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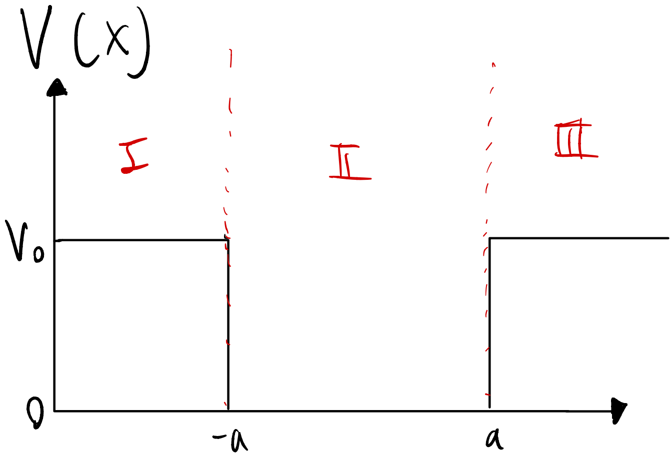


Exercise 1: Bound and Scattering states in the finite square well

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

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

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

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

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

Even Solutions:

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

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

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

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

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

$\gamma^2 + k^2 = \frac{2mV_0}{\hbar^2}$ $\therefore$ $k\tan(ka) = \gamma$

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:

$z = \gamma a$ $\qquad$ $ka\tan ka = \gamma a$

$w = ka$ $\qquad$ $w\tan w = z$

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

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

Find intersections

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

$$z = w \tan w$$

intersection points:

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

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

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

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

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

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

ODD:

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

$$la \tan ka = -ka$$

$$w = ka, \; z = la$$

$$z \tan w = -w$$

Find intersections for

$$z = -w \cot w$$

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

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

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

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

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

$\psi_0 = F_0 e^{\gamma_0 x} + \cancel{G e^{-\gamma_0 x}}$ for $x < -a$ $\quad \mathrm{I}$

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

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

Apply Boundary Conditions

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

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

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

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

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

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

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

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

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

Apply Boundary Conditions

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

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

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

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

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

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

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

ψ' at $x = -a$:

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

sin is odd, so

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

ψ at $x = a$:

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

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

ψ' at $x = a$:

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

Solve for constants
A, F, I

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

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

$$A\cos(ka) = Fe^{-\gamma a} = Ie^{-\gamma a}$$

$$\star \quad F = I$$

$$\therefore \quad F = I$$

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

satisfies odd condition

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

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

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

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

Normalize

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

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

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

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

Normalize

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

$F_0 \approx 21.666$ $\quad k_0 \approx 1.306446$

$E_0 \approx 1.7068$

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

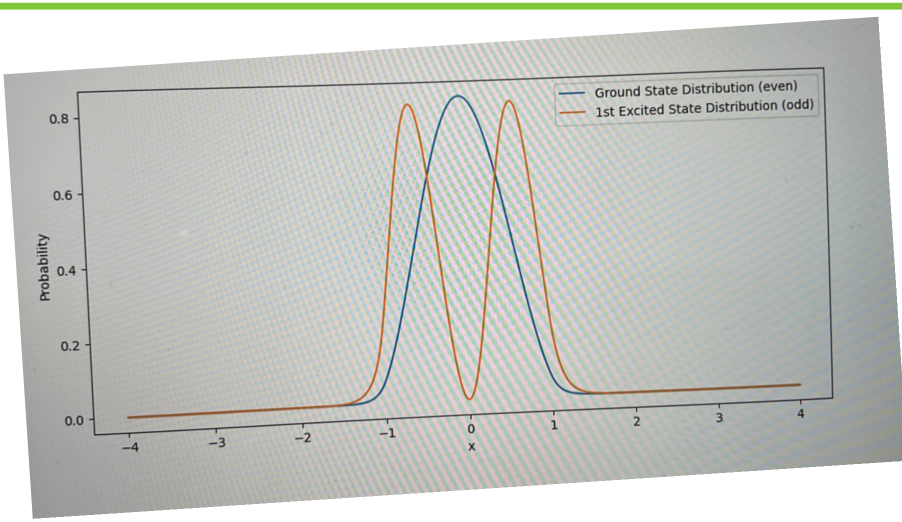
1st excited state (odd)

