2) Particles in an infinite square well potential

Schrödinger equation:

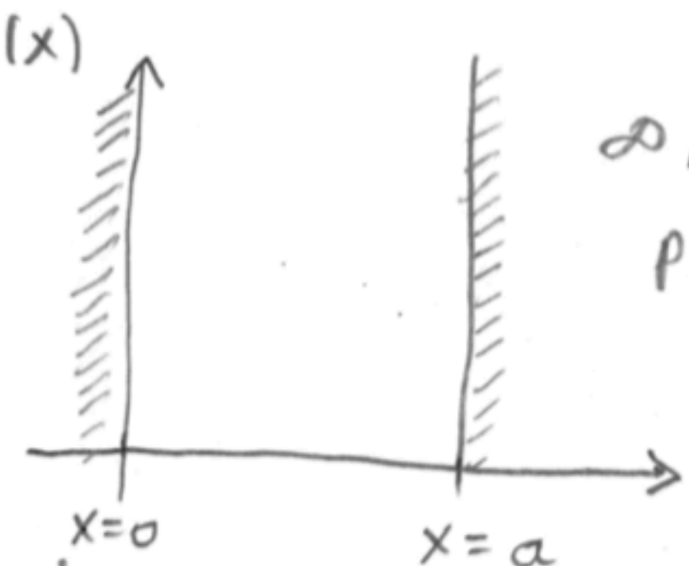
$$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 \Psi}{\partial x^2} + V\Psi \xrightarrow[V=V(x)]{\Psi = \psi(x)\varphi(t)} \begin{cases} \dfrac{d\varphi}{dt} = -\dfrac{iE}{\hbar}\varphi \;\rightarrow\; \varphi = e^{-i\frac{E}{\hbar}t} \\ -\dfrac{\hbar^2}{2m}\dfrac{d^2\psi}{dx^2}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

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:

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

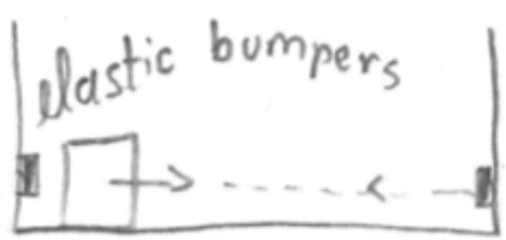


∞ □ well potential

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:



$\mu_k = 0$

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

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

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

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

2) Particles in an infinite square well potential

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

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

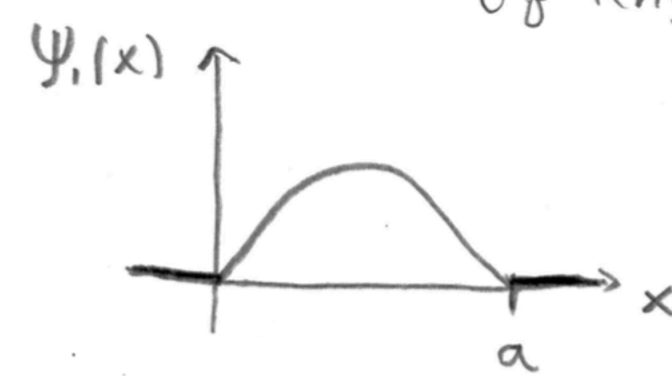
11) Inside the well, the sln reads:

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

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

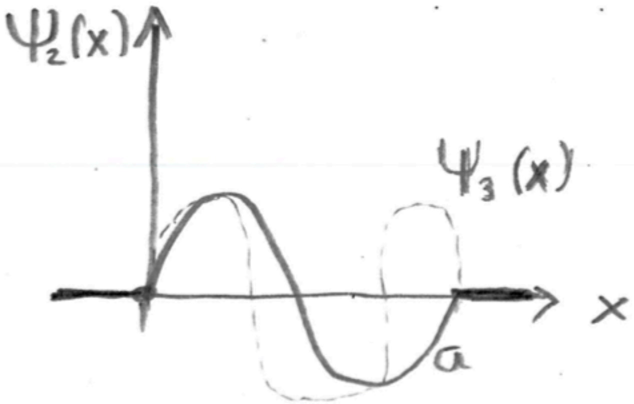
n = 1: Ground state.

