a}_+)^3 \psi_0.$
$\vdots$

$$\boxed{\psi_n(x) = A_n (\hat{a}_+)^n \psi_0}$$

Now,

$\hat{a}_+ \psi_n = C_n \psi_{n+1}$ as we know, $\hat{a}_\pm \psi_n \propto \psi_{n\pm1}.$

How ?

$$\hat{a}_+ \psi_n = C_n \psi_{n+1}$$

$$\hat{a}_- \psi_n = d_n \psi_{n-1}.$$

$\hat{a}_- = \hat{a}_+^{\,+}.$ → Hermitian conjugate (Adjoint)

$$\int_{-\infty}^{\infty} (\hat{a}_\pm \psi_n)^* (\hat{a}_\pm \psi_n)\, dx = \int_{-\infty}^{\infty} (\hat{a}_\mp \hat{a}_\pm \psi_n)^* \psi_n \, dx.$$

But using

$$\psi_n(x) = A_n (\hat{a}_+)^n \psi_0(x) \quad , \quad E_n = \left(n+\tfrac{1}{2}\right)\hbar\omega.$$

and $\hat{H} = \hbar\omega\left(\hat{a}_\pm \hat{a}_\mp \pm \frac{1}{2}\right)$ and $\hat{H}\psi = E\psi.$

$$\hbar\omega\left(\hat{a}_+\hat{a}_- + \tfrac{1}{2}\right)\psi = E\psi$$

$$\hbar\omega(\hat{a}_+ \hat{a}_- \psi_n) = \left(E_n - \frac{\hbar\omega}{2}\right)\psi_n$$

$$(\hat{a}_+ \hat{a}_- \psi_n) = \left(E_n - \frac{\hbar\omega}{2}\right)\frac{1}{\hbar\omega}\psi_n.$$

$$= \left\{\left[\left(n+\cancel{\tfrac{1}{2}}\right) - \cancel{\tfrac{1}{2}}\right]\cancel{\hbar\omega}\right\}\frac{1}{\cancel{\hbar\omega}}\psi_n = n\psi_n.$$

$$\therefore \ \hat{a}_+ \hat{a}_- \psi_n = n\psi_n$$

$|||^{ly}$, $\left(\hat{a}_- \hat{a}_+ - \frac{1}{2}\right)\hbar\omega\psi_n = E_n\psi_n$

$$a_- a_+ \psi_n = \frac{1}{\hbar\omega}\left[\left(E_n + \frac{1}{2}\right)\right]\psi_n$$

$$\hat{a}_- \hat{a}_+ \psi_n = (n+1)\psi_n$$

Using $\hat{a}_+ \hat{a}_- \psi_n$ & $\hat{a}_- \hat{a}_+ \psi_n$,

$$\hat{a}_+ \psi_n = \,?\; \int_{-\infty}^{\infty} (\hat{a}_+ \psi_n)^* (\hat{a}_+ \psi_n)\, dx = |c_n|^2$$

$$\Rightarrow \int_{-\infty}^{\infty} (\underline{\hat{a}_- \hat{a}_+ \psi_n})^* (\psi_n)\, dx = |c_n|^2$$

$$\downarrow$$

$$\Rightarrow \int_{-\infty}^{\infty} ((n+1)\psi_n)^* (\psi_n)\, dx = |c_n|^2$$

$$\Rightarrow \quad (n+1) \int_{-\infty}^{\infty} |\psi_n|^2 dx = |c_n|^2$$

Since ψ_n is already normalised, $\int_{-\infty}^{\infty} |\psi_n|^2 dx = 1.$

$$\therefore \quad c_n = \sqrt{n+1}$$

$$\therefore \quad \hat{a}_+ \psi_n = \sqrt{n+1}\, \psi_{n+1}$$

$$\hat{a}_- \psi_n \Rightarrow \int_{-\infty}^{\infty} (\hat{a}_- \psi_n)^* (\hat{a}_+ \psi_n)\, dx = |d_n|^2$$

$$\int_{-\infty}^{\infty} (\underline{\hat{a}_+ \hat{a}_- \psi_n})^* (\psi_n)\, dx = |d_n|^2$$