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 $\hbar=1$).

$$\boxed{\Psi(x,t) = \frac{1}{2}\psi_0(x)e^{-iE_0t/\hbar} + \frac{\sqrt{3}}{2}\psi_1(x)e^{-iE_1t/\hbar}}$$

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

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

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

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

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 3a.) $\Rightarrow$ groundstate of initial potential is now denoted as $\psi_{init}(x)$
* Result from Exercise 2 are $\psi_0(x)$ and $\psi_1(x)$ (time $=0$) ($V_0 = 25$)

At t_0, $t_0 = 0 \ldots$

General Expression

$$\psi_{init}(x) = C_1 \psi_0(x) + C_2 \psi_1(x)$$

Get coefficients by calculating overlap:

$$C_1 = \int_{-\infty}^{\infty} \psi_0 \psi_{init} \, dx, \quad C_2 = \int_{-\infty}^{\infty} \psi_1 \psi_{init} \, dx, \quad C_3 = \int_{-\infty}^{\infty} \psi_2 \psi_{init} \, dx, \quad C_4 = \int_{-\infty}^{\infty} \psi_3 \psi_{init} \, dx$$

$$C_1 = \int_{-\infty}^{-a} F_0 e^{\gamma_0 x} F_{init} e^{\gamma_{init} x} dx + \int_{-a}^{a} A_0 \cos(k_0 x) A_{init} \cos(k_{init} x) \, dx + \int_{a}^{\infty} F_0 e^{-\gamma_0 x} F_{init} e^{-\gamma_{init} x} dx$$

$$C_2 = \int_{-\infty}^{-a} F_1 e^{\gamma_1 x} F_{init} e^{\gamma_{init} x} dx + \int_{-a}^{a} B_1 \sin(k_1 x) A_{init} \cos(k_{init} x) \, dx + \int_{a}^{\infty} -F_1 e^{-\gamma_1 x} F_{init} e^{-\gamma_{init} x} dx$$

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

Numerical Integrator Results:

(Python code for integral in Github Repo)

$C_1 = 0.838546061$ $\quad C_2 = 0$ $\quad C_3 = -0.274176$ $\quad C_4 = 0$

Orthogonal to both odd solutions

Renormalize

$$|C_1|^2 + |C_3|^2 = 0.7783192405614446$$

So $|N|^2 (|C_1|^2 + |C_3|^2) = 1$, $N = 1.133489$

$\therefore$ $C_1 = N c_1$, $C_3 = N C_3$

since stationary wavefunctions are already normalized.

Finally normalized:

$$C_1 = 0.9504833 \quad c_2 = -0.310775563$$

where $|C_1|^2 + |C_3|^2 = 1$

Finally, add time dependency

$$\Psi_{init}(x,t) = C_1 \, \psi_0(x) e^{-iE_0 t/\hbar} + C_3 \, \psi_2(x) e^{-iE_2 t/\hbar}$$

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

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 $V_0 = 25$.

An instantaneous increase in the potential of the walls will increase the number of bound states, wavefunctions will adjust to the new potential (decay quicker in wall region as there is a stronger barrier), tunneling probability will decrease. It can also cause energy level transitions for bound states which can result in energy emission or absorption via photons.

Whereas a slow change from $V_0 = 1 \rightarrow V_0 = 25$ would allow the system to adjust smoothly. Bound states, wavefunctions, tunneling probabilities, and time evolution will change gradually. Transitions of bound state energy levels become likely to occur since under slow changes, the system will remain close to its instantaneous eigenstate.

This can be explained by the adiabatic theorem that undergoing slow change of a system's Hamiltonian (includes V_0) will remain in the Hamiltonian's energy eigenstate that corresponds to its initial energy eigenstate for its initial potential/Hamiltonian.