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



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

2) Particles in an infinite square well potential



Excited states:

n = 2:

$$\Psi_2(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{2\pi}{a}x\right)$$

$$E_2 = \frac{2^2 \pi^2 \hbar^2}{2 m a^2}$$

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: $\Psi_1 \rightarrow 0$, $\Psi_2 \rightarrow 1$, $\Psi_3 \rightarrow 2$, 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.

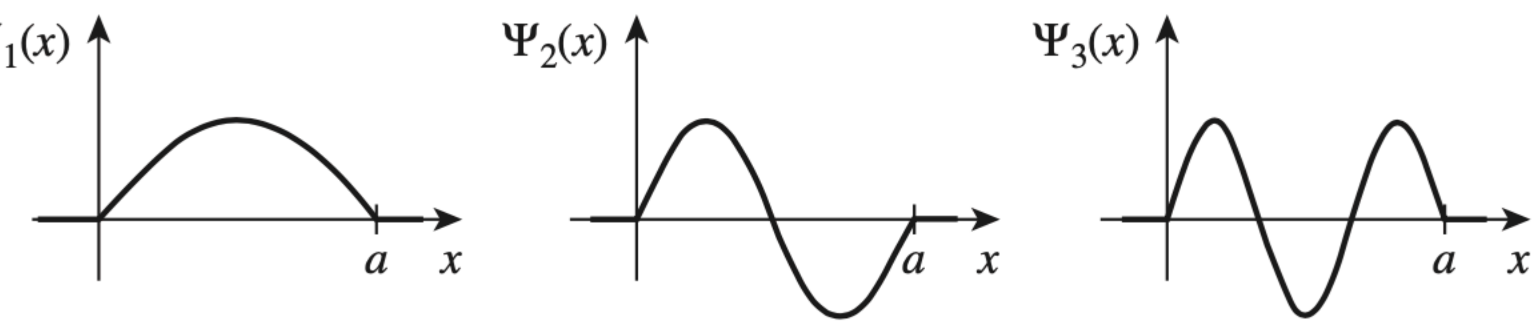
② is universal for all $V(x)$.

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:

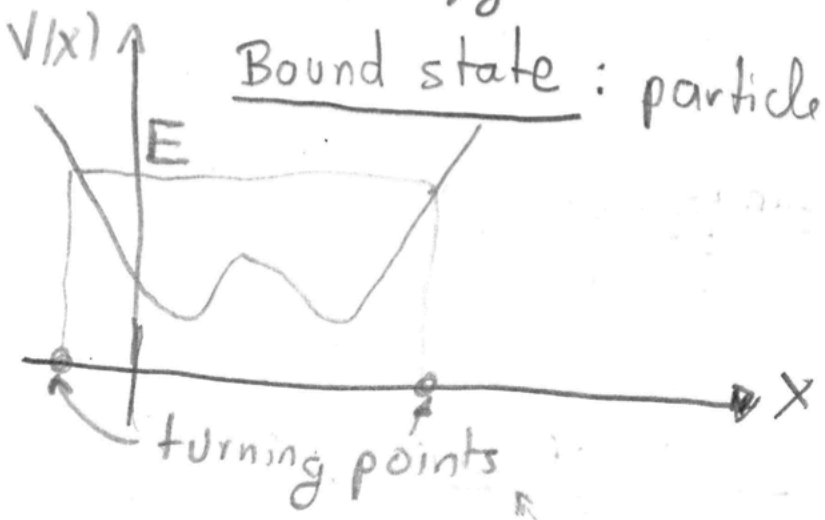
① Non-normalisable: free particle → labeled by continuous var. k $\int dk$

