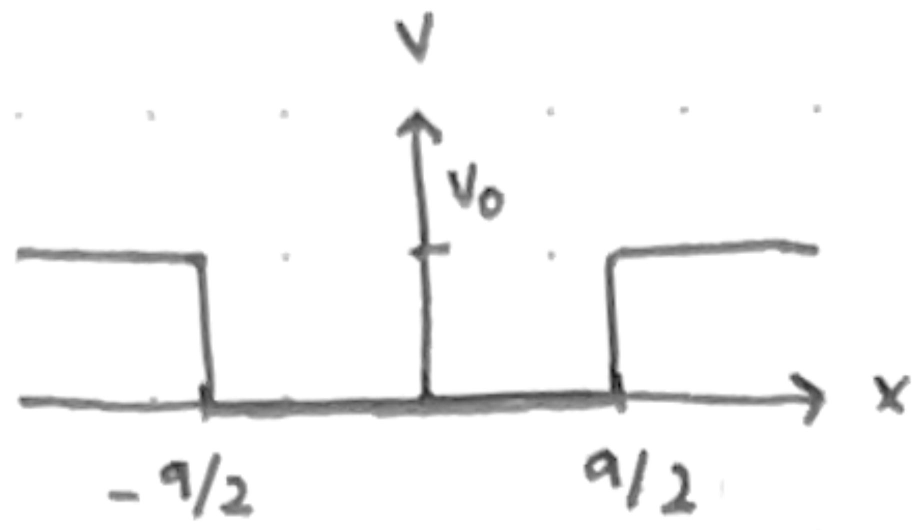
Week 12 - Some QM scenarios

Say we have a particle moving in 1D with the following potential:



$$V(x) = \begin{cases} V_0, & |x| > a/2 \\ 0; & |x| < a/2 \end{cases}$$

$$\hat{H} = \hat{P}^2/2m + V(\hat{x})$$

The spectum of $\hat{H}$ is:

- obviously real
- Not less than minimum V: $E < \min_{x \in \mathbb{R}} V(x) \Rightarrow E \notin \sigma(\hat{H})$

- for $0 < E < V_0$: $\mu(V^{-1}(\varepsilon < E)) = a < \infty$
  This says there is a finite set of values for x where the energy is between 0 and V_0. To be precise, their width / range is a.
  (also, $V^{-1}(\varepsilon < E) = \{x \mid \underline{V(x) < E}\}$
  This is the "classically accessible region", meaning kinetic energy is non-negative: $E = KE + PE$, $KE = E - PE$, so we want $\underline{V < E}$.

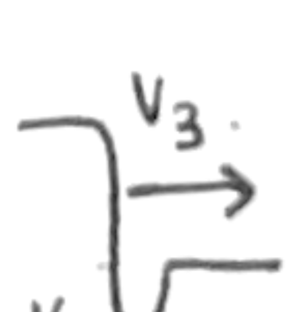
also this

- for $E > V_0$, $\mu(V^{-1}(\varepsilon < E)) = \infty$, since the "anti-image" / x values span the entire real axis. The associated E's are doubly degenerate since you can travel to $-\infty$ or $+\infty$, left/right.
- As mentioned, for $E < 0$, $\mu(V^{-1}(\varepsilon < E)) = 0$
- Within our classically accessible regions, are the values of E discrete or continuous?

If E is between 0 and V_0, x has to be from $-a/2$ to $a/2$. This means the wave function for <u>all</u> states where E is between 0 and V_0 <u>must</u> be <u>smooth</u> at $-a/2$ and $a/2$, $\therefore$ E's are <u>discrete</u>.

(Not the infinite potential well, so outside $-a/2 < x < a/2$, we can still have some wavefcn to describe the outside of the well. Classically, $0 < E < V_0$, $x < -a/2$ or $x > a/2$ would never happen, but this is QM!)

For $E > V_0$, No such condition is necessary, so it is <u>continuous</u>.

Note that a potential like this: 

is not degenerate for energies between V_1 & V_3, since you only move to the right. For $E > V_3$, though, you're doubly degenerate again.

