Quantum Mechanics I

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UC2
Quantum Mechanics in 1D

UC2 contents:

- Stationary states and the time-independent Schrödinger equation.
- Free particles and wave packets.
- Finite, Infinite potential wells, and the harmonic oscillator.
- Delta-function potentials, tunnelling and scattering states.

Matter waves of free particles

Particle $\left\{ \begin{array}{l} E = \hbar\omega \\ p = \hbar k \end{array} \right.$ what is the shape of a wave?

Plane wave in the +x direction:

(i) $\sin(kx - \omega t)$

(ii) $\cos(kx - \omega t)$

(iii) $e^{ikx - i\omega t}$ $\quad (e^{-i\omega t}$ always$)$

(iv) $e^{-ikx + i\omega t}$ $\quad (e^{+i\omega t}$ always$)$] phase.

Superposition + Probabilities:

↳ state of particle with the = prob. of moving to the left or right

(i) $\sin(kx - \omega t) + \sin(kx + \omega t) = 2\sin(kx)\cos(\omega t)$

but this vanishes at $\left(\omega t = \frac{\pi}{2}, \frac{3\pi}{2}, \frac{5\pi}{2}, \ldots\right)$

$\Rightarrow$ cannot be a matter particle.

ii) $\cos(kx - \omega t) + \cos(kx + \omega t) = 2\cos(kx)\cos(\omega t)$

Matter waves of free particles

iii) $e^{ikx-i\omega t} + e^{-ikx-i\omega t}$

$= \left(e^{ikx} - e^{-ikx}\right) e^{-i\omega t} = 2\cos(kx)\, e^{-i\omega t}$ (does not vanish)

(iv) $e^{-ikx} e^{i\omega t} + e^{ikx} e^{i\omega t}$

$= 2\cos(kx)\, e^{i\omega t}$ (does not vanish)

(iii) ∧ (iv) cannot be true at the same time.

Superimposing a state to itself does not change the state.

$e^{ikx-i\omega t} + e^{-i(kx-\omega t)} = 2\cos(kx-\omega t)$

energy part always has −

$\Rightarrow \boxed{\Psi(x,t) = e^{ikx-i\omega t}}$ in 1D $\Rightarrow \Psi(\vec{r},t) = e^{i\vec{k}\vec{r}-i\omega t}$

The above is the wave function for a particle with:

$p = \hbar k$

$E = \hbar\omega$

$\vec{p} = \hbar\vec{k}$

$E = \hbar\omega$

Wave function of a free particle

$$\Psi(x,t) = e^{ikx - i\omega t} \quad \text{with} \quad p = \hbar k, \quad E = \hbar\omega$$

Non-relativistic particles: $E = \frac{p^2}{2m}$

Momentum:

$$\frac{\hbar}{i}\frac{\partial}{\partial x}\Psi = \hbar k \Psi = p\Psi$$

momentum operator: $\hat{p} = \frac{\hbar}{i}\frac{\partial}{\partial x}$

$$\Rightarrow \hat{p}\Psi = p\Psi$$

If this holds:

1) $\Psi(x,t)$ is an eigenstate of $\hat{p}$ with eigenvalue "p".

Remember: $\begin{bmatrix} \text{matrix} \end{bmatrix} \begin{bmatrix} \text{vector} \end{bmatrix} = \alpha \begin{bmatrix} \text{vector} \end{bmatrix}$

↳ rotate ×, same vector × constant ✓ eigenvector.

2) $\Psi(x,t)$ is a state of definite momentum.

Wave function of a free particle

Energy:

$$i\hbar \frac{\partial}{\partial t}\Psi = i\hbar(-i\omega)\Psi = \hbar\omega\Psi = E\Psi$$

We know that: $E = \frac{p^2}{2m}$, let's find an operator:

Then: $E\Psi = \frac{p^2}{2m}\Psi = \frac{p}{2m}\overset{p\Psi}{\hat{p}\Psi} = \frac{p}{2m}\left(\frac{\hbar}{i}\frac{\partial}{\partial x}\Psi\right) = \frac{1}{2m}\frac{\hbar}{i}\frac{\partial}{\partial x}(\overset{\hat{p}\Psi}{p\Psi}) =$

$$= \frac{1}{2m}\frac{\hbar}{i}\frac{\partial}{\partial x}\left(\frac{\hbar}{i}\frac{\partial}{\partial x}\Psi\right) = \underbrace{-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}}_{\text{energy operator}}\Psi \quad (2^{\text{nd}} \text{ order PDE})$$

$$\boxed{\hat{E} = \frac{1}{2m}\hat{p}^2}$$

$\Rightarrow \hat{E}\Psi = E\Psi$

1) Ψ is an eigenstate of $\hat{E}$.

2) Ψ is a state of definite E.

Schrödinger equation of a free particle

$$i\hbar \frac{\partial \psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 \psi}{\partial x^2}$$

Let’s substitute this solution:

$$\psi = e^{ikx - i\omega t}$$

Into Schrödinger’s equation:

$$i\hbar(-i\omega)\cancel{\psi} = -\frac{\hbar^2}{2m}(ik)^2\cancel{\psi}$$

$$\hbar\omega = \frac{\hbar^2 k^2}{2m} \Rightarrow \boxed{E = \frac{p^2}{2m}}$$

relation tells we have a particle plane wave that exists.

- Eqn. is linear, so we can construct more general solutions.

The time-independent Schrödinger equation

How do we get $\Psi(x,t)$?

We need to solve Sch. eq:

$$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 \Psi}{\partial x^2} + V\Psi$$

for a specified potential $V = V(x,t)$

* For simplicity, we will assume that $V = V(x)$ is independent of t.

Then, we can use separation of variables, and look for solutions.

$$\Psi(x,t) = \psi(x)\,\varphi(t)$$

- Solutions of this type are only a subset, but they are interesting.
- We can patch together these solution to construct more general solutions.

The time-independent Schrödinger equation

Separation of variables: $$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 \Psi}{\partial x^2} + V\Psi$$

LHS:

$$\frac{\partial \Psi}{\partial t} = \psi(x)\frac{d\varphi(t)}{dt}$$

RHS:

$$\frac{\partial^2 \Psi}{\partial x^2} = \varphi(t)\frac{d^2\psi}{dx^2}$$

ordinary derivatives

Sch. Eq:

$$\Rightarrow \quad i\hbar\,\psi\,\frac{d\varphi}{dt} = -\frac{\hbar^2}{2m}\varphi\frac{d^2\psi}{dx^2} + V\psi\varphi$$

$\div\ \psi\varphi$

$$\Rightarrow \quad \underbrace{i\hbar\,\frac{1}{\varphi}\frac{d\varphi}{dt}}_{\text{function of } t} = \underbrace{-\frac{\hbar^2}{2m}\frac{1}{\psi}\frac{d^2\psi}{dx^2} + V}_{\text{function of } x}$$

The time-independent Schrödinger equation

Separation of variables: $$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 \Psi}{\partial x^2} + V\Psi$$

Temporal ODE:

$$i\hbar \frac{1}{\varphi}\frac{d\varphi}{dt} = E$$

$$\Rightarrow \boxed{\frac{d\varphi}{dt} = -\frac{i}{\hbar}E\varphi} \quad \text{ODE} \quad \Rightarrow \varphi(t) = Ce^{-\frac{iE}{\hbar}t}$$

the wiggle factor.

$$\varphi(t) = C\left(\cos\left(\frac{E}{\hbar}t\right) - i\sin\left(\frac{E}{\hbar}t\right)\right).$$

Spatial ODE:

$$-\frac{\hbar^2}{2m}\frac{1}{\psi}\frac{d^2\psi}{dx^2} + V = E$$

$$\boxed{-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V\psi = E\psi}$$

time-independent Sch. equation.

* $V(x)$ needs to be specified.

Separable Solutions

Why are separable solutions important?

Most sln to time-depende S.eq do not take this form.

1) They are stationary states:

$$\Psi(x,t) = \psi(x)\, e^{-i\frac{E}{\hbar}t}$$

$$\Rightarrow |\Psi(x,t)|^2 = \Psi\Psi^* = \psi e^{-i\frac{E}{\hbar}t}\, \psi^* e^{+i\frac{E}{\hbar}t} = |\psi(x)|^2$$

the probability density does not depend on time.

Expectation Values:

$$\langle Q(x,p)\rangle = \int \Psi^* \left[Q\left(x, -i\hbar\frac{\partial}{\partial x}\right)\right] \Psi \, dx$$

$$\Rightarrow \langle Q(x,p)\rangle = \int \psi^* \left[Q\left(x, -i\hbar\frac{\partial}{\partial x}\right)\right] \psi \, dx$$

- Every expectation value is constant in time
- If $\langle x\rangle$ is constant, $\Rightarrow$ $\langle p\rangle = 0$
- Nothing ever happens in a stationary state.

Separable Solutions

2) They are states of definite total energy.

$$H(x,p) = \frac{p^2}{2m} + V(x) \qquad \text{Hamiltonian}$$

The Hamiltonian operator is:

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x) \quad \overset{\text{Sch eq}}{\Longrightarrow} \quad \hat{H}\psi = E\psi$$

The expectation value is:

$$\langle H \rangle = \int \psi^* \hat{H} \psi \, dx = E\int |\psi|^2 dx = E\int |\Psi|^2 dx = E$$

Also: $\hat{H}^2\psi = \hat{H}(\hat{H}\psi) = \hat{H}(E\psi) = E\hat{H}\psi = E^2\psi$

$$\Rightarrow \langle H^2 \rangle = \int \psi^* \hat{H}^2 \psi \, dx = E^2 \int |\psi|^2 dx = E^2$$

The variance of H is

$$\sigma_H^2 = \langle H^2 \rangle - \langle H \rangle^2 = E^2 - E^2 = 0 \qquad \text{(zero spread)}$$

Every measurement of the total energy returns E in a separable sln.

Separable Solutions

3) The general solution is a linear combination of the separable slns.

$\psi_1(x),\ \psi_2(x),\ \psi_3(x) \Rightarrow \{\psi_n(x,t)\}$

$E_1 \quad E_2 \quad E_3 \qquad \{E_n\}$

$\Rightarrow \Psi_1(x,t) = \psi_1(x) e^{-i\frac{E_1}{\hbar}t}$, etc.

general $\Rightarrow$ solution

$$\boxed{\Psi(x,t) = \sum_{n=1}^{\infty} c_n \psi_n(x) e^{-\frac{iE_nt}{\hbar}}}$$

Every sln. to the time-dependent S. eq can be written in this form. We need to find c_n.

Once you solved ψ $\Rightarrow$ getting a general sln. is straightforward.

Structure of a typical QM problem

We need to solve the time-dependent Schrödinger equation:

$$\left.\begin{array}{l} V(x) \\ \Psi(x,0) \end{array}\right\} \text{are given} \Rightarrow \Psi(x,t) = ?$$

Assuming V=V(x), we can solve it via separation of variables:

1) Solve time-indep. S eq $\Rightarrow$ infinite set of slns. $\{\psi_n(x)\}$
$\{E_n\}$

2) To fit $\Psi(x,0)$, linear combination:

$$\Psi(x,0) = \sum_{n=1}^{\infty} c_n \psi_n(x)$$

You can always match the initial state choosing $\{c_n\}$.

Structure of a typical QM problem

3) To construct $\Psi(x,t)$, you add the wiggle factor.

$$\boxed{\Psi(x,t) = \sum_{n=1}^{\infty} c_n \psi_n(x) e^{-\frac{iE_n}{\hbar}t} = \sum_{n=1}^{\infty} c_n \Psi_n(x,t)}$$

4) The separable slns are stationary states.

$$\Psi_n(x,t) = \psi_n(x)\, e^{-\frac{iE_n t}{\hbar}}$$

- All prob. and expectation values are independent of t.
- Property not shared by the general solution
  ↳ energies are different for different ψ_n, so "e" do not cancel out.

Structure of a typical QM problem

What is the physical meaning of $\{c_n\}$?

$|c_n|^2$ is the prob. that a measurement of the energy return E_n.

* measurement yields one allowed value.

$$\Rightarrow \boxed{\sum_{n=1}^{\infty} |c_n|^2 = 1}$$

$$\Rightarrow \boxed{\langle H \rangle = \sum_{n=1}^{\infty} |c_n|^2 E_n}$$ Expectation value of the energy.

* $\{c_n\}$ do not depend on time.

$\Rightarrow \langle H \rangle$ do not " " " $\Rightarrow$ energy conservation in QM.

