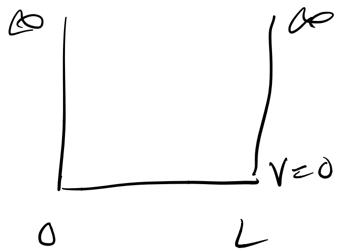
The Infinite Square Well (Reminder)

Earlier we solved for the values and eigenstates of the infinite square well potential.



⟸ Infinite Square well. Potential

- In solving this problem we found eigenvalues that were discrete (quantized) and yet infinite (no upper bound on "n")

$$\boxed{E_n = \frac{n^2\pi^2\hbar^2}{2mL^2} \qquad n > 1}$$

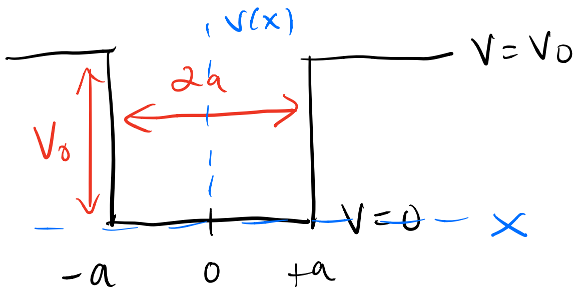
- In addition we made use of the position representation [$\varphi_n(x)$), which is a continuous function that represents each energy eigenstate.

$$\boxed{\langle x | E_n \rangle = \varphi_n(x) = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right)}$$

Here we see that though the position representation is continuous, the allowed eigenstates are discrete and infinite in number.

Pedagogically, the next most complicated potential is one where the walls are not infinite. That is the particle is bound in the <u>finite square well</u>.

Finite Square Well (Quantization Condition)



For the finite square well, we drop the walls down to a nominal level, $V = V_0$.

$$V = \begin{cases} V_0 & x < -a \\ 0 & -a < x < a \\ V_0 & x > a \end{cases}$$

This leads to two different descriptions of our problem → inside & outside the box,

$$\hat{H}\,\varphi_E(x) = E\varphi_E(x)$$

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + 0\right)\varphi_E(x) = E\varphi_E(x) \qquad (1)$$

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V_0\right)\varphi_E(x) = E\varphi_E(x) \qquad (2)$$

We can rewrite 1 & 2 in a way that 3 is similar,

$$\frac{d^2}{dx^2}\varphi_E(x) = \frac{-2mE}{\hbar^2}\varphi_E(x) \quad (1)$$

$$\frac{d^2}{dx^2}\varphi_E(x) = \frac{-2m(E-V_0)}{\hbar^2}\varphi_E(x) \quad (2)$$

We are only interested in "bound" states where $E < V_0$.*

* we will look at unbound states later

So $E > 0$ but $E < V_0$

For 1, this means,

$$\frac{d^2}{dx^2}\varphi_E(x) = -\underbrace{\left(\frac{2mE}{\hbar^2}\right)}_{>0}\varphi_E(x) \quad (1)$$

let $k^2 = \frac{2mE}{\hbar^2}$ like before. Then,

$$\frac{d^2\varphi_E(x)}{dx^2} = -k^2\varphi_E(x) \quad (1)$$

produces sinusoidal solutions as before

For 2, this means,

$$\frac{d^2}{dx^2}\varphi_E(x) = -\underbrace{\left(\frac{2m(E-V_0)}{\hbar^2}\right)}_{<0}\varphi_E(x) \quad ②$$

let $q^2 = \dfrac{2m(V_0-E)}{\hbar^2}$, $\Leftarrow$ switched order of E & V_0, then,

$$\frac{d^2\varphi_E(x)}{dx^2} = q^2\varphi_E(x) \quad ②$$

produces exponential solutions.

Thus, our general solution is,

$$\varphi_E(x) = \begin{cases} Ae^{qx} + Be^{-qx} & x<-a \\ C\sin(kx) + D\cos(kx) & -a<x<a \\ Fe^{qx} + Ge^{-qx} & x>a \end{cases}$$

Our job is now to find A, B, C, D, F, G & the allowed E's $\rightarrow$ k's & q's.

As before, we expect discrete E's and yet continuous φ's.

Solving the Boundary Value Problem

This seems like a lot of unknowns, but we can make our life easier by recognizing a few things.*

* We won't use the symmetry condition from pg. 130 in McIntyre

① $\psi_E(x)$ must be normalizable

$\Rightarrow \psi_E(x \to \pm\infty) = 0$

② $\psi_E(x)$ must be continuous

$\Rightarrow$ important at boundaries, $x = \pm a$

③ $\dfrac{d\psi_E(x)}{dx}$ must be continuous

$\Rightarrow$ important at boundaries, $x = \pm a$

Condition ① $\Rightarrow$ the exponential solutions must only decay, thus $B=0$ $(x<-a)$ & $F=0$ $(x>a)$

$$\psi_E(x) = \begin{cases} Ae^{\gamma x} & x < -a \\ C\sin kx + D\cos kx & -a < x < a \\ Ge^{-\gamma x} & x > a \end{cases}$$