$$\downarrow$$

$$\int_{-\infty}^{\infty} (n\psi_n)^* (\psi_n)\, dx = |d_n|^2$$

$$n \int_{-\infty}^{\infty} |\psi_n|^2 dx = |d_n|^2$$

$$n \cdot 1 = |d_n|^2$$

$$\therefore \quad d_n = \sqrt{n}.$$

$$\therefore \quad \hat{a}_- \psi_n = \sqrt{n}\, \psi_{n-1}$$

$$\psi_1 = \hat{a}_+ \psi_0 . \quad \psi_2 = \frac{1}{\sqrt{2}} \hat{a}_+ \psi_1 = \frac{1}{\sqrt{2}} (\hat{a}_+)^2 \psi_0$$

$$\psi_3 = \frac{1}{\sqrt{3\cdot 2}} \psi_2 = \frac{(\hat{a}_+)^3}{\sqrt{3\cdot 2}} \psi_0 \; ; \quad \psi_4 = \frac{1}{2\cdot\sqrt{6}} (a_+)^4 \psi_0 .$$

$$\boxed{\therefore \; \psi_n(x) = \frac{(\hat{a}_+)^n}{\sqrt{n!}} \psi_0}$$

Bound states and scattering states.

Normalisable — Non-normalisable

$E < V(-\infty)$ and $V(+\infty)$ — $E > V(-\infty)$ and $V(+\infty)$

But usually in real life, $V(-\infty)$ and $V(\infty) \to 0$.

$\therefore \quad E < 0 \qquad\qquad E > 0$

The delta function well.

$$\delta(x) = \begin{cases} 0 , & x \neq 0 \\ \infty , & x = 0 \end{cases} \quad \text{and} \quad \int_{-\infty}^{\infty} \delta(x)\, dx = 1 .$$

Not a function but a generalised function.

Let us consider a potential of the form $V(x) = -\alpha \, \delta(x)$.
$\alpha > 0$, $\alpha \in \mathbb{R}$.

$$\therefore \text{TISE} = -\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} - \alpha\, \delta(x) \psi = E \psi .$$

Is possible for both $E > 0$ & < 0.

$\therefore$ Case I : $E < 0$ – Bound state. In the region $x < 0$, $V(x) = 0$.

$$\frac{d^2\psi}{dx^2} = -\frac{2mE}{\hbar^2} \psi = k^2 \psi$$

$$\therefore k^2 = \frac{-2mE}{\hbar^2} \to k = \sqrt{\frac{-2mE}{\hbar^2}}$$

$\hbar^2 \qquad\qquad V \quad \hbar^2$

Since $E < 0$, k is +ve & Real.

$\therefore$ General sol^n = $\psi(x) = Ae^{-kx} + Be^{kx}$.

At $x \to -\infty$, Ae^{-kx} blows up. $\therefore \psi(x) = Be^{kx}$. $(x<0)$

|||^{ly} for $x > 0$, $\psi(x) = Fe^{-kx}$.

Now, we need to stitch these two.

We know the boundary conditions for ψ:

ψ is always continuous, $d\psi/dx$ is continuous except at points where the potential is infinite

$$\therefore \quad \psi(x) = \begin{cases} Be^{kx} & (x \leq 0) \\ Fe^{-kx} & (x \geq 0) \end{cases}$$

$\therefore$ At $x=0$, $Be^{kx} = Fe^{-kx} \Rightarrow B = F$.

$$\therefore \quad \psi(x) = \begin{cases} Be^{kx} & x \leq 0 \\ Be^{-kx} & x \geq 0 \end{cases} \quad \text{or} \quad Be^{-k|x|}$$

We haven't encountered delta potential anywhere! It determines the discontinuity in the derivative of ψ at $x = 0$.

So, we integrate the Schrödinger equation from $-\epsilon$ to ϵ then put $\epsilon \to 0$.

$$\lim_{\epsilon \to 0} \left\{ -\frac{\hbar^2}{2m} \int_{-\epsilon}^{\epsilon} \overbrace{\cancel{\frac{d^2\psi}{dx^2}}}^{d\psi/dx} dx + \int_{-\epsilon}^{\epsilon} V(x)\psi(x)\,dx = E \int_{-\epsilon}^{\epsilon} \overbrace{\cancel{\psi(x)}}^{0 \to \text{continuous}} dx. \right\}$$

$$\therefore \quad \left.\frac{d\psi}{dx}\right|_{-\epsilon} - \left.\frac{d\psi}{dx}\right|_{\epsilon} = \frac{2m}{\hbar^2} \lim_{\epsilon \to 0} \int_{-\epsilon}^{\epsilon} V(x)\psi(x)\,dx$$