1) Null potential: free QM particles

For a free particle: $V(x) = 0$, there are no boundary conditions

Sch. eq of a free particle:

$$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2}$$

A possible sln was: $\Psi = e^{ikx - i\omega t}$

$$E = \frac{p^2}{2m} = \frac{(\hbar^2 k^2)}{2m}$$

In a general way: $\Psi = \psi(x)\varphi(t)$

$$E = \cancel{\hbar}\omega = \frac{\hbar^{\cancel{2}} k^2}{2m}$$

Sch eq. $\Longrightarrow$
$$\begin{cases} i\hbar \dfrac{1}{\varphi}\dfrac{d\varphi}{dt} = E \\ -\dfrac{\hbar^2}{2m}\dfrac{1}{\psi}\dfrac{d^2\psi}{dx^2} + \cancelto{0}{V} = E \Rightarrow \boxed{-\dfrac{\hbar^2}{2m}\dfrac{d^2\psi}{dx^2} = E\psi} \end{cases}$$

$$\Rightarrow \omega = \frac{\hbar k^2}{2m}$$

time-independent Sch. eq

1) Null potential: free QM particles

$$\Rightarrow \frac{d^2\psi}{dx^2} = -k^2\psi \quad ; \quad \text{where } k = \frac{\sqrt{2mE}}{\hbar}$$

sln

$$\Rightarrow \boxed{\psi(x) = Ae^{ikx} + Be^{-ikx}}$$

General sln. for x.

↳ the particle can carry any (positive) energy.

$$\Rightarrow \Psi(x,t) = Ae^{ikx - i\frac{\hbar k^2}{2m}t} + Be^{-ikx - i\frac{\hbar k^2}{2m}t}$$

$$\Psi(x,t) = Ae^{ik[x - \frac{\hbar k}{2m}t]} + Be^{-ik[x + \frac{\hbar k}{2m}t]}$$

$$\boxed{\Psi(x,t) = A\underbrace{e^{ik(x - vt)}}_{\rightarrow} + B\underbrace{e^{-ik(x + vt)}}_{\leftarrow}}$$

This term $(x \mp vt)$ implies we have a wave of unchanging shape going in the $\pm x$ direction.

$$(x \mp vt) = \text{constant} \Rightarrow x = \text{constant} \pm vt$$

1) Null potential: free QM particles

$$\Rightarrow \boxed{\Psi_k(x,t) = A\, e^{i\left(kx - \frac{\hbar k^2}{2m} t\right)}}$$

$$k \equiv \pm \frac{\sqrt{2mE}}{\hbar} \quad \begin{cases} k>0 & \text{wave} \rightarrow \\ k<0 & \text{wave} \leftarrow \end{cases}$$

The stationary states of the free particle are propagating waves, with $\boxed{\lambda = \frac{2\pi}{|k|}}$, momentum $\boxed{p = \hbar k}$, and speed:

$$v_{quantum} = \frac{\hbar |k|}{2m} = \sqrt{\frac{E}{2m}}.$$

But, there are two problems.

1) Null potential: issues with plane wave solutions

1) The classical speed of a free particle with $E = \frac{1}{2}mv^2$ is

$$v_{classical} = \sqrt{\frac{2E}{m}} = 2\, v_{quantum}.$$

* The QM wave travels at ½ $v_{particle}$?! (Paradox)

2) This wave function is not normalisable.

$$\int_{-\infty}^{+\infty} \Psi_k^* \Psi_k \, dx = \int_{-\infty}^{+\infty} |A|^2 e^{i\alpha} e^{-i\alpha} dx = |A|^2 \int_{-\infty}^{+\infty} dx$$

$$= |A|^2 x \Big|_{-\infty}^{+\infty} = |A|^2 (\infty) \quad \text{(Big problem)}$$

* Sep. sln do not represent physical states!
* A free particle cannot exist in a stationary state!
* A free particle with definite E cannot exist!

1) Null potential: free QM particles

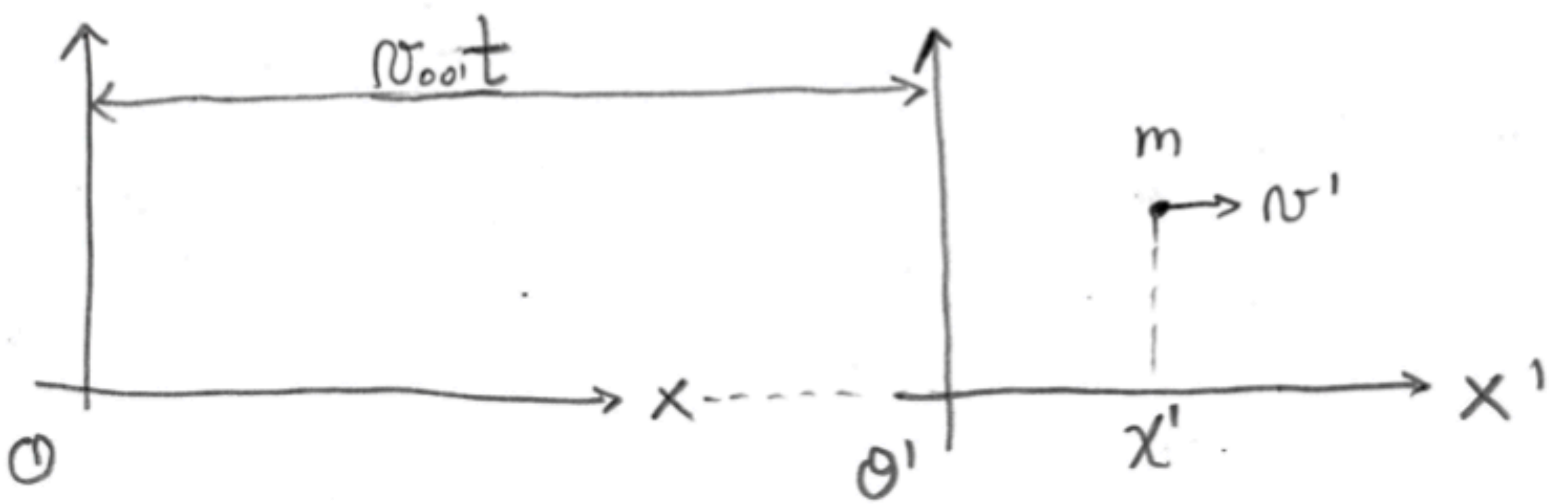
Problem 1: Quantum waves are <u>NOT</u> ordinary (classical) waves.

de Broglie: $\lambda = \dfrac{h}{p}$.

$\psi(x,t) \in \mathbb{C}$ $\begin{cases} \text{Is it measurable?} \\ \text{What's its meaning?} \end{cases}$

Imagine we have 2 observers who measure $\binom{\lambda}{p}$ moving at constant speeds with respect to each other, do their measurements agree?

$$p = \frac{h}{\lambda} = \left(\frac{h}{2\pi}\right)\left(\frac{2\pi}{\lambda}\right) = \hbar \underset{\uparrow \text{ wave number}}{k}$$



$\begin{cases} \text{velocity: } v,\ v' \\ \text{momentum: } p,\ p' \end{cases}$

1) Null potential: free QM particles

$$x' = x - v_{00}t \qquad t' = t \quad \Big\} \text{ Galilean transformation}$$

$$\frac{dx'}{dt'} = \frac{dx}{dt} - v_{00} \Rightarrow v' = v - v_{00}$$

$$\Rightarrow p' = p - m v_{00}$$

In the lab:

de Broglie λ do not agree.

$$\lambda = \frac{h}{p} \qquad \lambda' = \frac{h}{p'} = \frac{h}{p - m v_{00}} \Rightarrow \boxed{\lambda \neq \lambda'}$$

For ordinary waves, this does NOT happen. λ does not change.

Phase of the wave: $\phi = kx - \omega t$

ϕ is a Galilean invariant, 2 obs. will agree on the value of the phase.

$$\Rightarrow \phi = k\left(x - \frac{\omega}{k}t\right) = \frac{2\pi}{\lambda}(x - v\,t)$$

↳ velocity of the wave.

$$\phi = \overset{k}{\frac{2\pi x}{\lambda}} - \overset{\omega}{\frac{2\pi v}{\lambda}}\,t$$

1) Null potential: free QM particles

O' should see the same phase: $\phi' = \phi$ (same point, same t)

$$\phi' = \phi = \frac{2\pi}{\lambda}(x - Vt)$$

$$= \frac{2\pi}{\lambda}(x' + vt - Vt)$$

$$= \frac{2\pi}{\lambda}(x' + vt' - Vt') = \overbrace{\frac{2\pi}{\lambda}}^{k'} x' - \overbrace{\frac{2\pi V}{\lambda}\left(1 - \frac{v}{V}\right)}^{\omega'} t'$$

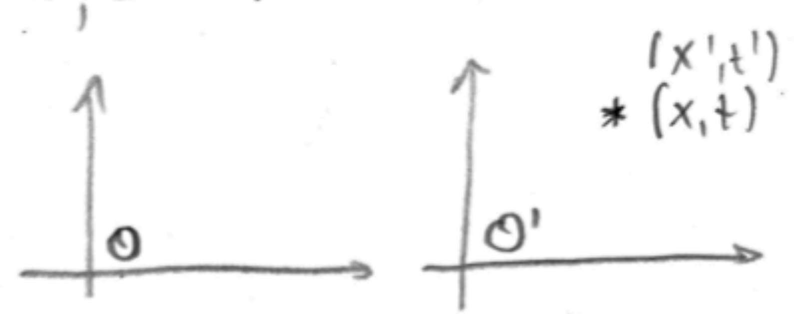
$$\Rightarrow \begin{cases} \omega' = \omega\left(1 - \frac{v}{V}\right) \\ k' = k \;\Rightarrow\; \frac{2\pi}{\lambda'} = \frac{2\pi}{\lambda} \;\Rightarrow\; \boxed{\lambda' = \lambda} \end{cases}$$ for ordinary waves.

⇒ QM waves are not ordinary waves.

⇒ 2 obs. would not agree on the value of the wavefunction Ψ.

⇒ Ψ is not directly measurable, but measurements can still be compared.

⇒ Ψ is not Galilean invariant.



$$\boxed{\Psi \neq \Psi'}$$

1) Null potential: free QM particles

Frequency of matter waves:

$p = \hbar k$

$E = \hbar\omega \Rightarrow \omega = \frac{E}{\hbar}$

Wave phase: $\phi = kx - \omega t$

phase velocity: $v_{phase} = \frac{\omega}{k} = \frac{E}{p} = \frac{\frac{1}{2}mv^2}{mv} = \frac{1}{2}v$.

$\Rightarrow \boxed{v_{phase} = \frac{1}{2}v}$ Same result!

- If the plane wave carries no real information, it is not a signal.
- Representing travelling information with plane waves is wrong,
- We need wave packets.
- Phase velocity is not meaningful physically.

1) Null potential: free QM particles

- We can use the group velocity.

$$v_{group} = \left.\frac{d\omega}{dk}\right|_{k_0} = \frac{dE}{dp} = \frac{d}{dp}\left(\frac{p^2}{2m}\right) = \frac{p}{m} = v$$

↑ value of k at which propagation occurs.

⇒ the v_{group} of a wave packet is the velocity of the particle.

Problem 2:

Wave packets

Can be constructed from the superposition of waves.

Remember:

$$\Psi_k(x,t) = A e^{i\underbrace{\left(kx - \frac{\hbar k^2}{2m} t\right)}_{\phi \equiv \text{phase of the wave}}} \quad ; \quad \omega(k) = \frac{\hbar k^2}{2m}$$

Superposition:

$$\Psi(x,t) = \sum_{n=1}^{\infty} c_n \Psi_n(x,t)$$

1) Null potential: wave packets

Wave packet:

k continuous

$$\boxed{\Psi(x,t) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty}\phi(k)\, e^{i\left(kx-\frac{\hbar k^2}{2m}t\right)}\,dk}$$

each state can have a different amplitude

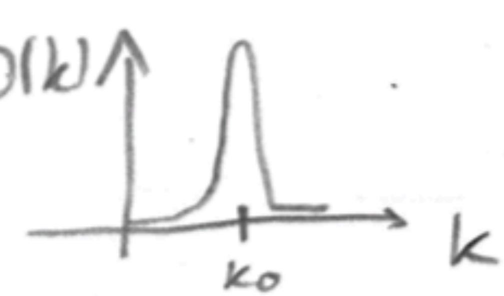
↳ wp is a superposition of sin functions modulated by ϕ

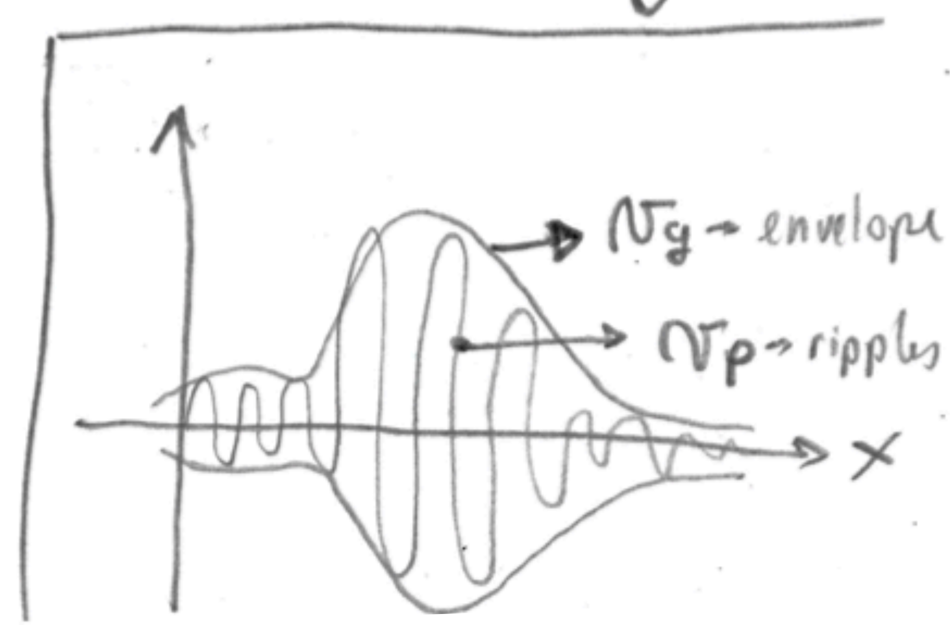
↳ ripples contained within an envelope (v_g) and

① $C_n \Rightarrow \frac{1}{\sqrt{2\pi}}\phi(k)\,dk$

② This can be normalised for an appropriate $\phi(k)$

$\phi(k)$ should peak:





③ wp. carries a range of k, E, v.