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

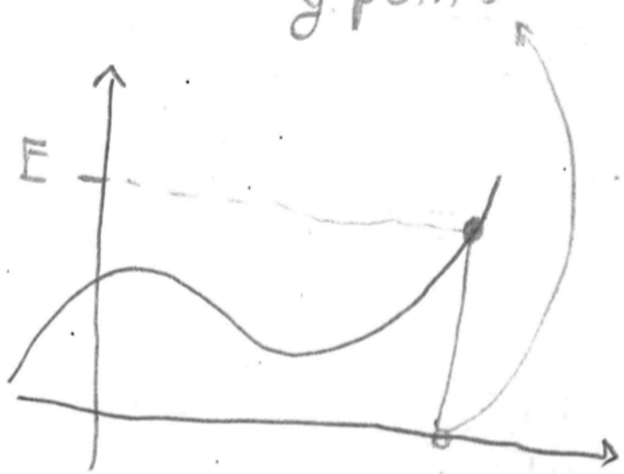
What is the physical distinction?

Classical analogy.

<u>Bound state</u>: particle cannot escape



<u>Scattering state</u>: 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:

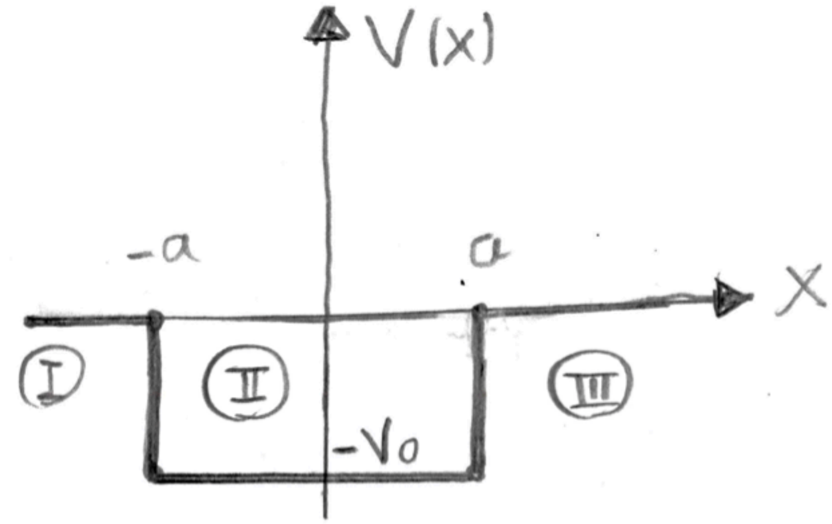
1) $\infty\square$ well: $V(x) \rightarrow \pm\infty$ when $x \rightarrow \pm\infty \Rightarrow$ only bound states

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:

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

I

ODE

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

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

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

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

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

III

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

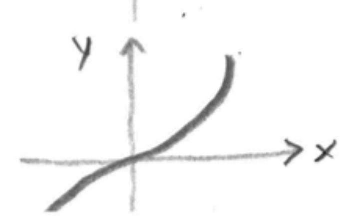
$x \to +\infty \Rightarrow e^{\kappa x} \to +\infty \Rightarrow$ $\boxed{\psi(x) = Fe^{-\kappa x} \text{ for } x>+a}$

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:

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

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

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

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

① in ②

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

Variable change: $z = \ell a \Rightarrow$

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

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

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

$z_0 = 4$:

$$\frac{\tan(z)}{\sqrt{\frac{16}{z^2} - 1}} = 1 \quad ; \quad z = ? \quad \rightarrow \text{see python notebook}$$

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: $z_0 >> 0$

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

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

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

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 gnal, 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

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

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

incident amplitude

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

reflected amplitude

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

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

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:

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

At x=+a:

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

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 □ well

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.