Solutions to Elementary Quantum Systems

§ A Free Particle

Consider a particle with no potential. That is $V(x)=0$. Then

$$H\,\psi(x) = E\,\psi(x)$$

takes the form

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

ODE's of this form are solved by

$$\psi(x) = Ae^{\pm ikx}$$

for some k value. Hence

$$\frac{d^2}{dx^2}\left(Ae^{\pm ikx}\right) = -k^2\,\psi(x)$$

$$\Rightarrow \quad \frac{-\hbar^2}{2m}(-k^2)\psi(x) = E\,\psi(x)$$

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

So we have a continuous set of states! $-\infty < k < +\infty$.
But note we have an issue of normalization:

$$\int_{-\infty}^{+\infty} dx\,\psi^*(x)\,\psi(x) = \int_{-\infty}^{+\infty} |A|^2 e^{ikx} e^{-ikx}\,dx = \int_{-\infty}^{+\infty} |A|^2 dx$$

Thus, since $|A|^2$ must be a real, positive number, the integral diverges! So we know nothing about where the particle is in space because of this!

Note that $E = \frac{-\hbar^2}{2m}\frac{d^2}{dx^2} = \frac{\hat{p}^2}{2m}$

Hence $\psi(x)$ is actually an "eigenstate" of the momentum operator, so we know definitely what the momentum of the particle is; however we do not know anything about where it is in space! This is an example of the uncertainty principle.

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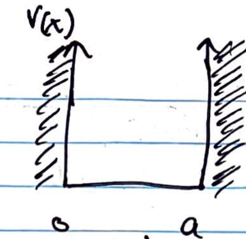
§ 1D Infinite Well potential



Let $V(x) = \begin{cases} 0 & 0 < x < a \\ \infty & \text{elese} \end{cases}$

Then outside the box, $\psi(x) = 0$ (must be). Inside the box, we have

$$H\psi(x) = E\psi(x)$$

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) = E\psi(x).$$

But we have just solved this! Namely

$$\psi(x) = Ae^{\pm ikx} \quad \text{for } k = \sqrt{\frac{2mE}{\hbar^2}}$$

A brief interlude,

$$e^{i\theta} = \cos\theta + i\sin\theta \quad \text{(Euler's identity)}$$

$$\frac{e^{i\theta} + e^{-i\theta}}{2} = \cos\theta \qquad \frac{e^{i\theta} - e^{-i\theta}}{2i} = \sin\theta$$

Hence, $\cos\theta + \sin\theta = \left(\frac{e^{i\theta} + e^{-i\theta}}{2}\right) + \left(\frac{e^{i\theta} - e^{-i\theta}}{2i}\right)$

So, since a linear combination, we must have

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

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

Must match $\psi(x)$ at the boundary. So $\psi(0) = \psi(a) = 0$.

$\psi(0) = A\cos(0) + B\sin(0) = A\cos(0) = A$.
So $A = 0$.

$\psi(a) = B\sin(ka) = 0 \Rightarrow \sin ka = 0 \Leftrightarrow ka = n\pi,\ n = 1, 2, \ldots$

So only certain allowed energies are allowed!

That is, $ka = n\pi \Rightarrow k = \frac{n\pi}{a}$ $\quad n=1,2,\dots$

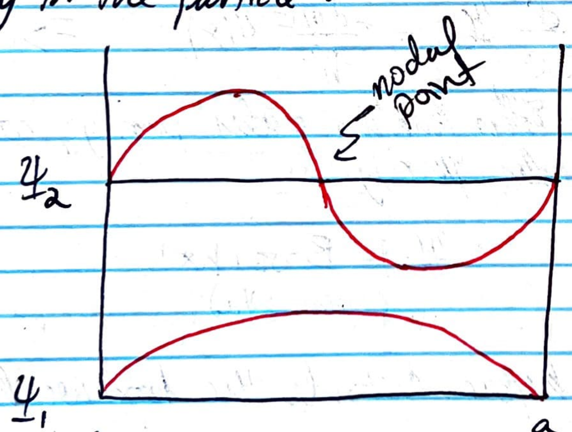
From before $k=\sqrt{\frac{2mE}{\hbar^2}} \Rightarrow$