1) Null potential: wave packets

How do wave packets move?

Principle of stationary phase $(kx - \omega(k)t)$

At $k \approx k_0$ the $\int$(function x wave) can be non-zero

$\phi = kx - \omega t \rightarrow$ phase should be stationary wrt k at k_0 → constant

$$\left.\frac{d\phi}{dk}\right|_{k_0} = x - \left.\frac{d\omega}{dk}\right|_{k_0} t = 0$$

$$\Rightarrow x = \left.\frac{d\omega}{dk}\right|_{k_0} t \Rightarrow \boxed{x = v_{group}\, t}$$

The shape of the wave moves with v_{group}.

In QM, we are given: $\Psi(x,0)$, and need to find $\Psi(x,t)$

=> we need to find $\phi(k)$ to match $\Psi(x,0)$

$$\Psi(x,0) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \phi(k)\, e^{ikx}\, dk$$

; $\phi(k)$ is F. transf of $\Psi(x,0)$.

1) Null potential: Plancherel's theorem

We can use Fourier analysis, in particular Plancherel's theorem:

$$\int_{-\infty}^{+\infty} |f(x)|^2 dx = \int_{-\infty}^{+\infty} |F(k)|^2 dk$$

$$\int_{-\infty}^{+\infty} f(x)\, g^*(x)\, dx = \int_{-\infty}^{+\infty} F(k)\, G^*(k)\, dk$$

$$\downarrow$$

$$\Psi(x,0) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \phi(k)\, e^{ikx}\, dk$$

$$\Leftrightarrow \quad \boxed{\phi(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \Psi(x,0)\, e^{-ikx}\, dx}$$

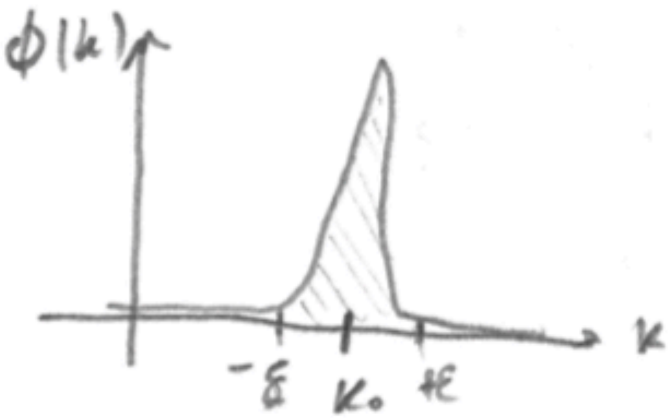
1) Null potential: Phase and Group Velocities

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \phi(k)\, e^{i(kx-\omega t)}\, dk$$

with $\omega = \frac{\hbar k^2}{2m}$, which is called the dispersion relation of the wp.

$\phi(k)$ is narrowly peaked at k_0,

$\Rightarrow$ we can taylor-expand $\omega(k)\big|_{k_0}$



$$\omega(k) = \omega(k_0) + (k-k_0)\frac{d\omega}{dk}\bigg|_{k_0} + \cancel{\mathcal{O}((k-k_0)^2)} \rightsquigarrow \text{distorsion of wave pattern.}$$

$$\Rightarrow \Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \phi(k)\, e^{ikx}\, e^{-i\omega_0 t}\, e^{-ik\omega_0' t}\, e^{+ik_0\omega_0' t}\, dk$$

1) Null potential: Phase and Group Velocities

①

$$\Rightarrow \Psi(x,t) = \frac{1}{\sqrt{2\pi}}\, e^{-i\omega_0 t}\, e^{+ik_0\omega_0' t} \underbrace{\int_{-\infty}^{+\infty} \phi(k)\, e^{ik(x-\omega_0' t)}\, dk}$$

pure phase

Similar to:

$$\Psi(x,0) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \phi(k)\, e^{ikx}\, dk$$

$$\Rightarrow \boxed{|\Psi(x,t)| = |\Psi(x-\omega_0' t, 0)|}$$

② $s \equiv k - k_0$

$$\Rightarrow \Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \phi(k_0+s)\, e^{i(s+k_0)x}\, e^{-i(\omega_0 t + (k_0+s)\omega_0' t - ik_0\omega_0' t)}\, ds$$

$$\Rightarrow \Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \phi(k_0+s)\, e^{i[(s+k_0)x - (\omega_0 + \omega_0' s t)}\, ds$$

1) Null potential: Phase and Group Velocities

Then: $$\Psi(x,t) = \underbrace{\frac{1}{\sqrt{2\pi}} e^{i(k_0 x - \omega_0 t)}}_{\text{sinusoidal wave "ripples"}} \underbrace{\int_{-\infty}^{\infty} \phi(k_0+s)\, e^{is(x-\omega_0' t)}\, ds}_{\text{envelope}}$$

$$\frac{\omega_0}{k_0} \qquad \omega_0'$$

<u>Phase velocity:</u>

$$v_{phase} = \frac{\omega}{k}\bigg|_{k_0}$$

<u>Group velocity</u>

$$v_{group} = \frac{d\omega}{dk}\bigg|_{k_0}$$

1) Null potential: Phase and Group Velocities

In our case:

$$\omega(k) = \frac{\hbar k^2}{2m} \Rightarrow \frac{d\omega}{dk} = \frac{\hbar k}{m}$$

$$\Rightarrow \boxed{v_{group} = v_{classical} = 2\, v_{phase}}$$

$$v_{group} = \frac{dE}{dt} = \frac{d}{dt}\left(\frac{p^2}{2m}\right) = \frac{p}{m} = v_{classical} \checkmark$$

Notes:

1) Ψ cannot be $\mathbb{R}$.

2) Sch. eq is not a wave equation of the classical type:

$$\frac{\partial^2 y}{\partial t^2} = v^2 \frac{\partial^2 y}{\partial x^2} \Rightarrow \boxed{y = f(x-vt) + g(x+vt)} \in \mathbb{R}$$

Example: $\boxed{y(x,t) = A\sin(x-vt) + B\sin(x+vt)}$

Canonical commutation relation

<u>The $\hat{x}$ operator</u>

$$\text{Sch. eq:}\ \underbrace{i\hbar\frac{\partial}{\partial t}}_{\text{operator}}\psi = \overbrace{\left(\underbrace{-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}}_{\text{operator}} + \underbrace{V}_{\text{operator} \to V(x,t)}\right)}^{\hat{H} \equiv \text{Hamiltonian}}\psi$$

We can introduce an operator $\hat{x}$, which is a multiplication operator. When applied on a function of x, it multiplies it by x.

$$\Rightarrow \hat{x}\cdot F(x) = x\cdot F(x)$$

In QM, we have a few operators: $\hat{x}$, $\hat{p}$, $\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{x},t)$

Operators are matrices, so the order in which we multiply them makes a difference. Does the order matter when multiplying $\hat{x}$ and $\hat{p}$? (Heisenberg)

$(\hat{x}\hat{p} - \hat{p}\hat{x})\psi = 0$?? $\Rightarrow \hat{x}\hat{p}\psi - \hat{p}\hat{x}\psi = ?$; $\psi(x,t)$

Canonical commutation relation

$$\hat{x}(\hat{p}\psi) - \hat{p}(\hat{x}\psi) = \hat{x}\left(\frac{\hbar}{i}\frac{\partial}{\partial x}\psi\right) - \hat{p}(x\psi)$$

$$= \frac{\hbar}{i} x \frac{\partial \psi}{\partial x} - \frac{\hbar}{i}\frac{\partial}{\partial x}(x\psi)$$

$$= \frac{\hbar}{i} x \frac{\partial \psi}{\partial x} - \frac{\hbar}{i} x \frac{\partial \psi}{\partial x} - \frac{\hbar}{i}\psi = -\frac{\hbar}{i}\psi = i\hbar\psi$$

$$\Rightarrow (\hat{x}\hat{p} - \hat{p}\hat{x})\psi = i\hbar\psi$$

$$\Rightarrow \boxed{(\hat{x}\hat{p} - \hat{p}\hat{x}) = i\hbar}$$ equality between operators.

This is called a commutator: $[\hat{x}, \hat{p}] = \hat{x}\hat{p} - \hat{p}\hat{x}$

$$\boxed{[\hat{x}, \hat{p}] = i\hbar}$$

Canonical commutation relation.

Operators : wavefunctions, eigenstates

Matrices : vectors , eigenvectors

2) Particles in an infinite square well potential

Schrödinger equation:

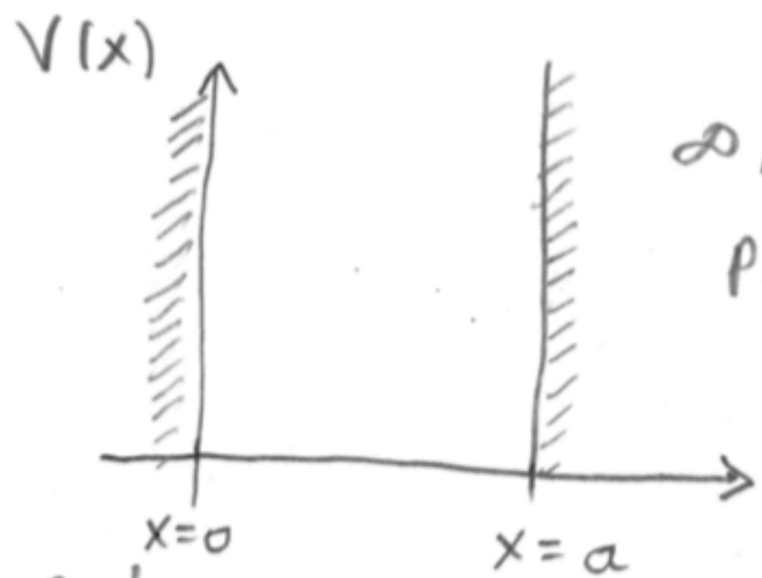
$$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 \Psi}{\partial x^2} + V\Psi \xrightarrow[V=V(x)]{\Psi=\psi(x)\varphi(t)} \begin{cases} \frac{d\varphi}{dt} = -\frac{iE}{\hbar}\varphi \rightarrow \varphi = e^{-\frac{iE}{\hbar}t} \\ -\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V\psi = E\psi \rightarrow \psi \end{cases}$$

Solution:

$$\Rightarrow \Psi(x,t) = \sum_{n=1}^{\infty} c_n \underbrace{\psi_n(x)\, e^{-i\frac{E}{\hbar}t}}_{\text{stationary states}}$$

we analyze the case where:

$$V(x) = \begin{cases} 0, & 0 \le x \le a \\ \infty, & \text{otherwise} \end{cases}$$

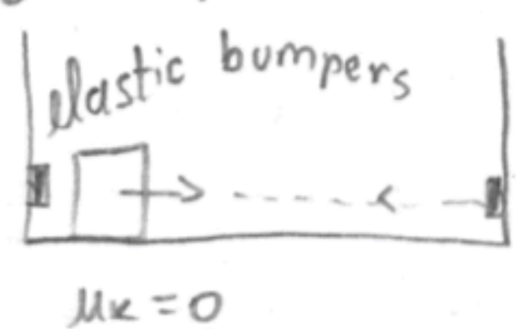


∞ □ well potential

1) A particle in V(x) is free, except at the ends.

2) At the ends, an ∞ force prevents it from escaping.

3) Analogy in CM:



2) Particles in an infinite square well potential

4) This $V(x)$ is artificial, but serves as a good test case

5) Outside the well: $\psi(x) = 0$ (the prob. of finding the particle is 0)

6) Inside the well: $V(x) = 0$, so the time independent Sch. eq reads:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx_2} = E\psi \Rightarrow \frac{d^2\psi}{dx^2} = -k^2\psi \quad \text{where } k = \sqrt{\frac{2mE}{\hbar^2}} = \frac{\sqrt{2mE}}{\hbar}$$

This is the classical simple harmonic oscillator eq. with general sln:

$$\psi(x) = A\sin(kx) + B\cos(kx)$$

where A & B are fixed by the boundary conditions

7) What are the appropriate B.Cs for $\psi(x)$?

$$\left.\begin{matrix} \psi(x) \\ \frac{d\psi}{dx} \end{matrix}\right\}$$ are ordinarily continuous, but when $V \to \infty$, only $\psi(x)$ is continuous.