Anyway. What is $\psi_E(x)$ for this potential? ($\psi_E(x)$ being $\langle x|\psi_E\rangle$ for $\hat{H}|\psi_E\rangle = E|\psi_E\rangle$ ...)

$$\langle x|\hat{H}|\psi_E\rangle = E\langle x|\psi_E\rangle = E\,\psi_E(x)$$

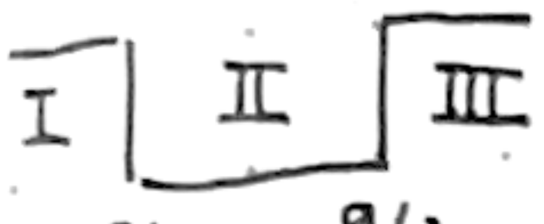
$$\langle x|\frac{\hat{p}^2}{2m}+V(\hat{x})|\psi_E\rangle = \left(\frac{1}{2m}\left(-i\hbar\frac{d}{dx}\right)^2 + V(x)\right)\langle x|\psi_E\rangle$$

$$= \left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)\right)\psi_E(x)$$

equating these two:

$$E\,\psi_E(x) = -\frac{\hbar^2}{2m}\psi_E''(x) + V(x)\,\psi_E(x)$$

we get a second order differential equation. To solve this, we consider the following three sections:



for $0 < E < V_0$, where we want continuity and know E's are discrete.

$$\psi(x) = \begin{cases} \psi_I(x) & x < -a/2 \\ \psi_{II}(x) & |x| < a/2 \\ \psi_{III}(x) & x > a/2 \end{cases}$$

I: $V(x)$ is V_0 for I (all $x < -a/2$), so:

$$E\,\psi_I(x) = -\frac{\hbar^2}{2m}\psi_I''(x) + V_0\,\psi_I(x)$$

$$\psi_I''(x) = \frac{(V_0 - E)2m}{\hbar^2}\psi_I(x), \text{ call } \beta = \sqrt{\frac{2m(V_0-E)}{\hbar^2}}, \text{ so}$$

$\psi_I'' = \beta^2\psi_I$ which has solution $\psi_I = A_1 e^{\beta x} + A_2 e^{-\beta x}$

we're considering $0 < E < V_0$, so $V_0 - E$ is positive and β is positive. However, in region I, x is negative. so βx is negative, $-\beta x$ is positive. $A_2 e^{-\beta x}$ then blows up as x goes to $-\infty$ (we constrained I so x can't go to $+\infty$). So $\underline{A_2 = 0}$ (we want $\underbrace{\int|\psi(x)|^2 dx = 1}_{\text{probability}}$ so we can't have any terms blow up!)

II: $V(x) = 0$ in this region, so:

$\psi_{II}'' = -\frac{2mE}{\hbar^2}\psi_{II}$ which has solution $\psi_{II} = B_1 e^{ikx} + B_2 e^{-ikx}$ for

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

III: Now, like I, $V_0 = V(x)$, so:

$\psi''_{\mathrm{III}} = \beta^2 \psi_{\mathrm{III}} \longrightarrow \psi_{\mathrm{III}} = C_1 e^{\beta x} + C_2 e^{-\beta x}$

since this time, x is positive, $C_1 e^{\beta x}$ blows up and so $C_1 = 0$.

We now have that:

$$\psi_I = A_1 e^{\beta x}, \quad \psi_{\mathrm{II}} = B_1 e^{ikx} + B_2 e^{-ikx}, \text{ and } \psi_{\mathrm{III}} = C_2 e^{-\beta x}$$

and need to find A_1, C_2, B_1, and B_2. We do this via boundary conditions: continuity!

$$\psi''(x) = \frac{2m(V(x)-E)}{\hbar^2}\psi(x) \text{ and we want:}$$

$$\psi'(x+\varepsilon) = \psi'(x-\varepsilon) + \int_{x-\varepsilon}^{x+\varepsilon} \underbrace{\frac{2m(V(x)-E)}{\hbar^2}\psi(x)}_{\text{both of these are bounded}} dx \text{ as } \varepsilon \to 0 \text{ to}$$

be true (so integral $\to 0$)

so ψ' is continuous and ψ is then also continuous.