When x is anything else, $\int^{\epsilon} V(x)\psi(x)\,dx = 0$ at lim as

$\psi(x)$ is continuous. But x is infinite at the boundary $x=0$.

$$\therefore \underbrace{\left.\frac{d\psi}{dx}\right|_{-\epsilon} - \left.\frac{d\psi}{dx}\right|_{\epsilon}} = \frac{2m}{\hbar^2} \lim_{\epsilon \to 0} \int_{-\epsilon}^{\epsilon} -\alpha\, \delta(x)\, \psi(x)\, dx.$$

$$\Rightarrow \quad -\Delta\left(\frac{d\psi}{dx}\right) = \frac{2m\alpha}{\hbar^2}\psi(0)$$

$$\therefore \quad \left.\frac{d\psi}{dx}\right|_{\epsilon} - \left.\frac{d\psi}{dx}\right|_{-\epsilon} = -\frac{2m\alpha}{\hbar^2}\psi(0)$$

$$\frac{d\psi}{dx} = -Bk e^{-kx}, \; x>0 \Rightarrow d\psi/dx|_{+} = -Bk$$

$$\frac{d\psi}{dx} = +Bk e^{kx}, \; x<0 . \Rightarrow d\psi/dx|_{-} = Bk.$$

$$\therefore \Delta = -2Bk \quad \text{and} \quad \psi(0) = \text{just } B$$

$$\therefore \quad k = -\frac{\cancel{2}m\alpha}{\cancel{2}\cancel{B}\hbar^2}\cdot \cancel{B} = +\frac{m\alpha}{\hbar^2}$$

$$\& \; k = \sqrt{\frac{-2mE}{\hbar^2}} \qquad \therefore \quad E = \frac{-k^2\hbar^2}{2m}$$

$$= \frac{-\cancel{\hbar^2}\, m^{\cancel{2}}\alpha^2}{\cancel{\hbar^4}\cdot 2\cancel{m}} = -\frac{m\alpha^2}{2\hbar^2} \qquad \therefore \; E = \frac{-m\alpha^2}{2\hbar^2}$$

Normalising it, we get $\Rightarrow \int_{-\infty}^{\infty} |\psi(x)|^2 dx$

$$= 2|B|^2 \int_0^{\infty} e^{-2kx} dx = \frac{|B|^2}{k} = 1$$

$$\therefore \quad B = \sqrt{k} = \frac{\sqrt{m\alpha}}{\hbar}.$$

$$\therefore \psi(x) = \frac{\sqrt{m\alpha}}{\hbar} e \quad \quad \& \quad E = \frac{-m\alpha}{2\hbar^2}$$

Bound states.

Scattering states?

$E > 0$

$$\therefore \text{for } x<0, \quad \frac{d^2\psi}{dx^2} = -\frac{2mE}{\hbar^2}\psi = -k^2\psi$$

$$\text{with } k = \frac{\sqrt{2mE}}{\hbar}$$

$\therefore \psi(x) = Ae^{ikx} + Be^{-ikx}$. Since the powers are now imaginary, neither of them blow up now.

|||ly for $x>0$, $\psi(x) = Fe^{ikx} + Ge^{-ikx}$.

Continuity of $\psi(x)$ still holds.

$\therefore F+G = A+B$ at $x=0$.

$$\frac{d\psi}{dx} = ik\left(Fe^{ikx} - Ge^{-ikx}\right), x>0, \quad \left.\frac{d\psi}{dx}\right|_{\epsilon} = ik(F-G)$$

$$\frac{d\psi}{dx} = ik\left(Ae^{ikx} - Be^{-ikx}\right), x<0, \quad \left.\frac{d\psi}{dx}\right|_{-\epsilon} = ik(A-B)$$

$$\therefore \Delta\frac{d\psi}{dx} = ik(F+B-A-G) = -\frac{2m\alpha}{\hbar^2}(A+B)$$