2) Particles in an infinite square well potential

8) A QM particle in an ∞ $\square$ well cannot have any E, it has to be one of the allowed values.

9) The quantisation of E emerges from the B.Cs

10) How do we find A?

$$1 = \int_{-\infty}^{+\infty} |\psi|^2 \, dx = \int_0^a |A \sin(kx)|^2 dx = \int_0^a |A|^2 \sin^2(kx)\, dx = |A|^2 \int_0^a \sin^2(kx)\, dx$$

Remember: $\cos(2x) = \sin^2 x - \cos^2 x$

$$\cos(2x) = \sin^2 x - 1 + \sin^2 x = 2\sin^2 x - 1$$

$$\Rightarrow \sin^2 x = \frac{\cos(2x) + 1}{2}$$

$$\int_0^a \sin^2(kx)\, dx = \int_0^a \frac{\cos(2x)+1}{2} dx = \left(-\frac{1}{4}\sin(2x) + \frac{x}{2}\right)\Big|_0^a =$$

2) Particles in an infinite square well potential

$$= -\frac{1}{4}\underbrace{\sin(2a)}_{0 \text{ because } \sin(ka)=0} + \frac{a}{2} = \frac{a}{2} \Rightarrow |A|^2\frac{a}{2} = 1 \Rightarrow \boxed{|A|^2 = \frac{2}{a}}$$

$\Rightarrow A = \sqrt{\frac{2}{a}}$, phase of A has no physical significance

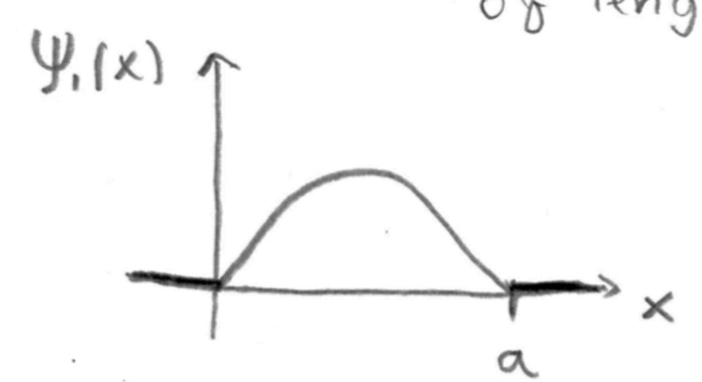
11) Inside the well, the sln reads:

$$\boxed{\psi_n(x) = \sqrt{\frac{2}{a}}\,\sin\left(\frac{n\pi}{a}x\right)}$$

We have an ∞ set of slns, one for each "n" (standing waves on string) of length a)

n = 1: Ground state.

$$\psi_1(x) = \sqrt{\frac{2}{a}}\,\sin\left(\frac{\pi}{a}x\right)$$

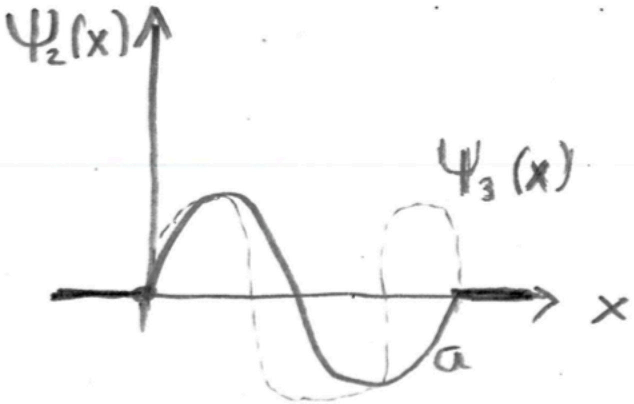


$E_1 = \frac{\pi^2\hbar^2}{2ma^2}$ (lowest energy)

2) Particles in an infinite square well potential

Excited states:

n = 2:



$$\psi_2(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{2\pi}{a}x\right)$$

$$E_2 = \frac{2^2 \pi^2 \hbar^2}{2ma^2}$$

Properties of the solutions:

i) With respect to the centre of the well, they are alternately even or odd.

ii) Zero crossings are called nodes, as $E\uparrow$, succesives states have one more node: $\psi_1 \to 0$, $\psi_2 \to 1$, $\psi_3 \to 2$, etc

iii) They are orthonormal:

$$\boxed{\int \psi_m^*(x)\, \psi_n(x)\, dx = \delta_{mn}}$$

where: $\delta_{mn} = \begin{cases} 0 & \text{for } m \neq n \\ 1 & \text{for } m = n \end{cases}$ is the Kronecker delta.

2) Particles in an infinite square well potential

iv) They are complete:

$$f(x) = \sum_{n=1}^{\infty} c_n \psi_n(x) = \sqrt{\frac{2}{a}} \sum_{n=1}^{\infty} c_n \sin\left(\frac{n\pi}{a} x\right)$$

This is the Fourier series for $f(x)$.

Dirichlet's theorem: any function can be expanded in this way.

* We can use "Fourier's trick" to evaluate c_n; using ψ_n orthonormality.

(only $m=n$ survives)

$$\int \psi_m(x)^* f(x)\, dx = \sum_{n=1}^{\infty} c_n \int \psi_m^* \psi_n\, dx = \sum_{n=1}^{\infty} c_n \delta_{mn} = c_m$$

$$\Rightarrow \boxed{c_n = \int \psi_n(x)^* f(x)\, dx}$$

In general:

① holds when $V(x)$ is symmetric.

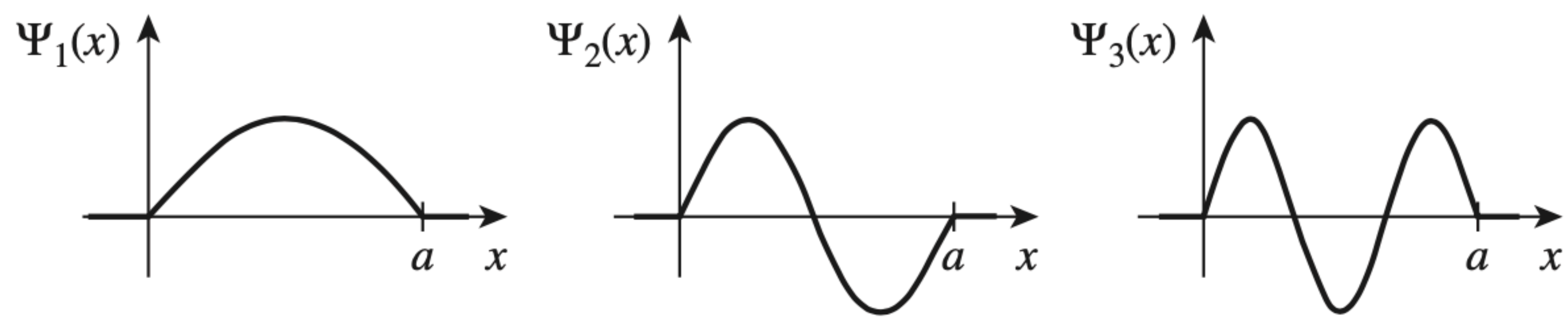
② is universal for all $V(x)$.

③ is general.

④ also holds.

2) Infinite square well: stationary states

$$\Psi_n(x,t) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a}x\right) e^{-i\left(\frac{n^2\pi^2\hbar}{2ma^2}\right)t} \qquad E_n = \hbar\omega = \frac{n^2\pi^2\hbar^2}{2ma^2}$$



General solution:

$$\Psi(x,t) = \sum_{n=1}^{\infty} c_n \Psi_n(x,t)$$

Initial conditions: given

$$\Psi(x,0) = \sum_{n=1}^{\infty} c_n \Psi_n(x,0)$$, we can use Fourier's trick:

$$\Rightarrow \boxed{c_n = \sqrt{\frac{2}{a}} \int_0^a \sin\left(\frac{n\pi}{a}x\right) \Psi(x,0)\, dx}$$

to compute the expansion coefficients.

* $\sum_{n=1}^{\infty} |c_n|^2 = 1$

* $\langle H \rangle = \sum_{n=1}^{\infty} |c_n|^2 E_n$

Bound states and stationary states

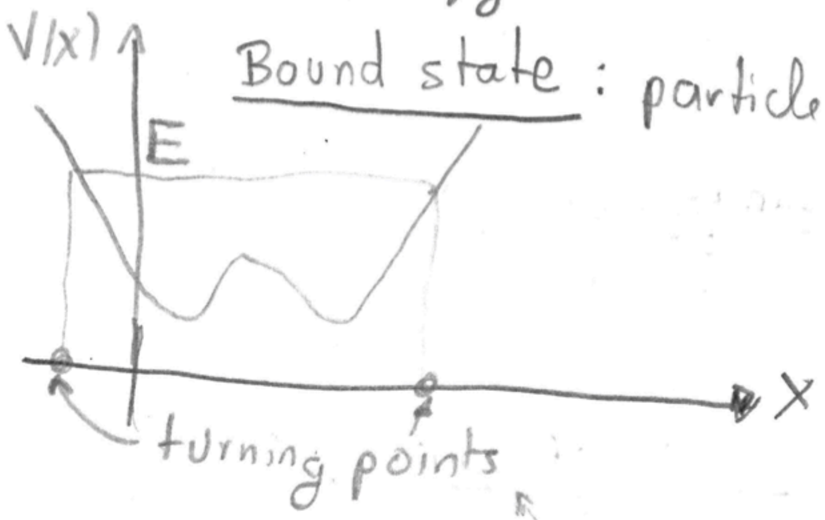
Sln to time independent Sch. eq:

① Non-normalisable: free particle → labeled by continuous var. k $\int dk$

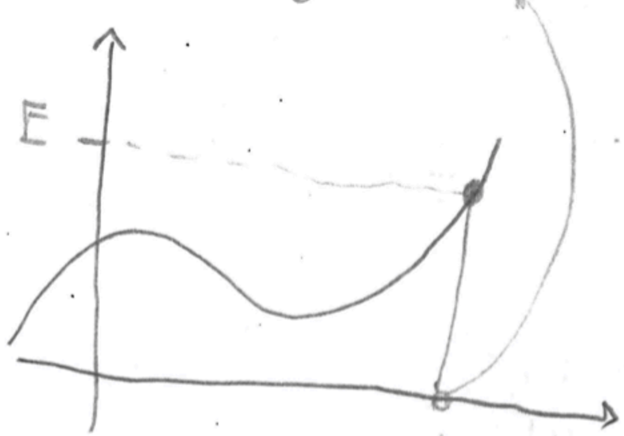
② Normalisable: ∞ □ well → labeled by discrete var. n. $\sum_n$

What is the physical distinction?

Classical analogy.



Bound state: particle cannot escape



Scattering state: particle comes from ∞ reacts to $V(x)$ and goes back.

Bound states and stationary states

In QM:

$$V(x) \begin{cases} \text{only bound states} \rightarrow \text{normalisable} \\ \text{only scattering states} \rightarrow \text{free particle} \\ \text{both depending on } E \end{cases}$$

* Tunneling allows particle to leak thru any finite potential barrier, so the kind of states only depends on $V(\pm\infty)$

Bound state: $E < V(-\infty) \wedge E < V(+\infty)$, also $E<0$

Scattering state: $E > V(-\infty)$ or $E > V(+\infty)$, also $E>0$

Examples:

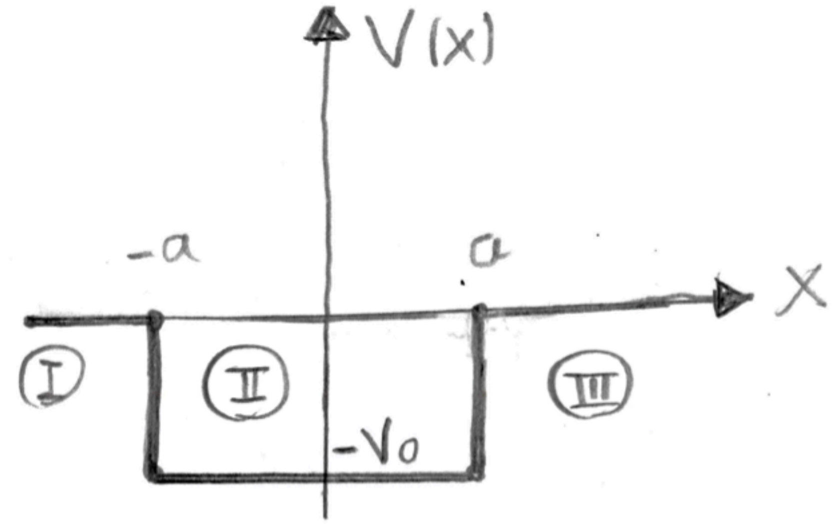
1) $\infty \square$ well: $V(x) \rightarrow \pm\infty$ when $x \rightarrow \pm\infty \Rightarrow$ only bound states

2) free particle: $V(x) = 0 \Rightarrow$ only scattering states

3) Finite square well potential

The finite square well potential:

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



where $V_0 > 0$.

This potential admits both kind of s/ns.

