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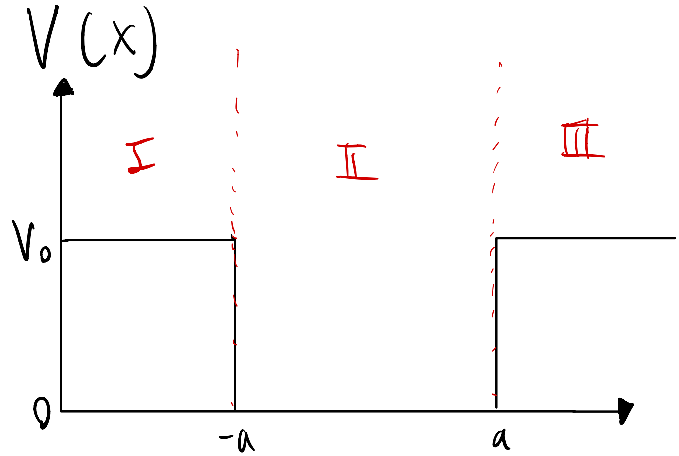


Exercise 1: Bound and Scattering states in the finite square well

A particle of mass m shall be in the finite square well potential as depicted above. For which energies is it in a bound state? scattering state? Which energies are not accessible?

The energies at which the particle is in a bound state, firstly must satisfy that they do not exceed, but remain within the potential energy well.

Corresponding to the diagram above,

this means $\boxed{E < V_0}$.

Secondly they must lie in specific discrete energy values within the potential energy well defined by

$$E_n = \frac{\hbar^2 \pi^2 n^2}{8 m a^2}$$

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

in well, $V = 0$, at walls: $V = V_0$,

I & III) $-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V_0\psi = E\psi$ II) $-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi$

Even Solutions:

$$\psi_I = Ae^{\gamma x}, \quad \psi_{II} = B\cos kx, \quad \psi_{III} = Ae^{-\gamma x}$$

$$\psi_{II}(a) = \psi_{III}(a) = B\cos(ka) = Ae^{-\gamma a}$$

where $\gamma = \sqrt{\dfrac{2m(V_0 - E)}{\hbar^2}}$

$$\psi_{II}'(a) = \psi_{III}'(a) = -Bk\sin(ka) = -\gamma Ae^{-\gamma a}$$

$$= Bk\sin(ka) = \ell Ae^{-\ell a}$$

$$\gamma^2 + k^2 = \frac{2mV_0}{\hbar^2}$$

$$\therefore \; k\tan(ka) = \gamma$$

even

Odd solutions

$$\psi_{II}(a) = \psi_{III}(a) = B\sin(ka) = -Ae^{-\gamma a}$$

$$\psi_{II}'(a) = \psi_{III}' = kB\cos(ka) = \gamma Ae^{-\gamma a}$$

$$\therefore \; \tan(ka) = -\frac{k}{\gamma}$$

odd

New Notation

even:

$z = \gamma a$

$w = ka$

$ka\tan ka = \gamma a$

$w\tan w = z$

$$w^2 + z^2 = \frac{2ma^2V_0}{\hbar^2} \quad R_0^2$$

$$w^2 + z^2 = R_0^2$$

Find intersections

$$z = \sqrt{R_0^2 - w^2}$$

$$z = w \tan w$$

intersection points:

$$w = 1.30644, \; z = 4.8263$$

$$w = 3.83747, \; z = 3.20528$$

$w = ka$, $z = \ell a$

$$k = 1.30644, \; \ell = 4.8263$$

$$k = \sqrt{E_0}, \; k^2 = E_0 = 1.7068$$

$$k = 3.83747 = \sqrt{E_1}, \; E_1 = k^2 = 14.7262$$

ODD:

$$\tan ka = -\frac{k}{\ell} \; ; \quad \ell \tan ka = -k$$

$$\ell a \tan ka = -ka$$

$$w = ka, \; z = \ell a$$

Find intersections for

$$z \tan w = -w$$

$$z = -w \cot w$$

$$z^2 + w^2 = V_0 = 25$$

$$z = \sqrt{25 - w^2}$$

ODD: $\omega = 2.595739, 4.90629515$

$E_0 = (2.595739)^2 = 6.7379$

$E_1 = (4.90629515)^2 = 24.0717$

The energies for which the particle is in a scattering state are those that exceed the potential energy well.