Specifically,

$$\psi_I(-a/2) = \psi_{\mathrm{II}}(-a/2) \text{ and } \psi'_I(-a/2) = \psi'_{\mathrm{II}}(-a/2)$$

$$\psi_{\mathrm{II}}(a/2) = \psi_{\mathrm{III}}(a/2) \text{ and } \psi'_{\mathrm{II}}(a/2) = \psi'_{\mathrm{III}}(a/2)$$

which gives relative magnitudes of A_1, C_2, B_1, B_2, and also enforces discrete $\sigma(\hat{H})$ between $\pm a/2$ for $0 < E < V_0$.

There's a long, tedious derivation, but quickly, we can exploit symmetry: we have symmetry via reflection over $x=0$, and:

$$\hat{\Pi}|x\rangle = |-x\rangle, \ [\hat{H}, \hat{\Pi}] = 0, \ \hat{H}(\hat{\Pi}|\psi\rangle) = E\hat{\Pi}|\psi\rangle$$

define $|\psi_\pm\rangle \equiv |\psi\rangle \pm \hat{\Pi}|\psi\rangle$ which can be even or odd, say we choose even to make things easier...

if even, $\psi(x) = \psi(-x)$, so $\psi_I(x) = \psi_{\mathrm{III}}(-x)$ and $\psi_{\mathrm{II}}(-x) = \psi_{\mathrm{II}}(x)$.

Meaning $A_1 = C_2 = C$ and:

$$B_1 e^{-ikx} + B_2 e^{ikx} = B_1 e^{ikx} + B_2 e^{-ikx}, \quad B_1 = B_2 \ \forall |x| < a/2$$

(in the odd case, $B_1 = -B_2$ instead.)

so: $\psi_{II} = B(e^{-ikx} + e^{ikx}) = B(2\cos(kx))$ and very simply,

$\psi_{III} = Ce^{-\beta x}$, so we can now enforce the second boundary condition.