Bound states when $E < 0$

Scattering states when $E > 0$

a) Bound states:

$x < -a$: $V(x) = 0 \Rightarrow -\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi \Rightarrow \frac{d^2\psi}{dx^2} = \overbrace{-\frac{2mE}{\hbar^2}}^{k^2}\psi$

I

$\Rightarrow \boxed{\frac{d^2\psi}{dx^2} = \kappa^2\psi}$ ODE where $\kappa = \frac{\sqrt{-2mE}}{\hbar}$

s/ns $\Rightarrow \psi(x) = Ae^{-\kappa x} + Be^{\kappa x}$

$x \to -\infty \Rightarrow e^{-\kappa x} \to +\infty \Rightarrow \boxed{\psi(x) = Be^{\kappa x} \text{ for } x < -a}$

3) Finite square well potential: bound states

$-a<x<a$: $V(x)=-V_0 \Rightarrow -\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}-V_0\psi=E\psi \Rightarrow \frac{d^2\psi}{dx^2}=-\overbrace{\frac{2m(E+V_0)}{\hbar^2}}^{\ell^2}\psi$

II

$$\Rightarrow \boxed{\frac{d^2\psi}{dx^2}=-\ell^2\psi}$$

ODE

where $\ell=\frac{\sqrt{2m(E+V_0)}}{\hbar}$; $E>-V_0$

slns $\Rightarrow$ $\boxed{\psi(x)=C\sin(\ell x)+D\cos(\ell x) \quad \text{for} \quad -a<x<a.}$

$x>a$: $V(x)=0 \Rightarrow -\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}=E\psi$

III

slns $\Rightarrow \psi(x)=Fe^{-\kappa x}+Ge^{\kappa x}$

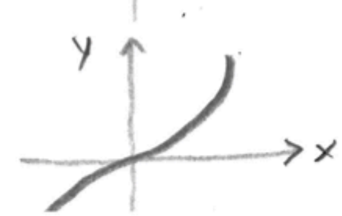
$x\to+\infty \Rightarrow e^{\kappa x}\to+\infty \Rightarrow$ $\boxed{\psi(x)=Fe^{-\kappa x} \quad \text{for} \quad x>+a}$

Remember:

Even functions: $f(-x)=f(x) \rightarrow$

cos (x)

Odd functions: $f(-x)=-f(x)$



sin (x)

3) Finite square well potential: even bound states

* $\psi(x)$ is an even function

Boundary conditions:

ψ ^ $d\psi/dx$ are continuous at, $x = \pm a$

Even solutions: $\psi(-x) = \psi(x)$

$$\psi(x) = \begin{cases} F e^{-\kappa x} & ; \; x > a \\ D\cos(\ell x) & ; \; 0 < x < a \\ \psi(-x) & ; \; x < 0 \end{cases}$$

At $x = a$: $\begin{cases} F e^{-\kappa a} = D\cos(\ell a) & \text{(c1)} \\ -\kappa F e^{-\kappa a} = -\ell D \sin(\ell a) & \text{(c2)} \end{cases}$

(c2) ÷ (c1) $\quad -\kappa = -\ell \tan(\ell a)$

$$\Rightarrow \boxed{\kappa = \ell \tan(\ell a)} \quad ①$$

3) Finite square well potential: even bound states

Remember:

$$\kappa = \kappa(E) = \frac{\sqrt{-2mE}}{\hbar}$$

$$l = l(E) = \frac{\sqrt{2m(E+V_0)}}{\hbar}$$

$$\Rightarrow \kappa^2 + l^2 = -\frac{2mE}{\hbar^2} + \frac{2m(E+V_0)}{\hbar^2}$$

$$\Rightarrow \boxed{\kappa^2 + l^2 = \frac{2mV_0}{\hbar^2}} \quad ②$$

D in ②

$$l^2\left(1+\tan^2(la)\right) = \frac{2mV_0}{\hbar^2}.$$

Variable change: $z = la \Rightarrow z^2\left(1+\tan^2(z)\right) = \underbrace{\frac{a^2 2mV_0}{\hbar^2}}_{z_0^2}$

$$\Rightarrow z^2\left(1+\tan^2(z)\right) = z_0^2$$

$$\Rightarrow \boxed{\tan(z) = \sqrt{\left(\frac{z_0}{z}\right)^2 - 1}} \quad \text{trascendental eq.}$$

$z_0 = 4$:

$$\frac{\tan(z)}{\sqrt{\frac{16}{z^2} - 1}} = 1 \; ; \; z = ?$$

→ see python notebook

3) Finite square well potential: even bound states

Limiting cases:

z_0 measures the size of the well because it depends on V_0.

1) Wide, deep well: $z_0 \gg 0$

$$Z_n = \frac{n\pi}{2} \quad \text{for} \quad n \equiv \text{odd number}$$

$$Z_n = \frac{n\pi}{2} = la = \frac{\sqrt{2m(E_n+V_0)}}{\hbar}\,a$$

$$\Rightarrow \frac{n^2\pi^2\hbar^2}{2^2a^2} = 2m(E_n+V_0) \Rightarrow \boxed{E_n+V_0 \approx \frac{n^2\pi^2\hbar^2}{2m(2^2a^2)}} \quad n = 1, 3, 5, \ldots\ldots$$

odd

Energy above the bottom of the well

half of the $\infty\,\square$ well energies for a well of width $2a$

$\Rightarrow$ finite square well $\rightarrow$ infinite square well for $V_0 \rightarrow \infty$

In gral, for any finite $V_0 \Rightarrow$ finite # of bound states

2) Shallow, narrow well: z_0 small $\rightarrow z_0 < \frac{\pi}{2} \Rightarrow 1$ bound state

3) Finite square well potential: scattering states

Limiting cases:

b) Scattering states: $E > 0 \rightarrow$ Asymmetric

$x < -a$: $V(x) = 0 \Rightarrow -\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi \Rightarrow \frac{d^2\psi}{dx^2} = -\overbrace{\frac{2mE}{\hbar^2}}^{k^2}\psi$

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

incident amplitude

slns $\Rightarrow$ $\boxed{\psi(x) = Ae^{ikx} + Be^{-ikx} \text{ for } x < -a.}$ $\rightarrow$ travelling waves come from one side only.

reflected amplitude

$-a < x < a$: $V(x) = -V_0$

slns $\Rightarrow$ $\boxed{\psi(x) = C\sin(lx) + D\cos(lx) \text{ for } -a < x < a}$

where: $l = \frac{\sqrt{2m(E+V_0)}}{\hbar}$

$x > +a$: $\boxed{\psi(x) = Fe^{ikx}}$ (no incoming wave)

transmitted amplitude

3) Finite square well potential: scattering states

Boundary conditions: ψ and $d\psi/dx$ are continuous.

At x=-a:

$$\begin{cases} \psi: \; Ae^{-ika} + Be^{+ika} = -C\sin(la) + D\cos(la) & (1) \\ \dfrac{d\psi}{dx}: \; ik\left[Ae^{-ika} - Be^{+ika}\right] = l\left[C\cos(la) + D\sin(la)\right] & (2) \end{cases}$$

At x=+a:

$$\begin{cases} \psi: \; C\sin(la) + D\cos(la) = Fe^{ika} & (3) \\ \dfrac{d\psi}{dx}: \; l\left[C\cos(la) - D\sin(la)\right] = ikFe^{ika} & (4) \end{cases}$$

From (3):

$$C = \frac{Fe^{ika} - D\cos(la)}{\sin(la)}$$

From (4):

$$C = \frac{\frac{ik}{l}Fe^{ika} + D\sin(la)}{\cos(la)}$$

3) Finite square well potential: scattering states

$$\Rightarrow \quad F\cos(la)\,e^{ika} - D\cos^2(la) = \frac{ikF}{l}\sin(la)\,e^{ika} + D\sin^2(la)$$

$$\Rightarrow \quad \boxed{D = \left[\cos(la) - \frac{ik}{l}\sin(la)\right]e^{ika}F}$$

$$\Rightarrow \quad \boxed{C = \left[\sin(la) + \frac{ik}{l}\cos(la)\right]e^{ika}F}$$

$$\Rightarrow \quad \boxed{B = i\,\frac{\sin(2la)}{2kl}\,(l^2-k^2)\,F}$$

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

3) Finite square well: transmission coefficient

Transmission coefficient: $T = \dfrac{|F|^2}{|A|^2}$

$$\Rightarrow T^{-1} = 1 + \frac{V_0^2}{4E(E+V_0)} \sin^2\left(\frac{2a}{\hbar}\sqrt{2m(E+V_0)}\right).$$

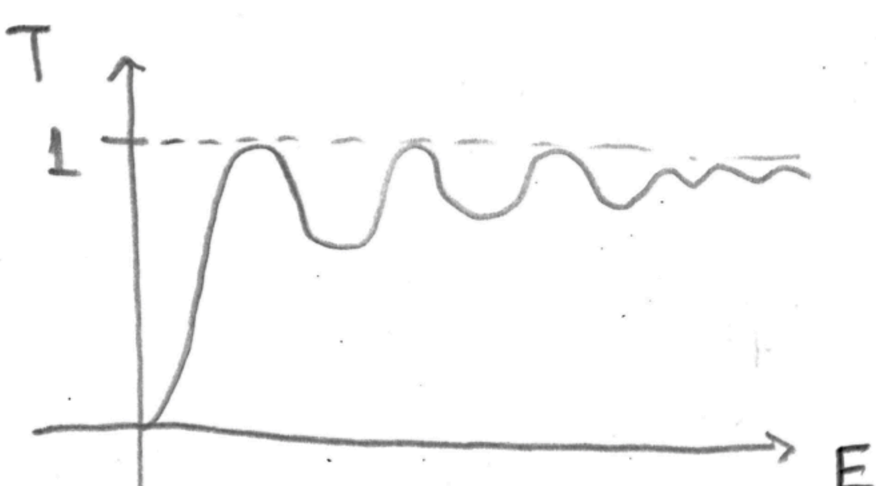
For $T=1 \Rightarrow$ well becomes transparent when $\sin^2(-)=0$

$$\Rightarrow \frac{2a}{\hbar}\sqrt{2m(E_n+V_0)} = n\pi \quad ; \quad n=1,2,3,4,\ldots$$

Perfect transmission:

$$\Rightarrow \boxed{E_n + V_0 = \frac{n^2\pi^2\hbar^2}{2m(2a)^2}}$$

which are precisely the allowed E_n for the infinite $\square$ well



4) Quantum Harmonic Oscillator

In Classical Mechanics:

$$F = -kx = m\frac{d^2x}{dt^2} \Rightarrow x(t) = A\sin(\omega t) + B\cos(\omega t) \; ; \quad \omega = \sqrt{\frac{k}{m}}$$

Hooke's law ↑ for a potential $V(x) = \frac{1}{2}kx^2$

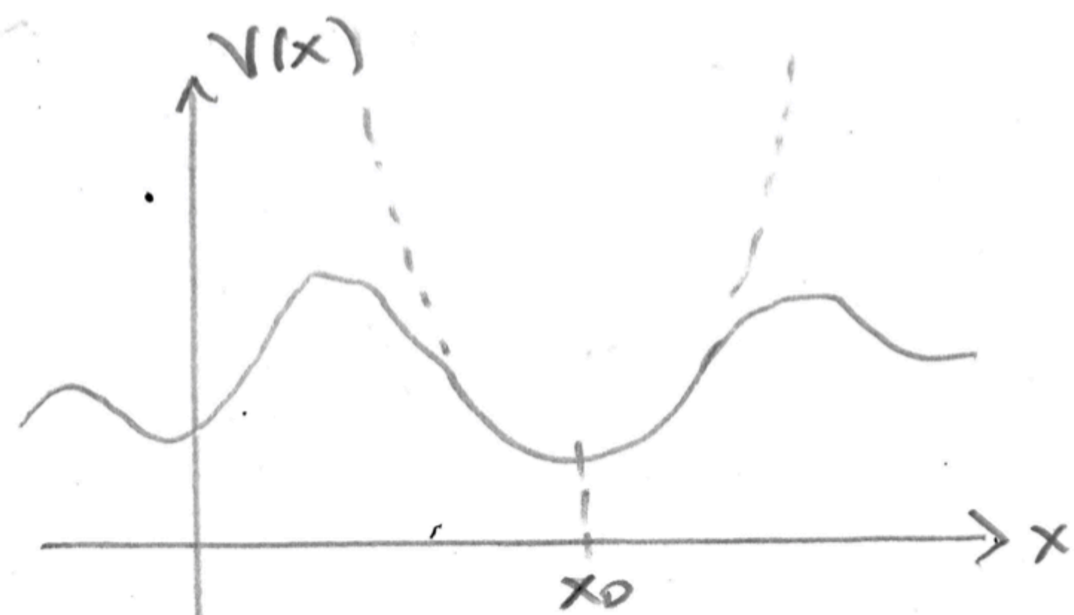
↑ force constant

- Any potential is approx. parabolic around a local minimum.
- Taylor expansion of $V(x)$ about x_0:

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

- We can subtract a constant: $(V(x_0))$
- $V'(x_0) = 0$ (minimum)
- $(x-x_0)$ is small

$$\Rightarrow \boxed{V(x) \approx \frac{1}{2}V''(x_0)(x-x_0)^2}$$



4) Quantum Harmonic Oscillator

For a constant: $K = V''(x_0) \geq 0$

Any oscillatory motion is aprox. simple harmonic for small amplitudes.