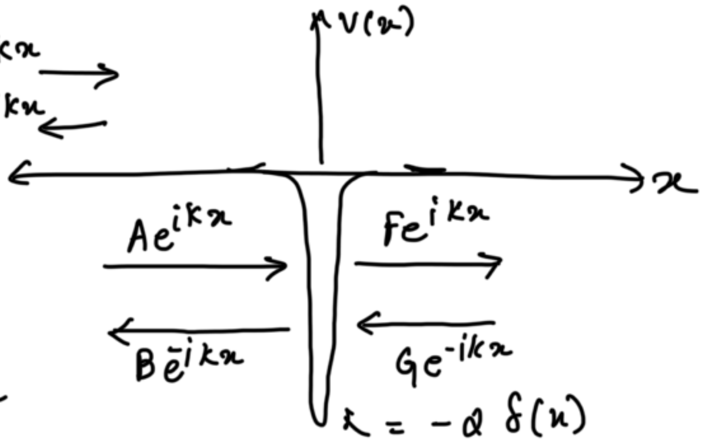
$\psi(0) = (A+B)$

$$\Rightarrow F-G = A(1+2i\beta) - B(1-2i\beta)$$

where $\beta = \dfrac{m\alpha}{\hbar^2 k}$.

All boundary conditions imposed, yet we have 4 unknowns (A, B, F, G) but 2 equations → Hence non-normalisable state.

Recall from Free particle: $e^{ikx} \rightarrow$
$e^{-ikx} \leftarrow$



Physical interpretation :

In a scattering experiment,

A → amplitude of incident wave
B → Reflected wave
F → Transmitted wave.

Solving for B & F in terms of A (the incident wave):

$$B = \frac{i\beta}{1-i\beta}A \quad ; \quad F = \frac{1}{1-i\beta}A.$$

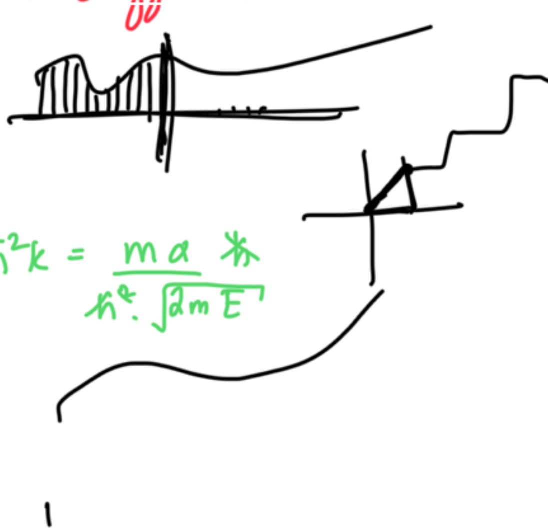
Studying scattering from right : set $A=0$,

G → incident, F → reflected, B → Transmitted.

Probability of finding a particle is $|\Psi|^2$, so the relative probability that an incident particle will be reflected back:

$$\frac{|B|^2}{|A|^2} = \frac{\beta^2}{1+\beta^2} \equiv R \rightarrow \text{reflection coefficient.}$$

lllly, $\frac{|F|^2}{|A|^2} = \frac{1}{1+\beta^2} \equiv T \rightarrow$ Transmission Coefficient.



and as expected, $R+T=1$.

R & T → functions of β, $\beta = m\alpha/\hbar^2 k = \frac{m\alpha\,\hbar}{\hbar^2\cdot\sqrt{2mE}}$

$= \frac{\sqrt{m}\,\alpha}{\hbar\sqrt{2E}} = \beta \qquad \therefore \beta^2 = \frac{m\alpha^2}{2\hbar^2 E}$

$\therefore R = \frac{1}{\dots}$ and $T = \frac{1}{\dots}$

$1+(2\hbar^2 E/m\alpha^2)$ $\qquad\qquad$ $1+(m\alpha^2/2\hbar^2 E)$

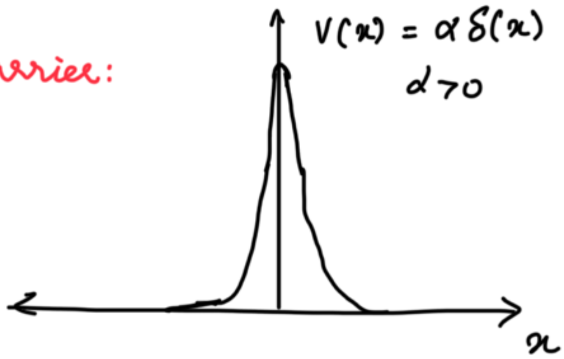
NOTE:

a) Scattering wave functions are not normalisable - Can only form normalisable linear combinations of stationary states.

b) It is impossible to create a normalisable wavefunctions without involving a range of Energies $\Rightarrow$ Hence Values of R & T are approximate.