Corresponding to the diagram above, this means $\boxed{E > V_0}$.

The energies that are not accessible are those where $E < 0$ as the potential energy well bottoms out at $V(x) = 0$ $-a < x < a$.

Exercise 2: Bound states of the finite square well

We now assume that the particle is in a bound state and we set $\frac{2m}{\hbar^2} = 1$ to make the other quantities dimensionless. We choose $a = 1$, $V_0 = 25$

a) Determine Eigen-Energies and wavefunctions $\psi_0(x)$ and $\psi_1(x)$ of two stationary states

a.) Accidentally already solved for these in Exercise 1

Numerical Solver

$E_{even} = 1.7067, 14.726$

E_2

E_0 Ground State

Numerical solver

$E_{odd} = 6.7378$ 24.072

E_3

E_1 First Excited State

Now, find wavefunctions ψ_0 & ψ_1 for even and odd

We already have K from Exercise 1:

Even

$$\gamma_0 = \sqrt{\frac{2m(V_0 - E_0)}{\hbar^2}} = \sqrt{25 - E_0}$$

$$\gamma_1 = \sqrt{\frac{2m(V_0 - E}{\hbar^2}} \quad \sqrt{25 - E_1}$$

ODD

$$\gamma_0 = \sqrt{\frac{2m(V_0 - E_0)}{\hbar^2}} = \sqrt{25 - E_0}$$

$$\gamma_1 = \sqrt{\frac{2m(V_0 - E_1)}{\hbar^2}} = \sqrt{25 - E_1}$$

Even

General Solution

$$\psi_0 = A_0 \cos(k_0 x) \quad \text{for } -a < x < a \quad \text{II}$$

$x \to -\infty,\ \psi^*\psi \to 0$

$$\psi_0 = F_0 e^{\gamma_0 x} + \cancel{G_0 e^{-\gamma_0 x}}^{\,0} \quad \text{for } x < -a \quad \text{I}$$

$x \to +\infty,\ \psi^*\psi \to 0$

$$\psi_0 = \cancel{H_0 e^{\gamma_0 x}} + I_0 e^{-\gamma_0 x} \quad \text{for } x > a \quad \text{III}$$

Apply Boundary Conditions

ψ at $x = -a$ $\quad \psi_{\text{I}}(-a) = \psi_{\text{II}}(-a)$

$$A_0 \cos(-k_0 a) = F_0 e^{-\gamma_0 a}$$

$$A_1 \cos(-k_1 a) = F_1 e^{-\gamma_1 a}$$

cos is even, so

$$A_0 \cos(k_0 a) = F_0 e^{-\gamma_0 a}$$

$$A_1 \cos(k_1 a) = F_1 e^{-\gamma_1 a}$$

Odd

General solution

$$\psi_1 = B_1 \sin(k_1 x) \quad \text{for } -a < x < a \quad \text{II}$$

$x \to -\infty,\ \psi\psi = 0$

$$\psi_1 = F_1 e^{\gamma_1 x} - \cancel{G_1 e^{-\gamma_1 x}}^{\,0} \quad \text{for } x \leq -a \quad \text{I}$$

$x \to \infty,\ \psi^*\psi \to 0$

$$\psi_1 = \cancel{H_1 e^{\gamma_1 x}}^{\,0} - I_1 e^{-\gamma_1 x} \quad \text{for } x > a \quad \text{III}$$