In Quantum mechanics:

$$\boxed{V(x) = \frac{1}{2} k x^2 = \frac{1}{2} m\omega^2 x^2}$$

Time independent Schrödinger eq:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + \frac{1}{2} m\omega^2 x^2 \psi = E\psi$$

Method 1: Algebraic solution using ladder operators

ewrite as operators: $\hat{p} = -i\hbar \frac{d}{dx} \Rightarrow \hat{p}^2 = -\hbar^2 \frac{d^2}{dx^2}$; $\hat{x}$

$$\Rightarrow \underbrace{\left(\frac{\hat{p}^2}{2m} + \frac{1}{2} m\omega^2 \hat{x}^2\right)}_{\hat{H} \equiv \text{Hamiltonian}} \psi = E\psi \Rightarrow \frac{1}{2m}\left[\hat{p}^2 + (m\omega\hat{x})^2\right]\psi = E\psi$$

4) Quantum Harmonic Oscillator: ladder operators

Analogous to: $u^2 + v^2 = (iu+v)(-iu+v)$

So we define ladder operators:

$$\boxed{\hat{a}_{\pm} = \frac{1}{\sqrt{2\hbar m\omega}}\left(\mp i\hat{p} + m\omega x\right)} = \frac{1}{\sqrt{2\hbar m\omega}}\left(\mp \hbar\frac{d}{dx} + m\omega x\right)$$

And we calculate the product:

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

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

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

4) Quantum Harmonic Oscillator: ground state

Lowest state of energy:

$\hat{a}_- \psi_0 = 0$, let us find ψ_0.

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

$$\Rightarrow \boxed{\frac{d\psi_0}{dx} = -\frac{m\omega}{\hbar}x\psi_0} \quad \text{ODE}$$

$$\frac{d\psi_0}{\psi_0} = -\frac{m\omega x}{\hbar}dx \Rightarrow \ln(\psi_0) = -\frac{m\omega x^2}{2\hbar} + C_1$$

$$\Rightarrow \boxed{\psi_0(x) = A\, e^{-\frac{m\omega x^2}{2\hbar}}} \quad (*)$$

Let us normalise it:

$$\int_{-\infty}^{+\infty} |\psi_0|^2 dx = 1 \Rightarrow \int_{-\infty}^{+\infty} |A|^2 e^{-\frac{m\omega x^2}{\hbar}} dx = I_1 \quad \text{Remember: } \int_{-\infty}^{+\infty} e^{-\lambda y^2} = \sqrt{\frac{\pi}{\lambda}}$$

$$\Rightarrow I_1 = |A|^2 \cdot \sqrt{\frac{\pi\hbar}{m\omega}} = 1 \Rightarrow |A|^2 = \sqrt{\frac{m\omega}{\pi\hbar}} \Rightarrow A = \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}}$$

4) Quantum Harmonic Oscillator: ground state

Therefore:

$$\boxed{\psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} e^{-\frac{m\omega}{2\hbar}x^2}}$$ → State of lowest energy, E_0

What is E_0? → Use Sch. eq:

$$\hbar\omega\left(\hat{a}_+\hat{a}_- + \frac{1}{2}\right)\psi_0 = E_0\psi_0$$

$$\hbar\omega\,\hat{a}_+\underbrace{\hat{a}_-\psi}_{=0} + \frac{1}{2}\hbar\omega\psi_0 = E_0\psi_0$$

$$\Rightarrow \boxed{E_0 = \frac{1}{2}\hbar\omega}$$ Ground state energy of the quantum harmonic oscillator.

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

$$\Rightarrow \hat{a}_-\hat{a}_+ = \frac{\hat{p}^2}{2m}\cdot\frac{1}{\hbar\omega} + \frac{1}{2\hbar}m\omega\hat{x}^2 + \frac{1}{2}$$

$$\Rightarrow \hat{a}_-\hat{a}_+ = \frac{1}{\hbar\omega}\underbrace{\left[\frac{\hat{p}^2}{2m} + m\omega^2\hat{x}^2\right]}_{\hat{H}} + \frac{1}{2} \Rightarrow \hat{a}_-\hat{a}_+ = \frac{1}{\hbar\omega}\hat{H} + \frac{1}{2}$$

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

4) Quantum Harmonic Oscillator: ground state

Similarly:

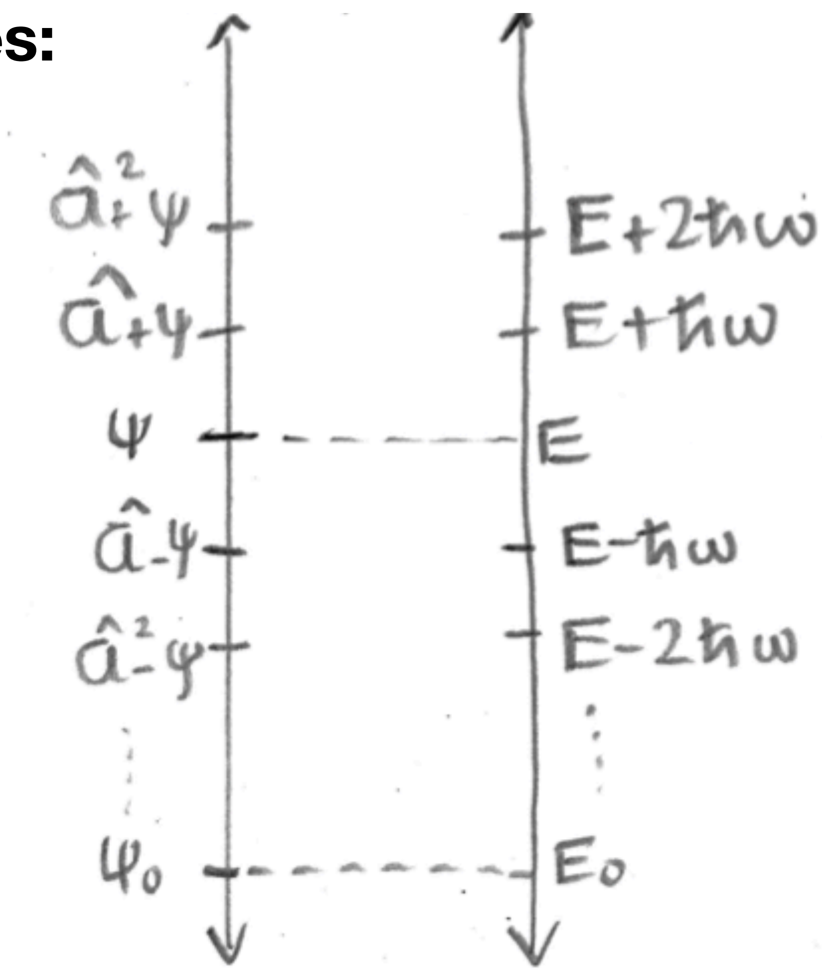
$$a_+ a_- = \frac{1}{\hbar\omega}\hat{H} - \frac{1}{2} \quad \Rightarrow \quad \overset{\text{commutator}}{[\hat{a}_-, \hat{a}_+]} = 1$$

$$\Rightarrow \boxed{\hat{H} = \hbar\omega\left[\hat{a}^+\hat{a}^- + \frac{1}{2}\right]}$$

going back to Sch. eq:

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

Ladder of states:



Therefore:

If $\hat{H}\psi = E\psi$

$$\Rightarrow \begin{cases} \hat{H}(\hat{a}_+\psi) = (E+\hbar\omega)(\hat{a}_+\psi) \; ; \; \hat{a}_+ \equiv \text{raising op.} \\ \hat{H}(\hat{a}_-\psi) = (E-\hbar\omega)(\hat{a}_-\psi) \; ; \; \hat{a}_- \equiv \text{lowering op.} \end{cases}$$

4) Quantum Harmonic Oscillator: excited states

$$\psi_n(x) = A_n \left(a_+\right)^n \psi_0(x) \,, \quad \text{with} \quad E_n = \left(n + \frac{1}{2}\right)\hbar\omega$$

normalisation constant

allowed energies

stationary states

Hermitian Adjoint / Conjugate

$\langle Ax, y\rangle = \langle x, A^* y\rangle$, $x, y \in H$ ($\mathbb{C}$ Hilbert space)

In our case: $\hat{a}_\mp$ is the Hermitian conjugate of $\hat{a}_\pm$.

$$\int_{-\infty}^{+\infty} f^* (\hat{a}_\pm g)\, dx = \int_{-\infty}^{+\infty} (\hat{a}_\mp f)^* g \, dx$$

Proof:

$$\int_{-\infty}^{+\infty} f^* (\hat{a}_\pm g)\, dx = \frac{1}{\sqrt{2\hbar m\omega}} \int_{-\infty}^{+\infty} f^* \left(\mp \hbar \frac{d}{dx} + m\omega \hat{x}\right) g \, dx = (*)$$

$\int u\, dv = uv - \int v\, du$ (Integration by parts)

4) Quantum Harmonic Oscillator: excited states

$$(*) = \frac{1}{\sqrt{2\hbar m\omega}}\left[\int_{-\infty}^{+\infty} \overset{\nearrow u}{f^*}\Big(\mp\hbar \overbrace{\frac{d}{dx}\Big) g\, dx}^{dv} + \int_{-\infty}^{+\infty} f^*(m\omega\hat{x})\, g\, dx\right]$$

$$= \frac{1}{\sqrt{2\hbar m\omega}}\left[\left[\mp\hbar\, \cancel{\left[f^* g\right]_{-\infty}^{+\infty}} - \int_{-\infty}^{+\infty} \mp\hbar \left(\frac{df}{dx}\right)^* g\, dx\right] + \int f^*(m\omega\hat{x})\, g\, dx\right]$$

$$= \frac{1}{\sqrt{2\hbar m\omega}} \int_{-\infty}^{+\infty} \left(\pm\hbar\frac{d}{dx} + m\omega\hat{x}\right) f^* g\, dx = \int (\hat{a}_{\mp} f)^* g\, dx$$

$$f = \hat{a}_{\pm}\psi_n \quad , \quad g = \psi_n$$

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

Remember:

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

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

4) Quantum Harmonic Oscillator: excited states

$$\Rightarrow \hat{a}_+\hat{a}_- = n \quad \Rightarrow \quad \boxed{\hat{a}_+\hat{a}_-\psi_n = n\psi_n}$$

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

Normalisation:

$$\hat{a}_\pm \psi_n \propto \psi_{n\pm 1} \Rightarrow \begin{cases} \hat{a}_+\psi_n = c_n\psi_{n+1} \\ \hat{a}_-\psi_n = d_n\psi_{n-1} \end{cases}$$

What are c_n & d_n?

$$\left.\begin{aligned} \int_{-\infty}^{+\infty} (\hat{a}_+\psi_n)^*(\hat{a}_+\psi_n)\,dx &= |c_n|^2 \int |\psi_{n+1}|^2 dx \\ = \int_{-\infty}^{+\infty} \hat{a}_-\hat{a}_+|\psi_n|^2 dx &= (n+1)\int |\psi_n|^2 dx \end{aligned}\right\} |c_n|^2 = (n+1)$$

$$\left.\begin{aligned} \int_{-\infty}^{+\infty} (\hat{a}_-\psi_n)^*(a_-\psi_n)\,dx &= |d_n|^2 \int |\psi_{n-1}|^2 dx \\ = \int_{-\infty}^{+\infty} \hat{a}_+\hat{a}_-|\psi_n|^2 dx &= n\int |\psi_n|^2 dx \end{aligned}\right\} |d_n|^2 = n$$

4) Quantum Harmonic Oscillator: excited states

Therefore:

$$\boxed{\begin{aligned} \hat{a}_+ \psi_n &= \sqrt{n+1}\, \psi_{n+1} \\ \hat{a}_- \psi_n &= \sqrt{n}\, \psi_{n-1} \end{aligned}}$$

For $n=0$: $\psi_1 = \hat{a}_+ \psi_0$

$n=1$: $\psi_2 = \frac{1}{\sqrt{2}} \hat{a}_+ \psi_1 = \frac{1}{\sqrt{2}} \hat{a}_+^2 \psi_0$

$n=2$: $\psi_3 = \frac{1}{\sqrt{3}} \hat{a}_+ \psi_2 = \frac{1}{\sqrt{3}\sqrt{2}} \hat{a}_+^3 \psi_0$

$n=3$: $\psi_4 = \frac{1}{\sqrt{4}} \hat{a}_+ \psi_3 = \frac{1}{\sqrt{4}\sqrt{3}\sqrt{2}} \hat{a}_+^4 \psi_0$

$$\Rightarrow \boxed{\psi_n = \frac{1}{\sqrt{n!}} (\hat{a}_+)^n \psi_0}$$

Compare: $\psi_n(x) = A_n (\hat{a}_+)^n \psi_0 \Rightarrow \boxed{A_n = \frac{1}{\sqrt{n!}}}$ Normalisation factor