$$\boxed{E_n = \frac{n^2\pi^2\hbar^2}{2ma^2}} \qquad n=1,2,\dots$$

If we enforce the normalization condition, $B=\sqrt{\frac{2}{a}}$. So

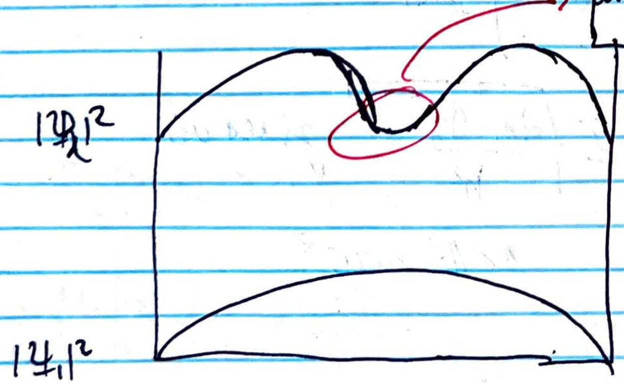
$$\boxed{\psi_n(x)=\sqrt{\frac{2}{a}}\sin\left(\frac{n\pi x}{a}\right)}$$ Energy states

Notice that $E_1 = \frac{\pi^2\hbar^2}{2ma^2} > 0$, so this is our zero-point energy. That is, we must have some amount of kinetic energy for the particle!

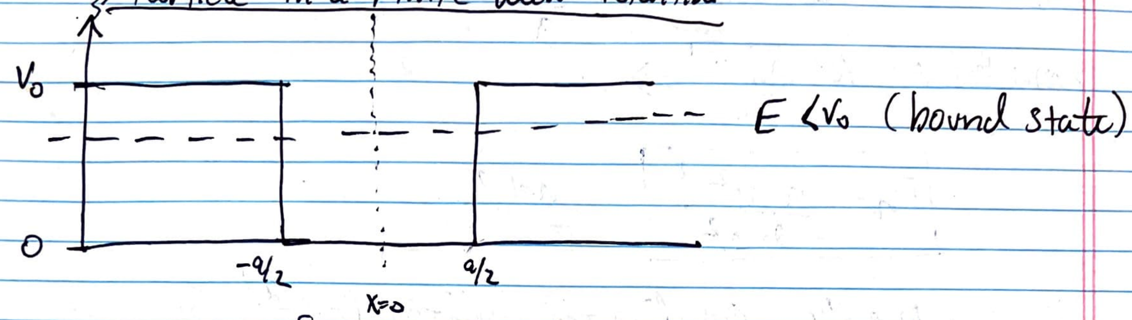


around the node, 0% chance to find particle at the node

probability density



§ Particle in a Finite Well Potential



$$V(x) = \begin{cases} 0 & -a/2 < x < a/2 \\ V_0 & \text{else} \end{cases}$$

For reasons which may not seem obvious, we seek solution of the bound state such that

$$\psi(x) = \pm \psi(-x)$$

Ie, even or odd under parity.

Inside the box, $\frac{d^2}{dx^2}\psi(x) = -\frac{2mE}{\hbar^2}\psi(x)$ $E > 0$.

Now, $\sin(x)$ is an ~~even~~ odd function under parity, $\cos(x)$ is an even function under parity. So

$\psi(x) = A\sin(kx)$ (odd) $\psi(x) = B\cos(kx)$ (even soln)

$k = \sqrt{\frac{2mE}{\hbar^2}}$, like before. Outside the box we have

$$\frac{d^2}{dx^2}\psi(x) = \frac{2m}{\hbar^2}\left[V_0 - E\right]\psi(x)$$

where $V_0 > E \Rightarrow \eta = \sqrt{\frac{2m(V_0-E)}{\hbar^2}}$ gives us

$$\psi(x) = e^{\pm\eta x}$$ $\eta \in \mathbb{R}$ now!

Outside the box

$$\psi(x) = \begin{cases} A'e^{\eta x} & x < -a/2 \\ A'e^{-\eta x} & x > a/2 \end{cases}$$

We don't have $\psi(x) = A' e^{\eta x} + B' e^{-\eta x}$ $x < -a/2$

since $e^{-\eta x} \to \infty$ as $x \to -\infty$. (Need them to go to zero for bound states. Hence

$$\psi(x) = \begin{cases} A' e^{\eta x} & x < -a/2 \\ A' e^{-\eta x} & x > a/2 \end{cases}$$