Apply Boundary Conditions

$\psi(-a) \to \psi_{\text{I}}(-a) = \psi_{\text{II}}(-a)$

$$-B \sin(ka) = F e^{-\gamma a}$$

$$F = -B \sin(ka)\, e^{\gamma a}$$

$\psi'(-a) \to \psi_{\text{I}}'(-a) = \psi_{\text{II}}'(-a)$

$$B k \cos(ka) = \gamma F e^{-\gamma a}$$

$\psi(a) \to \psi_{\text{II}}(a) = \psi_{\text{III}}(a)$

$$B \sin(ka) = -I e^{-\gamma a} = -F e^{-\gamma a}$$

ψ' at $x = -a$:

$$-A_0 k_0 \sin(-k_0 a) = \gamma_0 F_0 e^{-\gamma_0 a}$$

sin is odd, so

$$A_0 k_0 \sin(k_0 a) = \gamma_0 F_0 e^{-\gamma_0 a}$$

ψ at $x = a$:

$$F = \frac{A k \sin(ka)}{\gamma} e^{\gamma a}$$

$$A_0 \cos(k_0 a) = I_0 e^{-\gamma_0 a}$$

ψ' at $x = a$:

$$-A_0 k_0 \sin(k_0 a) = -\gamma_0 I_0 e^{-\gamma_0 a}$$

Solve for constants
A, F, I

$$A_0 \cos(k_0 a) = F_0 e^{-\gamma_0 a}$$

$$F = A \cos(ka) e^{\gamma a}$$

$$A \cos(ka) = F e^{-\gamma a} = I e^{-\gamma a}$$

$$F = I$$

$\therefore$ $F = I$

$\therefore$ $\psi_{III}(x) = -\psi_{I}(x)$

satisfies odd condition

$$\psi(x) = \begin{cases} F e^{\gamma x} & \text{for } x < -a \\ B \sin(kx) & \text{for } -a < x < a \\ -F e^{-\gamma x} & \text{for } x > a \end{cases}$$

where $F = -B e^{\gamma a} \sin(ka)$

$$|F|^2 = |B|^2 \underbrace{\left(e^{\gamma a} \sin(ka)\right)^2}_{\zeta}$$

$$|F|^2 = |B|^2 \zeta$$

Normalize

$$1 = \int_{-\infty}^{\infty} |\psi|^2 dx$$

$$= |B|^2 \left[\zeta \int_{-\infty}^{-a} e^{2\gamma x} dx + \int_{-a}^{a} \sin^2(kx) dx + \zeta \int_{a}^{\infty} e^{-2\gamma x} dx \right]$$

$$\therefore \Psi(x) = \begin{cases} F e^{\gamma x} & \text{for } x<a \\ A\cos(kx) & \text{for } -a<x<a \\ F e^{-\gamma x} & \text{for } x>a \end{cases}$$

where $F = A e^{\gamma a}\cos(ka)$

<u>Normalize</u>

$$1 = \int_{-\infty}^{\infty} |\Psi|^2\, dx$$

$$= |A|^2 \left[|e^{\gamma a}\cos(ka)|^2 \int_{-\infty}^{-a} e^{2\gamma x}\, dx + \int_{-a}^{a} \cos^2(kx)\, dx \right.$$

$$\left. \ldots + \underbrace{|e^{\gamma a}\cos(ka)|^2}_{\xi} \int_{a}^{\infty} e^{-2\gamma x} \right]$$

$$= |A|^2 \left[\xi \left[\frac{e^{2\gamma x}}{2\gamma} \right]_{-\infty}^{-a} + \left[\frac{x}{2} + \frac{1}{4k}\sin(2kx) \right]_{-a}^{a} + \xi \left[-\frac{1}{2\gamma} e^{-2\gamma x} \right]_{a}^{\infty} \right]$$

$$= |A|^2 \left[\xi \left[\frac{e^{-2\gamma a}}{2\gamma} - 0 \right] + \left[a + \frac{1}{2k}\sin(2ka) \right] + \xi \left[0 + \frac{1}{2\gamma} e^{-2\gamma a} \right] \right]$$

$$1 = |A|^2 \left[\frac{\xi}{\gamma} e^{-2\gamma a} + a + \frac{1}{2k}\sin(2ka) \right]$$

$$= |B|^2 \left[\xi \left[\frac{e^{2\gamma x}}{2\gamma} \right]_{-\infty}^{-a} + \left[\frac{x}{2} - \frac{\sin 2kx}{4k} \right]_{-a}^{a} + \xi \left[-\frac{1}{2\gamma} e^{-2\gamma x} \right]_{a}^{\infty} \right]$$