4) Quantum Harmonic Oscillator: excited states

Properties:

- Stationary states are orthogonal

$$\int_{-\infty}^{+\infty} \psi_m^* \psi_n \, dx = \delta_{mn}$$

Proof: $$\int_{-\infty}^{+\infty} \psi_m^* \left(\hat{a}_+ \hat{a}_-\right) \psi_n \, dx = n \int_{-\infty}^{+\infty} \psi_m^* \psi_n \, dx$$

- We can use Fourier's trick to evaluate c_n, we can expand $\Psi(x,0)$ as a linear combination of stationary states: $\Psi(x,0) = \sum_{n=1}^{\infty} c_n \psi_n(x)$

- $|c_n|^2$ is prob $(E) = E_n$

$$c_n = \int \psi_n^*(x) \, f(x) \, dx \quad \text{where } f(x) = \sum_{n=1}^{\infty} c_n \psi_n(x)$$

4) Quantum Harmonic Oscillator: power series

Time-independent Schrödinger equation for harmonic oscillator:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + \frac{1}{2}m\omega^2 x^2\psi = E\psi$$

$$\Rightarrow \quad \frac{d^2\psi}{dx^2} - \frac{m^2\omega^2}{\hbar^2}x^2\psi = -\frac{2m}{\hbar^2}E\psi$$

Variable change: $\xi = \sqrt{\frac{m\omega}{\hbar}}\,x \;\Rightarrow\; \xi^2 = \left(\frac{m\omega}{\hbar}\right)x^2$

$$d\xi = \sqrt{\frac{m\omega}{\hbar}}\,dx$$

$$\Rightarrow \quad \frac{d^2\psi}{d\xi^2}\left(\frac{m\omega}{\hbar}\right) - \left(\frac{m\omega}{\hbar}\right)\xi^2 = -\frac{2m}{\hbar^2}E\psi$$

$$\Rightarrow \quad \frac{d^2\psi}{d\xi^2} - \xi^2\psi = -\frac{2m}{\hbar^2}\cdot\frac{\hbar}{m\omega}E\psi$$

$$\Rightarrow \quad \frac{d^2\psi}{d\xi^2} - \xi^2\psi = -\frac{2E}{\hbar\omega}\psi$$

Variable change: K energy in units of $\frac{1}{2}\hbar\omega$: $K \equiv \frac{2E}{\hbar\omega}$

$$\Rightarrow \quad \boxed{\frac{d^2\psi}{d\xi^2} = (\xi^2 - K)\psi}$$

4) Quantum Harmonic Oscillator: power series

Time-independent Schrödinger equation for harmonic oscillator:

when x, ξ are very large: $\xi^2 >> K$

$$\Rightarrow \frac{d^2\psi}{d\xi^2} \approx \xi^2 \psi$$

sln: $\psi(\xi) = A e^{-\frac{\xi^2}{2}} + B e^{+\frac{\xi^2}{2}}$

when $x \to +\infty$, $\xi \to \infty$: $B e^{+\frac{\xi^2}{2}} \to +\infty$ (non normalisable)

physical solutions:

$$\psi(\xi) \propto e^{-\frac{\xi^2}{2}} \quad \text{at large } \xi$$

Method 2: Power series method

1) stripping off asymptotic behaviour:

$$\psi(\xi) = h(\xi) e^{-\frac{\xi^2}{2}}$$

↳ simpler functional form than $\psi(\xi)$

Differentiating:

$$\frac{d\psi}{d\xi} = \frac{dh}{d\xi} e^{-\frac{\xi^2}{2}} - \xi \cdot e^{-\frac{\xi^2}{2}} h$$

$$\Rightarrow \frac{d\psi}{d\xi} = \left(\frac{dh}{d\xi} - \xi h\right) e^{-\frac{\xi^2}{2}}$$

4) Quantum Harmonic Oscillator: power series

A second time:

$$\frac{d^2\psi}{d\xi^2} = \frac{dh^2}{d\xi^2} e^{-\frac{\xi^2}{2}} - \xi e^{-\frac{\xi^2}{2}} \frac{dh}{d\xi}$$

$$\Rightarrow \frac{d^2\psi}{d\xi^2} = \left(\frac{d^2h}{d\xi^2} - 2\xi \frac{dh}{d\xi} + (\xi^2 - 1)h \right) e^{-\frac{\xi^2}{2}}$$

Sch: eq:

$$\frac{d\psi^2}{d\xi^2} = (\xi^2 - K)\psi \Rightarrow \frac{d^2h}{d\xi^2} - 2\xi \frac{dh}{d\xi} + (K-1)h = 0$$

Solutions in the form of power series:

$$h(\xi) = a_0 + a_1\xi + a_2\xi^2 + \dots = \sum_{j=0}^{\infty} a_j \xi^j$$

Differentiating:

$$\frac{dh}{d\xi} = a_1 + 2a_2\xi + 3a_3\xi^2 + \dots = \sum_{j=0}^{\infty} j a_j \xi^{j-1}$$

$$\frac{d^2h}{d\xi^2} = 2a_2 + 2 \cdot 3a_3\xi + 3 \cdot 4a_4\xi^2 + \dots = \sum_{j=0}^{\infty} (j+1)(j+2)a_{j+2}\xi^j$$

4) Quantum Harmonic Oscillator: power series

The Schrödinger equation becomes:

$$\sum_{j=0}^{\infty}\left[(j+1)(j+2)a_{j+2} - 2ja_j + (k-1)a_j\right]\xi^j = 0$$

Uniqueness of power series expansion.

The coef. of each power of ξ must vanish:

$$(j+1)(j+2)a_{j+2} - 2ja_j + (k-1)a_j = 0$$

$$\Rightarrow \boxed{a_{j+2} = \frac{(2j+1-k)}{(j+1)(j+2)}a_j}$$ Recursion formula equivalent to the Sch. eq.

Generates: $\begin{cases} a_0 \rightarrow \text{all even-numbered coef.} \\ a_1 \rightarrow \text{all odd coef.} \end{cases}$

$$a_0 \rightarrow a_2 = \frac{1-k}{2}a_0, \quad a_4 = \frac{5-k}{12}a_2 = \frac{(5-k)(1-k)}{24}a_0, \dots\dots$$

$$a_1 \rightarrow a_3 = \frac{3-k}{6}a_1, \quad a_5 = \frac{7-k}{20}a_3 = \frac{(7-k)(3-k)}{120}a_1, \dots\dots$$

4) Quantum Harmonic Oscillator: power series

Complete Solution: $h(\xi) = h_{even}(\xi) + h_{odd}(\xi)$

Where: $h_{even} = a_0 + a_2\xi^2 + a_4\xi^4 + \cdots$

$h_{odd} = a_1 + a_3\xi^3 + a_5\xi^5 + \cdots$

olutions depend on 2 arbitrary constants: a_0, a_1

Can we normalise all solutions? Not all of them.

For large j: $a_{j+2} \approx \frac{2}{j} a_j$

With approximate solutions: $a_j \approx \frac{C}{\left(\frac{j}{2}\right)!}$

At large ξ: $h(\xi) \approx C \sum \frac{1}{\left(\frac{j}{2}\right)!} \xi^j \approx C \sum \frac{1}{j!} \xi^{2j} \approx C e^{\xi^2}$

Then: $\psi \propto e^{+\frac{\xi^2}{2}}$, so it is non-normalisable.

4) Quantum Harmonic Oscillator: power series

For normalisable solutions:

1) The power series must terminate, at some highest j ("n"), $a_{n+2} = 0$
2) This truncates h_{even}, $a_1 = 0$ if n is even
   h_{odd}, $a_0 = 0$ if n is odd

For physically acceptable slns:

$$K = 2n + 1 \quad , \quad n > 0$$

Remember that: $K = \frac{2E}{\hbar\omega} \Rightarrow \boxed{E_n = \left(n + \frac{1}{2}\right)\hbar\omega}$ for $n = 0, 1, 2, \ldots$

Recursion formula:

$$a_{j+2} = \frac{-2(n-j)}{(j+1)(j+2)} a_j$$

$n=0$: $h_0(\xi) = a_0 \Rightarrow \psi_0(\xi) = a_0 e^{-\frac{\xi^2}{2}}$; $a_1 = 0 \Rightarrow a_2 = 0$ ($j=0$)

$n=1$: $h_1(\xi) = a_1\xi \Rightarrow \psi_1(\xi) = a_1 \xi e^{-\frac{\xi^2}{2}}$; $a_0 = 0 \Rightarrow a_3 = 0$ ($j=1$)

$n=2$: $h_2(\xi) = a_0(1-2\xi^2) \Rightarrow \psi_2(\xi) = a_0(1-2\xi^2)e^{-\frac{\xi^2}{2}}$; $a_2 = -2a_0 \Rightarrow a_4 = 0$ ($j=2$

4) Quantum Harmonic Oscillator: power series

For normalisable solutions:

In general: $h_n(\xi)$ polynomial of degree n in ξ $\begin{cases} \text{even powers if } n \equiv \text{even} \\ \text{odd powers if } n \equiv \text{odd} \end{cases}$

$\downarrow$

$H_n(\xi) \equiv$ Hermite polynomials

- Coef of highest power of ξ is 2^n

$$\psi_n(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} \frac{1}{\sqrt{2^n n!}} H_n(\xi) e^{-\frac{\xi^2}{2}}$$

We had found: $\psi_n(x) = \frac{1}{\sqrt{n!}} (\hat{a}_+)^n \psi_0(x)$

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

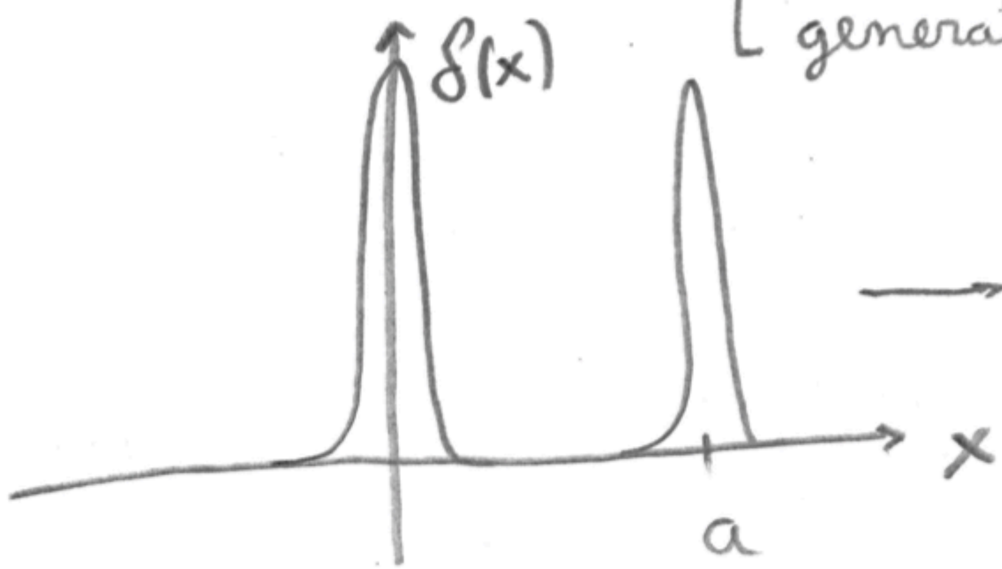
$H_0 = 1,$
$H_1 = 2\xi,$
$H_2 = 4\xi^2 - 2,$
$H_3 = 8\xi^3 - 12\xi,$
$H_4 = 16\xi^4 - 48\xi^2 + 12,$
$H_5 = 32\xi^5 - 160\xi^3 + 120\xi.$

The first few Hermite polynomials, $H_n(\xi)$.