Condition (2) gives two equations, (6)

$$\varphi_E(x=-a) = \varphi_E(x=-a)$$

$$Ae^{-qa} = C\sin(-ka) + D\cos(-ka)$$

$\cos(-x) = \cos(x)$
$\sin(-x) = -\sin(x)$

$$Ae^{-qa} = -C\sin(ka) + D\cos(ka)$$

$$\varphi_E(x=a) = \varphi_E(x=a)$$

$$C\sin(ka) + D\cos(ka) = Ge^{-qa}$$

$$\boxed{\begin{aligned} Ae^{-qa} &= -C\sin(ka) + D\cos(ka) \\ Ge^{-qa} &= C\sin(ka) + D\cos(ka) \end{aligned}}$$

2 equ's from continuity of φ_E

Condition (3) also gives two equations,

$$\left.\frac{d\varphi_E(x)}{dx}\right|_{x=-a} = \left.\frac{d\varphi_E(x)}{dx}\right|_{x=-a}$$

$$\left.\frac{d}{dx}\left(Ae^{+qx}\right)\right|_{x=-a} = \left.\frac{d}{dx}\left(C\sin(kx) + D\cos(kx)\right)\right|_{x=-a}$$

$$\left.qAe^{qx}\right|_{x=-a} = \left.kC\cos(kx) - kD\sin(kx)\right|_{x=-a}$$

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$$qAe^{-qa} = kC\cos(-ka) - kD\sin(-ka)$$

$$qAe^{-qa} = kC\cos(ka) + kD\sin(ka)$$

similarly for $\left.\frac{d\psi_E(x)}{dx}\right|_{x=a} = \left.\frac{d\psi_E(x)}{dx}\right|_{x=a}$ gives,

$$-qGe^{-qa} = kC\cos(ka) - kD\sin(ka)$$

$$\boxed{\begin{aligned} Ae^{-qa} &= \frac{k}{q}\left(C\cos(ka) + D\sin(ka)\right) \\ Ge^{-qa} &= \frac{-k}{q}\left(C\cos(ka) - D\sin(ka)\right) \end{aligned}}$$

2 eqns from continuity of $\frac{d\psi}{dx}$

OK with these 4 eqns,

(1) $Ae^{-qa} = -C\sin(ka) + D\cos(ka)$; $\psi_E(x=-a)$

(2) $Ge^{-qa} = C\sin(ka) + D\cos(ka)$; $\psi_E(x=a)$

(3) $Ae^{-qa} = \frac{k}{q}\left(C\cos(ka) + D\sin(ka)\right)$; $d\psi/dx\,(x=-a)$

(4) $Ge^{-qa} = -\frac{k}{q}\left(C\cos(ka) - D\sin(ka)\right)$; $d\psi/dx\,(x=a)$

Add 2 & 1, $2D\cos(ka) = (A+G)e^{-qa}$ 5

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Subtract 1 from 2, $2C\sin(ka) = (G-A)e^{-qa}$ 6

Add 3 & 4, $2D\sin(ka) = \frac{q}{k}(A+G)e^{-qa}$ 7

Subtract 4 from 3, $2C\cos(ka) = -\frac{q}{k}(G-A)e^{-qa}$ 8

substitute 5 into 7,

$$2D\sin(ka) = \frac{q}{k}\,2D\cos(ka))$$

or,

$$\boxed{2D\left(\sin(ka) - \frac{q}{k}\cos(ka)\right) = 0}$$

Similarly sub 6 into 8

$$2C\cos(ka) = -\frac{q}{k}(2C\sin(ka))$$

or

$$\boxed{2C\left(\cos(ka) + \frac{q}{k}\sin(ka)\right) = 0}$$

C & D cannot both be zero b/c then $\psi = 0$ inside the box.

Recall $C\sin(kx)$ and $D\cos(kx)$ are the solutions we are trying.

if $C \neq 0$ & $D = 0$ then we have pure odd solutions b/c $\sin(x)$ is odd.

in that case,

$$\cos(ka) + \frac{q}{k}\sin(ka) = 0$$

or

$$q = -k\,\frac{\cos(ka)}{\sin(ka)} = -k\cot(ka)$$

if $D \neq 0$ & $C = 0$ then we have pure even solutions b/c $\cos(x)$ is even.

in that case,

$$\sin(ka) - \frac{q}{k}\cos(ka) = 0$$

or

$$q = +k\,\frac{\sin(ka)}{\cos(ka)} = +k\tan(ka)$$

Ok we just did a ton of math! Why?

We seek the energy eigenvalues that satisfy $\hat{H}|E_n\rangle = E_n|E_n\rangle$.

What we have obtained are two equations that tell us the allowed energies,

$$\boxed{\begin{aligned} q &= -k\cot(ka) \\ q &= +k\tan(ka) \end{aligned}}$$

How do these equations give rise to energy eigenvalues?

Recall $k = \sqrt{\frac{2mE}{\hbar^2}}$ and $q = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}}$,

so that

$$\sqrt{\frac{2m(V_0 - E)}{\hbar^2}} = -\sqrt{\frac{2mE}{\hbar^2}} \cot\left(\sqrt{\frac{2mE}{\hbar^2}}\, a\right)$$

&

$$\sqrt{\frac{2m(V_0 - E)}{\hbar^2}} = \sqrt{\frac{2mE}{\hbar^2}} \tan\left(\sqrt{\frac{2mE}{\hbar^2}}\, a\right)$$

describe transcendental energy relationships. (everything is known except E!)

☆ We can plot these curves to find intersections on a graph or we can perform root finding by setting the whole equation to zero