$a - \frac{\sin 2ka}{2k}$ $\quad \frac{a}{2} - \frac{\sin 2ka}{4k} + \left(\frac{+a}{2} + \frac{\sin 2k\cdot -a}{4k} \right)$

$$1 = |B|^2 \left[\xi \left[\frac{e^{-2\gamma a}}{2\gamma} - 0 \right] + \left[a - \frac{\sin 2ka}{2k} \right] + \xi \left[0 + \frac{1}{2\gamma} e^{-2\gamma a} \right] \right]$$

Now solve for B for ground and first excited states by plugging in $\gamma_0, k_0, \gamma_1, k_1, a$

$$B_1 = \sqrt{\frac{1}{\frac{|e^{\gamma a}\sin ka|^2}{\gamma} e^{-2\gamma a} + a - \frac{\sin 2ka}{2k}}}$$

$$F_1 = -B e^{\gamma a} \sin ka$$

$$A_0 = \sqrt{\frac{1}{\left|\frac{e^{\gamma a}\cos(ka)}{\gamma}\right|^2 e^{-2\gamma a} + a + \frac{1}{2k}\sin(2ka)}}$$

$$F_0 = A e^{\gamma a}\cos(ka)$$

ψ_0 even

Finally, for odd case

ψ_1 odd

$$\psi_0(x) = \begin{cases} F_0 e^{\gamma_0 x} & \text{for } x < -a \\ A_0 \cos(k_0 x) & \text{for } -a < x < a \\ F_0 e^{-\gamma_0 x} & \text{for } x > a \end{cases}$$

Ground state (even)

where

$A_0 \approx 0.91$ $\quad$ $\gamma_0 \approx 4.8263$

$F_0 \approx 29.666$ $\quad$ $k_0 \approx 1.306446$

$E_0 \approx 1.7068$

$$\psi_1(x) = \begin{cases} F_1 e^{\gamma_1 x} & \text{for } x < -a \\ B_1 \sin(k_1 x) & \text{for } -a < x < a \\ -F_1 e^{-\gamma_1 x} & \text{for } x > a \end{cases}$$

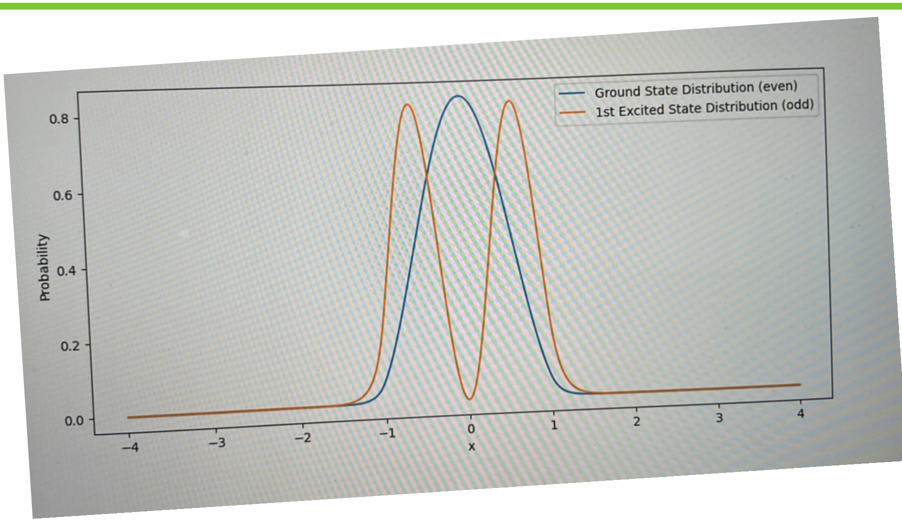
1st excited state (odd)

where

$B_1 \approx 0.90$ $\quad$ $\gamma_1 \approx 4.27342$

$F_1 \approx -33.54$ $\quad$ $k_1 \approx 2.59574$

$E_1 \approx 6.73786$



2.b.