We were able to analyse a time dependent problem using stationary states!

Now, delta function Barrier:



→ Kills the bound states
→ R & T remains unchanged.

A particle is just as likely to pass through the barrier as to cross over the well! → Quantum Mechanical Tunelling: Particle has some non-zero probability of passing through the potential even if $E > V_{max}$.

Finite Square Well.

$$V(x) = \begin{cases} -V_0, & -a \le x \le a \\ 0, & |x| > a. \end{cases}$$

Case 1: $E < 0$ (Bound states)

at $x < -a$, $V = 0$, TISE:

$$\frac{-\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi \quad \text{or} \quad \frac{d^2\psi}{dx^2} = k^2\psi$$

where $k^2 = \sqrt{-2mE}$ $\quad$ k is real + positive.

$$\hbar^2$$

Gen. sol^n : $\psi(x)$ $Ae^{-kx} + Be^{kx}$, but at $x \to -\infty$, Ae^{-kx} blows up.

$\therefore \psi(x) = Be^{kx}, x < -a.$

in region $x \in [-a,a]$, $V(x) = V_0$.

$$\therefore -\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} - V_0\psi = E\psi \text{ or } \frac{d^2\psi}{dx^2} = -l^2\psi.$$

where $l = \sqrt{\frac{2m(E+V_0)}{\hbar}}$, real & +ve.

$\therefore \psi(x) = C\sin lx + D\cos lx, x \in [-a,a]$

For region $x > a$, $\psi(x) = Fe^{-kx}, x > a.$

Now, impose boundary conditions :

ψ & $\frac{d\psi}{dx}$ $\to$ continuous everywhere, & at $-a$ & a.

$$\psi(x) = \begin{cases} Fe^{-kx}, & (x > a) \\ D\cos(lx), & (0 < x < a) \\ \psi(-x), & x < 0. \end{cases}$$

Assuming ψ is even.

and $\psi(x)$ continuous at $x = a$,

$\therefore \cancel{F}e^{\cancel{-ka}} = \cancel{D}\cos(la)$ &

$\frac{d\psi}{dx}$ contn at $x = a$,

$-Fk\,e^{\cancel{-ka}} = -\cancel{D}l\sin(la)$

Sec. 2.6: The Finite Square Well

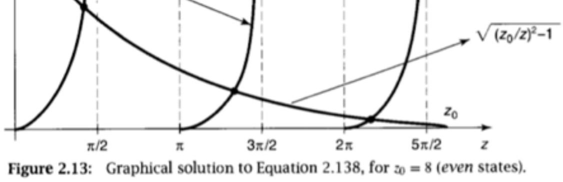


Figure 2.13: Graphical solution to Equation 2.138, for $z_0 = 8$ (*even* states).

$\Rightarrow \quad -k = -l\tan(la), \quad k = l\tan(la)$

defining $z = la$, $z_0 = \frac{a}{\hbar}\sqrt{2mV_0}$

$k^2+l^2 = \frac{2mV_0}{\hbar^2}$. $\therefore Ka = \sqrt{z_0^2 - z}$

$\therefore$ $\underline{\tan(z) = \sqrt{(z_0/z)^2 - 1}}$

This is a transcendental equation for z (and hence for E) as a function of z_0 (which is a measure of the size of the well)

Case 2 : Scattering states : $E > 0$.

To the left, $\psi(x) = Ae^{ikx} + Be^{-ikx}$, $k = \sqrt{\frac{2mE}{\hbar}}$

Inside the well, $\psi(x) = C\sin(lx) + D\cos(lx)$.

To the right (assuming no incoming wave) : $\psi(x) = Fe^{ikx}$.

Again, $A \rightarrow$ incident, $B \rightarrow$ Reflected, $F \rightarrow$ Transmitted.