5) Delta function potential well

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

Dirac delta function : { infinitely high
infinitesimally narrow
generalised function



spike at point a:
$\delta(x-a)$

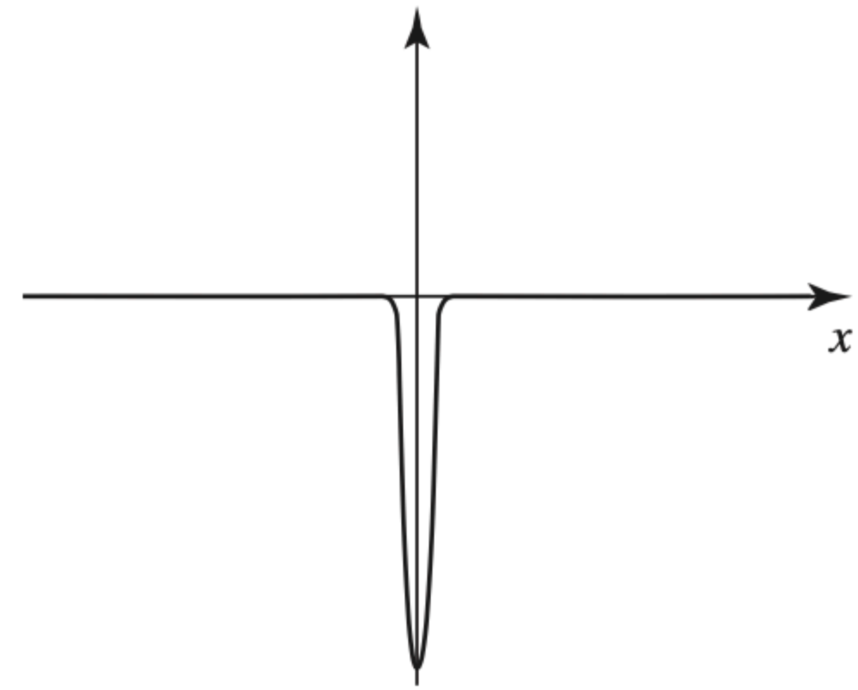
$$f(x)\,\delta(x-a) = f(a)\,\delta(x-a)$$

$$\Rightarrow \int_{-\infty}^{+\infty} f(x)\,\delta(x-a)\,dx = \int_{-\infty}^{+\infty} f(a)\,\delta(x-a)\,dx = f(a)\int_{-\infty}^{+\infty} \delta(x-a) = f(a)$$

* the delta function allows us to pick out the value of $f(x)$ at a.
* we just need to $\int$ between $a-\varepsilon \wedge a+\varepsilon$

5) Delta function potential well: bound states

In QM, we can study: $\boxed{V(x) = -\alpha\,\delta(x)}$



where $\alpha > 0$ ^ $[\alpha] = [\text{Energy}] \times [\text{length}]$

$[\delta(x)] = [\text{length}]^{-1}$

Sch. eq reads:

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

Bound states: $E<0$

Scattering states: $E>0$

Bound states: $E<0$

Ⓘ $x<0$: $V(x)=0$

$$\Rightarrow -\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi \quad \Rightarrow \quad \frac{d^2\psi}{dx^2} = \overbrace{-\frac{2mE}{\hbar^2}}^{K^2}\psi$$

$$K \equiv \frac{\sqrt{-2mE}}{\hbar}, \quad K \in \mathbb{R}, \quad K>0$$

5) Delta function potential well: bound states

(II) $x>0$: $V(x)=0$ $\Rightarrow \frac{d^2\psi}{dx^2} = -\frac{2mE}{\hbar^2}\psi$

sln: $\psi(x) = Fe^{-\kappa x} + Ge^{+\kappa x}$

If $x \to +\infty$: $Ge^{\kappa x} \to +\infty$

$\Rightarrow \boxed{\psi(x) = Fe^{-\kappa x}}$ for $x>0$

Boundary conditions $(x=0)$:

(1) ψ is continuous

(2) $\frac{d\psi}{dx}$ is continuous except where the potential is ∞.

(1) $\psi(0) = Be^{0} = Fe^{-0} \Rightarrow B=F$

$$\Rightarrow \psi(x) = \begin{cases} Be^{\kappa x}, & x \leq 0 \\ Be^{-\kappa x}, & x \geq 0 \end{cases}$$

(2) $\delta(x)$ determines the discontinuity in $\frac{d\psi}{dx}$ at $x=0$.

i) Integrate Sch. eq between $-\varepsilon$ & ε

ii) $\lim_{\varepsilon \to 0}$

5) Delta function potential well: bound states

$$-\frac{\hbar^2}{2m}\int_{-\varepsilon}^{+\varepsilon}\frac{d^2\psi}{dx^2}\,dx + \int_{-\varepsilon}^{+\varepsilon}V(x)\,\psi(x)\,dx = \cancel{E\int_{-\varepsilon}^{+\varepsilon}\psi(x)\,dx}^{\to 0}$$

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

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

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

$$\psi(x) = \begin{cases} Be^{kx}, & x \le 0 \\ Be^{-kx}, & x \ge 0 \end{cases} \Rightarrow \frac{d\psi}{dx} = \begin{cases} +Bke^{kx} \\ -Bke^{-kx} \end{cases} \overset{\varepsilon\to 0}{\Longrightarrow} \begin{cases} \left.\frac{d\psi}{dx}\right|_{-\varepsilon} = +Bk \\ \left.\frac{d\psi}{dx}\right|_{+\varepsilon} = -Bk \end{cases}$$

$$\Rightarrow \psi(0) = B$$

5) Delta function potential well: bound states

$$\Rightarrow \quad -2Bk = -\frac{2m\alpha}{\hbar^2} B$$

$$\Rightarrow \quad \boxed{k = \frac{m\alpha}{\hbar^2}} \quad \Rightarrow \text{allowed } E \Rightarrow \boxed{E = -\frac{\hbar^2 k^2}{2m} = -\frac{m\alpha^2}{2\hbar^2}}$$

Normalisation:

$$\int_{-\infty}^{+\infty} |\psi(x)|^2 dx = 2\int_0^{+\infty} |B e^{-kx}|^2 dx = 2|B|^2 \int_0^{+\infty} e^{-2kx} dx = 1$$

$$= 2|B|^2 \frac{2}{k} = 1 \Rightarrow B = \sqrt{k} = \frac{\sqrt{m\alpha}}{\hbar}$$

One bound state:

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

5) Delta function potential well: scattering states

Scattering states : $E > 0$

(I) $x < 0$: $\dfrac{d^2\psi}{dx^2} = -\dfrac{2mE}{\hbar^2}\psi = -k^2\psi$; $k \equiv \dfrac{\sqrt{2mE}}{\hbar}$

sln: $\psi(x) = Ae^{+ikx} + Be^{-ikx}$

(II) $x > 0$: $\dfrac{d^2\psi}{dx^2} = -\dfrac{2mE}{\hbar^2}\psi = -k^2\psi$

sln: $\psi(x) = Fe^{ikx} + Ge^{-ikx}$

Boundary conditions:

① $\psi(x)$ continuous $\rightarrow$ $\psi(0) = \boxed{A + B = F + G}$

② $\dfrac{d\psi}{dx}$ continuous $\begin{cases} \left.\dfrac{d\psi}{dx}\right|_{-} = ik\left(Ae^{ikx} - Be^{-ikx}\right), & x < 0 \\ \left.\dfrac{d\psi}{dx}\right|_{+} = ik\left(Fe^{ikx} - Ge^{-ikx}\right), & x > 0 \end{cases}$

5) Delta function potential well: scattering states

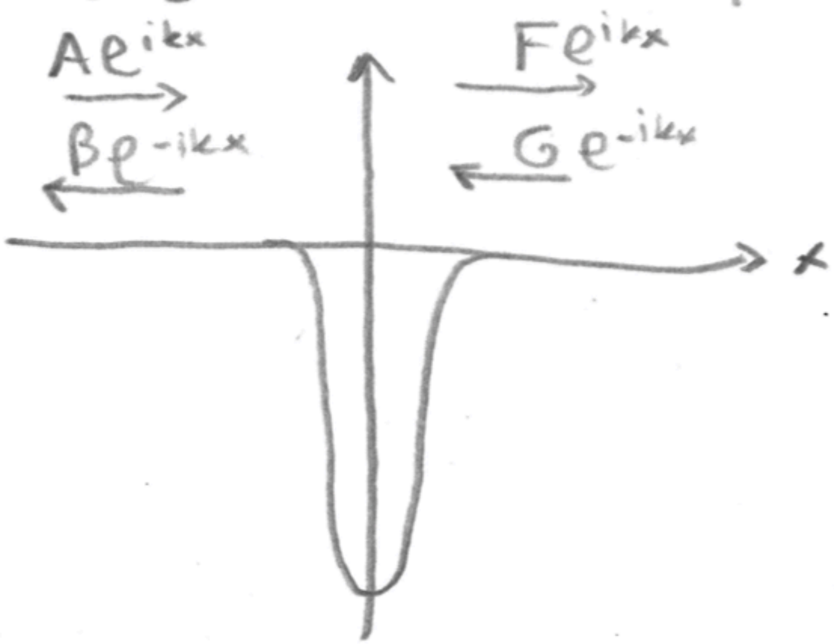
$$x \to 0: \quad \left.\frac{d\psi}{dx}\right|_+ = ik(F-G), \quad \left.\frac{d\psi}{dx}\right|_- = ik(A-B) \quad \Bigg\} \quad \Delta\left(\frac{d\psi}{dx}\right) = ik(F-G-A+B) = -\frac{2m\alpha}{\hbar^2}\psi(0)$$

$$\Rightarrow ik(F-G-A+B) = -\frac{2m\alpha}{\hbar^2}(A+B)$$

$$\Rightarrow \boxed{F-G = A(1+2i\beta) - B(1-2i\beta)}, \quad \beta \equiv \frac{m\alpha}{\hbar^2 k}$$

Normalisation won't help

We have 5 variables $\wedge$ 2 equations.



scattering from the left

$G = 0$

$A \equiv$ amplitude of incident wave.

$B \equiv$ " of reflected wave

$F \equiv$ " of transmitted wave

5) Delta function potential well: R & T coefficients

$$\Rightarrow B = \frac{i\beta}{1 - i\beta} A$$

$$\Rightarrow F = \frac{1}{1 - i\beta} A$$

We can define:

$R = \frac{|B|^2}{|A|^2} \equiv$ reflection coefficient $\Big\}$ fraction of particles that bounces back.

$$R = \frac{|B|^2}{|A|^2} \equiv \frac{\beta^2}{1+\beta^2} = \frac{1}{1 + (2\hbar^2 E / m\alpha^2)}$$

$T = \frac{|F|^2}{|A|^2} \equiv \frac{1}{1+\beta^2}$ $\Big\}$ prob of particle continues

$$\frac{1}{1 + (m\alpha^2 / 2\hbar^2 E)}$$

$\wedge\ R + T = 1$

5) Delta function potential well: R & T coefficients

Reflection (R) and transmission (T) coefficients:

- The higher E, the higher the prob. of transmission.
- These scattering wave functions are non-normalisable
- They are not possible particle states
- We need to form normalisable linear combinations of the stationary states
- True particles are represented by the resulting wavepackets
- R & T are approximate reflection & transmitted coef. around E.

Summary: general QM problem

Time-dependent Schrödinger equation:

$$i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} + V\Psi,$$

Separation of variables, assuming V=V(x).

$$\Psi(x,t) = \psi(x)\,\varphi(t),$$

We obtain 2 ODEs:

(wiggle factor)

1. $$\frac{d\varphi}{dt} = -\frac{iE}{\hbar}\varphi,$$ $$\varphi(t) = e^{-iEt/\hbar}.$$

Time-independent Schrödinger equation:

2. $$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V\psi = E\psi.$$

To solve it we need V(x).

Separable Solutions:

- They are stationary states.

- Every expectation value is constant in time

- They are states of definite total energy, i.e., every measurement of the total energy is certain to return the value E.

$$\sigma_H^2 = \langle H^2 \rangle - \langle H \rangle^2 = E^2 - E^2 = 0.$$

- The general solution is a linear combination of separable solutions, i.e., there is a different wave function for each allowed energy:

$$\Psi(x,t) = \sum_{n=1}^{\infty} c_n \psi_n(x) e^{-iE_n t/\hbar}.$$

General Solution:

- The strategy is first to solve the time-*in*dependent Schrödinger equation.

- This yields, in general, an infinite set of solutions, $\{\psi_n(x)\}$, each with its own associated energy, $\{E_n\}$.

- To fit $\psi(x, 0)$ you write down the general linear combination of these solutions:

$$\Psi(x, 0) = \sum_{n=1}^{\infty} c_n\, \psi_n(x);$$

- Construct global solution from the stationary states:

$$\boxed{\Psi(x,t) = \sum_{n=1}^{\infty} c_n \psi_n(x) e^{-iE_n t/\hbar} = \sum_{n=1}^{\infty} c_n \Psi_n(x,t).}$$

- Coefficients:

$\lvert c_n \rvert^2$	is the *probability* that a measurement of the energy would return the value E_n.

Bound states versus scattering states

Bound states are *normalisable*, and labeled by a *discrete index n.* They are physically realisable states on their own.

Scattering states are *non-normalisable*, and labeled by a *continuous variable k*.

$$\begin{cases} E < V(-\infty) \text{ and } V(+\infty) \;\Rightarrow & \text{bound state,} \\ E > V(-\infty) \text{ or } V(+\infty) \;\Rightarrow & \text{scattering state.} \end{cases}$$

$$\begin{cases} E < 0 \;\Rightarrow & \text{bound state,} \\ E > 0 \;\Rightarrow & \text{scattering state.} \end{cases}$$

Time-independent Schrödinger equation

Time-independent Schrödinger equation:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V\psi = E\psi.$$

To solve it we need V(x).

Steps:

1. Define and sketch V(x).
2. Divide the problem into regions of interest.
3. Analyse the expected type of solutions (e.g. bound states or scattering states)
4. Divide the problem based on the energy of the particle.
5. Re-write Schrödinger equation for each region.
6. Define an appropriate and real wavenumber.
7. Solve the resulting ODE.
8. Analyse the asymptotic behaviour of the ODE solutions, remove diverging terms.
9. Analyse boundary conditions (usually two: ψ(x) and ψ'(x) have to be continuous).
10. Find energies and normalise the solution.
11. Append the wiggle factor and construct a general solution.