So $\psi_{in}(x = \pm a/2) = \psi_{out}(x = \pm a/2)$

and $\psi'_{in}(x = \pm a/2) = \psi'_{out}(x = \pm a/2)$

to ensure continuity of 1st & 2nd derivative of $\psi(x)$. If we match at $x = a/2$ for the <u>even</u> soln,

$$A\cos(ka/2) = A' e^{-\eta a/2}$$

$$-kA\sin(ka/2) = -\eta A' e^{-\eta a/2}$$

If we divide these eqn's, we get

$$k\tan\left(\frac{ka}{2}\right) = \eta$$

This actually is a condition on the bound state energies! Replace $\alpha = \frac{ka}{2}$, then $\Rightarrow$

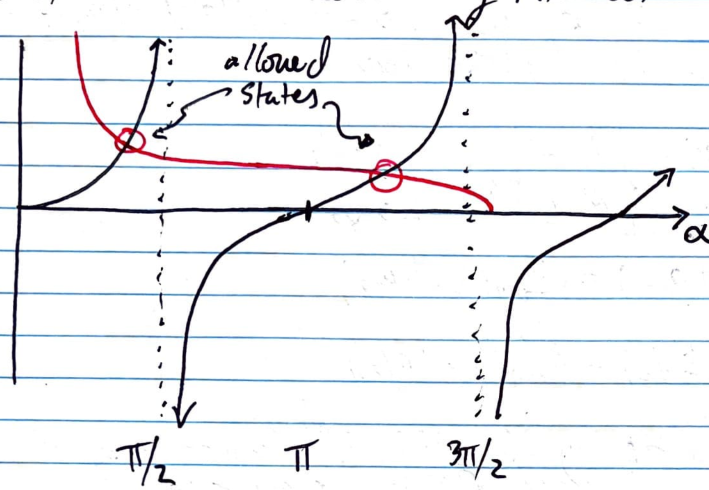
$$\tan(\alpha) = \frac{\eta a}{2\alpha}$$

Note that $\eta^2 = \frac{2mV_0 - 2mE}{\hbar^2} = C - k^2$, so

$$\frac{\eta a}{2} = \sqrt{\frac{Ca^2}{4} - \frac{k^2 a^2}{4}} = \sqrt{\frac{Ca^2}{4} - \alpha^2}$$

$\Rightarrow$ $\tan(\alpha) = \sqrt{\frac{\xi}{\alpha^2} - 1}$ with $\xi = \frac{mV_0 a^2}{2\hbar^2}$

This is a transcendental eqn. That is we can't solve this analytically, Need to solve numerically? Well, lets plot these function to see where they intersect.



Note, for even solutions, we are guaranteed to have a state $0 < \frac{ka}{2} < \frac{\pi}{2}$, we may also have some states

$$\frac{(2n-1)\pi}{2} < \frac{ka}{2} < \frac{(2n+1)\pi}{2} \quad \text{for } n = 1, 2, 3, \ldots$$

but only unless,

$$\frac{ka}{2} > \frac{a^2 m V_0}{2\hbar^2}$$

Lets solve numerically for $\xi = 100$ (note ξ is dimensionless!)

The minimum $\alpha = 1.428$ is where the graphs intersect. Hence

$$E_1 = \frac{2\hbar^2}{ma^2}(1.428)^2$$

$$\Rightarrow k = \frac{2.856}{a}$$

Then $\psi_{in}(x) = A\cos\left(\frac{2.856}{a}x\right)$

$$\eta = \frac{19.795}{a} \Rightarrow \psi_{out} = \begin{cases} A' e^{19.795/a\, x} & x < -a/2 \\ A' e^{-19.795/a\, x} & x > a/2 \end{cases}$$

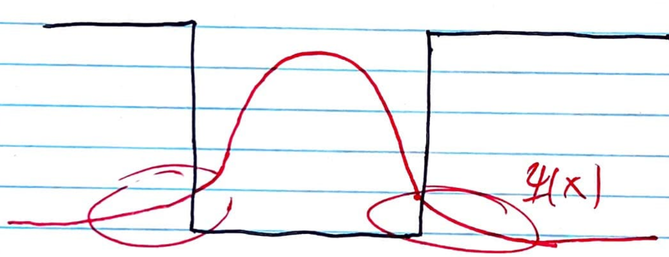
The A : A' have to due with normalization. In fact,

$$\frac{A}{A'} = \frac{e^{-19.795/2}}{\cos(1.428)} \simeq 3.5 \times 10^{-4}$$

by applying continuity at the boundary! So in fact

$$\psi_{out}(x) \neq 0$$

We have leakage! This is forbidden classically and ultimately implies there is a chance for the particle to leave the box:



The particle can leave the box (some probability)

This is a very small example of quantum tunneling.