But what are C & D ? $\rightarrow$ Let us first impose the boundary conditions and then figure out !

Continuity of ψ at $-a \Rightarrow Ae^{-ika} - Be^{ika} = -C\sin(la) + D\cos(la)$.

Continuity of $\frac{d\psi}{dx}$ at $-a \Rightarrow ik\left[Ae^{-ika} - Be^{ika}\right] = l\left[C\cos la + D\sin la\right]$

Contn. of ψ at $a \Rightarrow Fe^{ika} = C\sin la + D\cos la$

Contn of $\frac{d\psi}{dx}$ at $a \Rightarrow ikFe^{ika} = l\left[C\cos la - D\sin la\right]$

Eliminating C & D using last 2 eq^{n}s & 1^{st} 2 eq^{n}s,

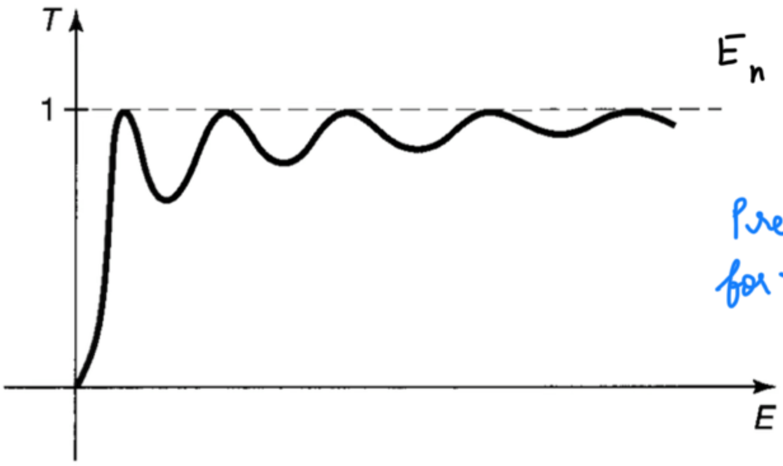
$$B = i\frac{\sin 2la}{2kl}(l^2-k^2)F.$$

$$F = \frac{e^{-2ika}A}{\cos(2la) - i\frac{(k^2+l^2)}{2kl}\sin(2la)}$$

$$T = \frac{|F|^2}{|A|^2} = \left[1 + \frac{V_0^{\,2}}{4E(E+V_0)} \sin^2\left(\frac{2a}{\hbar}\sqrt{2m(E+V_0)}\right)\right]^{-1}$$

$T = 1$ whenever sine is zero, i.e., $\frac{2a}{\hbar}\sqrt{2m(E_n+V_0)} = n\pi$.

$\therefore$ Energies for perfect transmission :



$$E_n + V_0 = \frac{n^2\hbar^2\pi^2}{8ma^2} \rightarrow$$

Precisely the allowed energies for the infinite square well!

Figure 2.14: Transmission coefficient as a function of energy (Equation 2.151).

Formalism

There is not much here that is genuinely new — the idea is to make coherent sense of what we have already discovered earlier.

The Hilbert Space

Quantum theory $\rightarrow$ 2 constructs : Wave functions & Operators.

state of a system   observables

Wave functions $\rightarrow$ Abstract vectors

Operators $\rightarrow$ linear transformations that act on vectors.

BUT THIS IS NOT LINEAR ALGEBRA THAT WE ARE FAMILIAR WITH.

But it is Linear Algebra. Slightly different.

How?

$\begin{bmatrix}3\\4\end{bmatrix} \longrightarrow \begin{bmatrix}\vdots\\\vdots\\\vdots\end{bmatrix}$

Vectors in QM are functions, and thus we do not work in N-Dim. Vector space, but an infinite dimensional vector space.

Now that we are in infinite dim. Vector space, the integral may not converge! → To tackle this, obviously, we restrict our domain of functions in QM to a particular type of fns.

Since $\int_{-\infty}^{\infty} |\Psi|^2 dx = 1$, Ψ belongs to a set of $f(x)$ such that

$$\boxed{\int_{-\infty}^{\infty} |f(x)|^2 dx < \infty} \longrightarrow$$

Mathematicians call it $\mathcal{L}_2(a,b)$

Physicists call it Hilbert Space.