Assume that the particle at time $t=0$ is in the state

$$\Psi(x, t=0) = \frac{1}{2}\psi_0(x) + \frac{\sqrt{3}}{2}\psi_1(x)$$

Make an animation of the probability distribution of the particles state from $t=0$ to $t=10\hbar$ (you may set $\hbar=1$).

$$\Psi(x,t) = \frac{1}{2}\psi_0(x)e^{-iE_0 t/\hbar} + \frac{\sqrt{3}}{2}\psi_1(x)e^{-iE_1 t/\hbar}$$

MP4, GIF, and python code submitted as Github link and File upload.

Search Github for:

Natsoulas / FiniteSquareWell_Animations

if the link fails.

Exercise 3: A Sudden Change

We now assume that the particle with mass m is in the ground state of a finite square well potential with $V_0 = 1$ and $a = 1$ ($\frac{2m}{\hbar^2} = 1$ according to Exercise 2).

a.) Derive the wavefunction of the ground state

Even

$$z = \sqrt{R_0^2 - w^2} \qquad \text{where} \quad R_0^2 = \frac{2ma^2V_0}{\hbar^2} = 1$$

$$z = w\tan(w)$$

$$z = \sqrt{1-w^2} = w\tan w,$$

Numerical Solver

$$w = 0.739085$$

ODD

$$z = \sqrt{1-w^2} = -w\cot(w)$$

Numerical Solver

$w =$ No real solutions . . .

$\therefore$ Ground State must be 1st even solution

$w = k, \quad E_0 = k^2 = (0.739085)^2$

Ground State Energy for New potential ($V_0 = 1$):

$E_0 = 0.5462$

Because this from the even energy groundstate, the general solution is the same as exercise 2:

$$\psi_0(x) = \begin{cases} F_0 e^{\gamma_0 x} & \text{for } x < a \\ A_0 \cos(k_0 x) & \text{for } -a < x < a \\ F e^{-\gamma_0 x} & \text{for } x > a \end{cases}$$

where $k_0 = \sqrt{E_0} = 0.739085$

$$\gamma_0 = \sqrt{\frac{2m(V_0 - E_0)}{\hbar^2}} = \sqrt{1 - E_0} = 0.673572565$$

$$A_0 = \sqrt{\frac{1}{\left|\frac{e^{\gamma_0 a}\cos(k_0 a)}{\gamma_0}\right|^2 e^{-2\gamma_0 a} + a + \frac{1}{2k_0}\sin(2k_0 a)}} = 0.63442529$$

$$F_0 = A_0 e^{\gamma_0 a}\cos(k_0 a) = 0.91958$$

All expressions derived in exercises 1 & 2

3 b.) Suddenly (and instantaneously) at time $t=0$ the potential changes to $V_0 = 25$. Calculate the new wavefunction as a function of position and time.

* Result from 3 a.) → groundstate of initial potential is now denoted as Ψ_{old}
* Result from Exercise 2 are $\Psi_0(x)$ and $\Psi_1(x)$ (time = 0) ($V_0 = 25$)

At t_0, $t_0 = 0$ . . . .

General Expression

$$\Psi_{old}(x) = C_1 \Psi_0(x) + C_2 \Psi_1(x)$$

Get coefficients by calculating overlap:

$$C_1 = \int_{-\infty}^{\infty} \Psi_0 \Psi_{old}\, dx, \quad C_2 = \int_{-\infty}^{\infty} \Psi_1 \Psi_{old}\, dx, \quad C_3 = \int_{-\infty}^{\infty} \Psi_2 \Psi_{old}\, dx, \quad C_4 = \int_{-\infty}^{\infty} \Psi_3 \Psi_{old}\, dx$$