Wave functions live in Hilbert Space.

Hence we define inner product to be

$$\langle f|g\rangle \equiv \int_a^b f^*(x)\, g(x)\, dx.$$

Schwarz inequality:

$$\left| \int_a^b f(x)^* g(x)\, dx \right| \leq \sqrt{\int_a^b |f(x)|^2 dx \int_a^b |g(x)|^2 dx}$$

$$|\langle f|g\rangle|^2 \leq \langle f|f\rangle \langle g|g\rangle.$$ → Prove it!

Orthonormal basis $\{f_n\} \rightarrow \langle f_m|f_n\rangle = \delta_{mn}$.

Completeness: $f(x) = \sum_{n=1}^{\infty} c_n f_n(x)$

Fourier's trick

How??

if $f_n(x)$ are orthonormal. $c_n = \langle f_n|f\rangle$

The stationary states of the infinite square well constitute a complete orthonormal set on the interval $(0, a)$.

The stationary states of the Harmonic oscillator are a complete orthonormal set on the interval $(-\infty, \infty)$

Observables

Observables are represented by Hermitian Operators.

Let Q be an Observable → Real...

$$\therefore \langle Q \rangle = \int \Psi^* \hat{Q} \Psi \, dx = \langle \Psi | \hat{Q} | \Psi \rangle$$

$$= \langle \Psi | \hat{Q} \Psi \rangle$$

$$\langle Q \rangle^* = \int \Psi^* \hat{Q}^+ \Psi \, dx = \langle \Psi | \hat{Q}^+ \Psi \rangle$$

$$= \langle \hat{Q} \Psi | \Psi \rangle$$

But $\langle Q \rangle^* = \langle Q \rangle$ as $\langle Q \rangle$ is Real.

$$\therefore \langle \Psi | \hat{Q} \Psi \rangle = \langle \hat{Q} \Psi | \Psi \rangle \quad \forall \, \Psi(x)$$

$$\therefore \hat{Q} = \hat{Q}^+ \longrightarrow \text{Hermitian.}$$

More stronger definition → $\langle f | \hat{Q} g \rangle = \langle \hat{Q} f | g \rangle \ \forall f, g$.

Hermitian – Transpose conjugate.

Is momentum operator Hermitian?

$$\langle f | \hat{p} g \rangle = \int_{-\infty}^{\infty} f^* (-i\hbar) \frac{dg}{dx} \, dx = \cancelto{0}{-i\hbar f^* g \Big|_{-\infty}^{\infty}} + \int_{-\infty}^{\infty} \left(-i\hbar \frac{df}{dx}\right)^* g \, dx.$$

Integration by parts.

$$= \langle \hat{p} f | g \rangle.$$

Determinate States

Ordinarily if you measure an observable Q on an ensemble of identically prepared systems, all in the same state ψ, you don't get the same result each time - this is the indeterminacy of Quantum Mechanics

But, there are states where every measurement of Q would return the same value (say, q). These states are called determinate states, for the observable Q.

$$\therefore \sigma^2 = 0 = \langle (\hat{Q} - \langle Q \rangle)^2 \rangle$$

$$= \langle \psi | (\hat{Q} - q)^2 \psi \rangle = \langle (\hat{Q} - q)\psi | (\hat{Q} - q)\psi \rangle = 0$$

as $\langle Q \rangle = q$ as Q is always giving q.

$$(\hat{Q} - q)\psi = 0$$

for $\psi \neq 0$ (non-trivial):

$\hat{Q}\psi = q\psi$. → The eigen value equation for the operator $\hat{Q}$.

ψ is the eigen function of $\hat{Q}$ and q is the corresponding eigen value.

Hence determinate states of Q are eigen functions of $\hat{Q}$.

Collection of all eigen values of an operation is called its spectrum.

Eigen functions of Hermitian Operator

→ Discrete Spectra

The normalisable eigen functions of a hermitian operator have two important properties:

1) Their eigenvalues are real

2) Eigen functions belonging to distinct eigenvalues are orthogonal.

Axiom : The eigen functions of an observable operator are complete. Any function (in Hilbert space) can be expressed as a linear combination of them.

→ Continuous spectra

Eigen functions are not normalisable. So, the 2 theorems fail.

But essential properties → reality, orthogonality, and completeness still hold.