$$C_1 = \int_{-\infty}^{-a} F_0 e^{r_0 x} F_{old} e^{r_{old} x}\, dx + \int_{-a}^{a} A_0 \cos(k_0 x) A_{old} \cos(k_{old} x)\, dx + \int_{a}^{\infty} F_0 e^{-r_0 x} F_{old} e^{-r_{old} x}\, dx$$

$$C_2 = \int_{-\infty}^{-a} F_1 e^{r_1 x} F_{old} e^{r_{old} x}\, dx + \int_{-a}^{a} B_1 \sin(k_1 x) A_{old} \cos(k_{old} x)\, dx + \int_{a}^{\infty} -F_1 e^{-r_1 x} F_{old} e^{-r_{old} x}\, dx$$

$C_3 = \ldots (2)$ $\quad C_4 = \ldots (4)$

Numerical Integrator Results: (Python code for integral in Github Repo)

$C_1 = 0.938546061$ $\quad C_2 = 0$ $\quad C_3 = -0.274176$ $\quad C_4 = 0$

Orthogonal to both odd solutions

Renormalize

$$|c_1|^2 + |c_3|^2 = 0.7783192405614446$$

So $|N|^2 \left(|c_1|^2 + |c_3|^2\right) = 1$, $N = 1.133489$

$\therefore \quad c_1 = N c_1 , \quad c_3 = N c_3$

since stationary wavefunctions are already normalized!

Finally normalized:

$$c_1 = 0.9504833 \qquad c_2 = -0.310775563$$

where $|c_1|^2 + |c_3|^2 = 1$

Finally, add time dependency

$$\Psi_{old}(x,t) = c_1 \, \psi_0(x) e^{-iE_0 t/\hbar} + c_3 \, \psi_2(x) e^{-iE_2 t/\hbar}$$

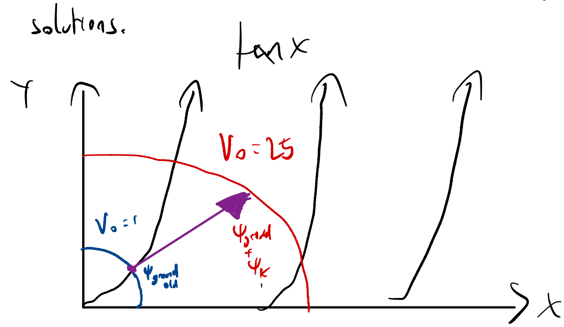
$\Psi_{old}(x,t)$ is a linear combination of the $V_0 = 25$ potential's energy eigenstates denoted by constants c_1 and c_3.

Where ψ_0 and ψ_2 are the ground state and 2nd excited state wavefunctions for the new potential.

3c.) Describe Qualitatively what happens when instead of a sudden change, the potential is slowly changing from $V_0 = 1$ to $V_0 = 25$.

A sudden increase in the potential of the walls will increase the number of bound states. This can be reasoned by the R-value from earlier where I found the discrete bound energy solutions.

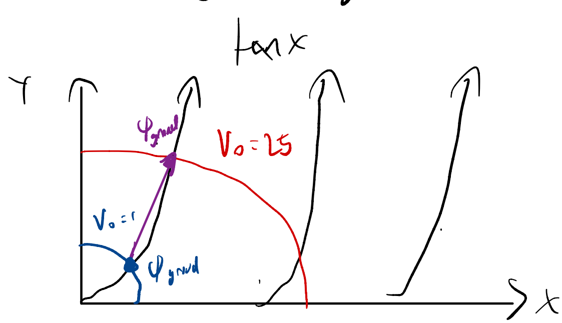
sudden...



Something like this being instantaneos would be quite messy as all of the sudden, the original ground state from 3a would become a superposition of multiple higher energy states.

Whereas a slow change from $V_0 = 1 \rightarrow V_0 = 25$ would allow the particle to adjust to the change. This means we would see the particle remain in the ground state of whatever potential between 1 and 25 during the change rather than suddenly jumping to energies it was never at initially.

slowly...



Hopefully this visual helps