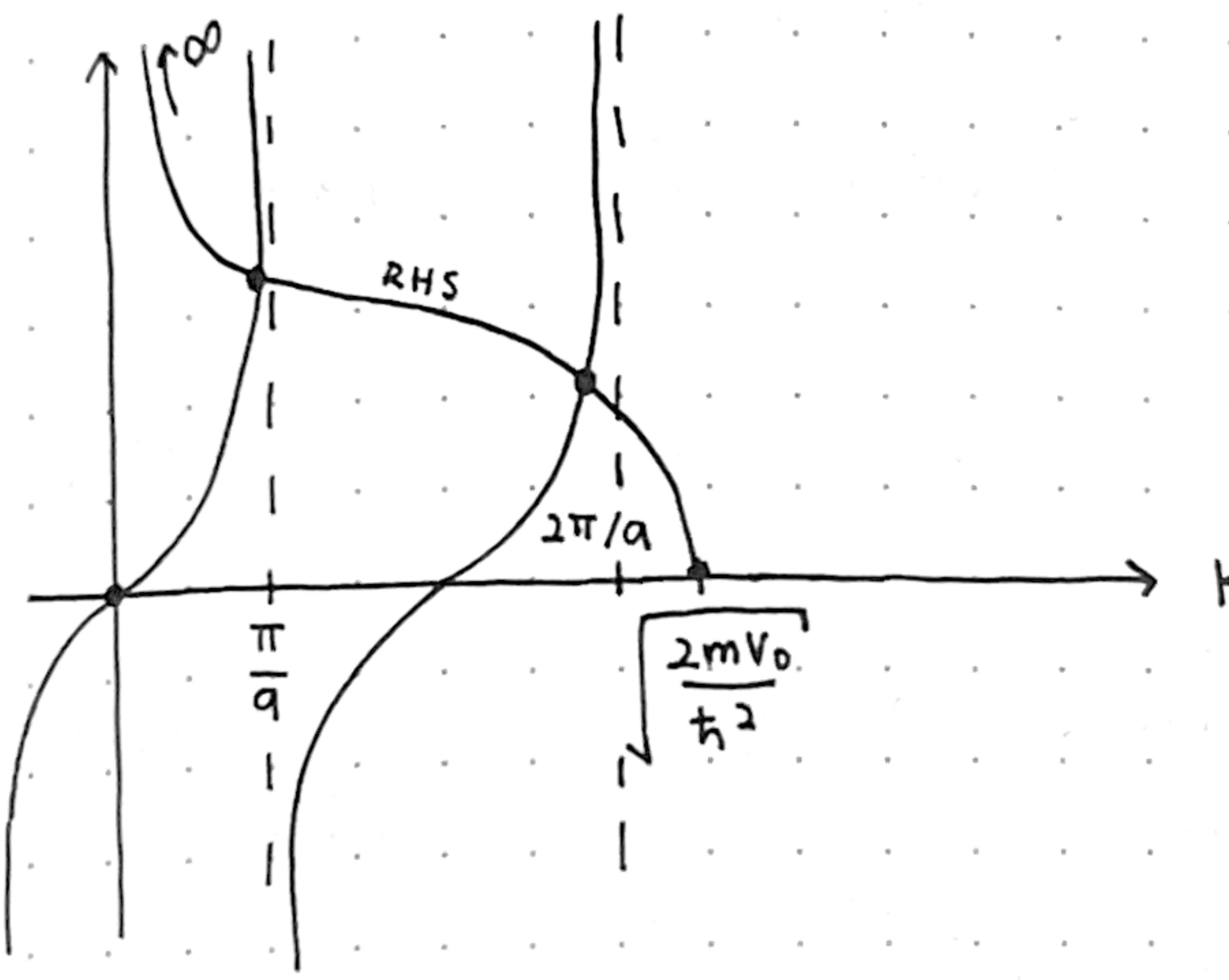
① $2B\cos(k\,a/2) = Ce^{-\beta a/2}$ and ② $-2Bk\sin(k\,a/2) = -\beta Ce^{-\beta a/2}$

②/① gives: $k\tan(ka/2) = \beta$ and we know β already:

$$k\tan(ka/2) = \sqrt{\frac{2m(V_0-E)}{\hbar^2}} = \sqrt{\frac{2mV_0}{\hbar^2} - k^2}$$

$$\tan(ka/2) = \sqrt{\frac{2mV_0}{(\hbar k)^2} - 1}$$, which is always real because we say $0 < E < V_0$, and $\frac{2mV_0}{(\hbar k)^2} = \frac{2mV_0\hbar^2}{\hbar^2 2mE} = \frac{V_0}{E} > 1$.

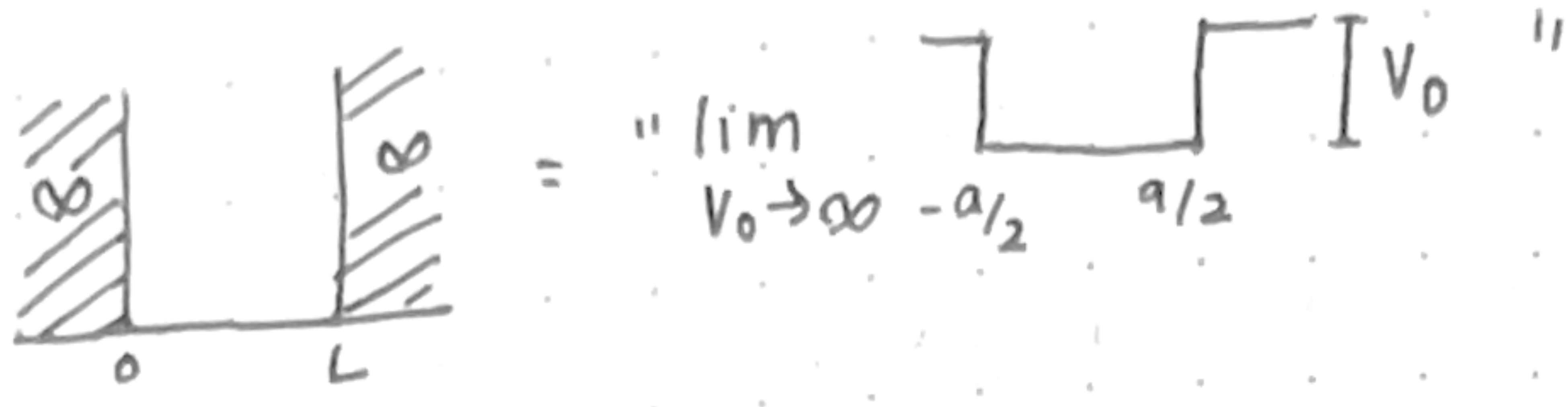
a trig fcn = polynomial is not analytically solvable (it's a transcendental fcn!) but graphically:



- $\tan(x)$ has asymptotes $\pi/2, 3\pi/2$, etc. so $\tan(ka/2)$ has π/a, $\pi/a + 2\pi/a$, etc.
- the largest possible k is $\sqrt{\frac{2mV_0}{\hbar^2}}$ since a sqrt can never yield a value less than 0.

we can see there are intersections, so bound states. If $k_{max} >> \pi/a$, you can approximate analytically, and clearly increasing a or increasing V_0 will lead to more bound states.

Particle in a box



$$V(x) = \begin{cases} \infty & x<0,\ x>L \\ 0 & 0<x<L \end{cases}$$

Eigenstates of $\hat{H}$: conditions are $\psi(0) = \psi(L) = 0$ and $\psi'(0^+) \neq 0$ $\psi'(L^-) \neq 0$ (else we have a perfectly flat line?)
*Also, no longer $L^2(\mathbb{R})$ but $L^2([0,L])$

$$\hat{H}|\psi\rangle = E|\psi\rangle$$
$$\langle x|\hat{H}|\psi\rangle = \langle x|E|\psi\rangle \rightarrow -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) = E\psi(x)$$

so:
$$\psi'' = -\frac{2m}{\hbar^2}E\psi \rightarrow \psi'' + \frac{2mE}{\hbar^2}\psi = 0$$

call $k = \sqrt{2mE/\hbar^2}$, then we have known solution:

$$\psi = A\sin(kx) + B\cos(kx)$$ (same as II from finite well!)

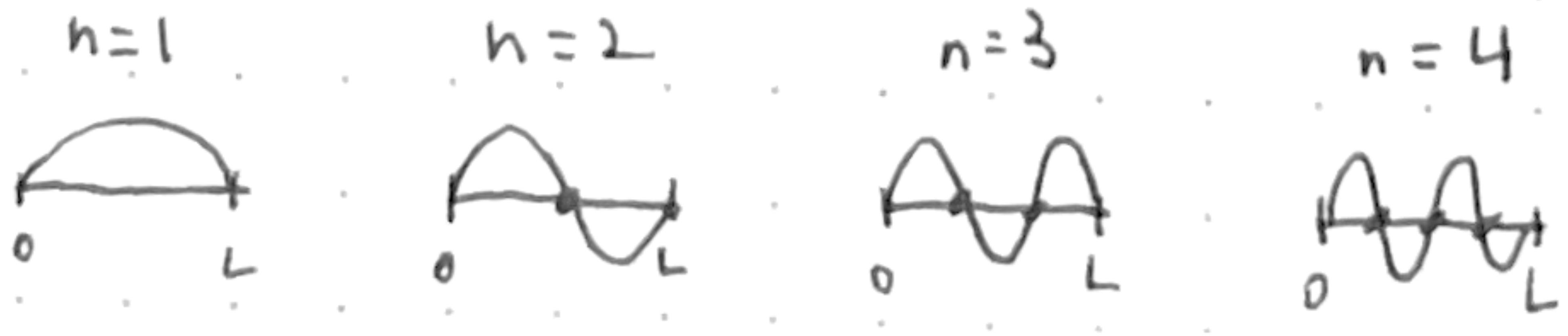
To enforce $\psi(0)=0$, $B=0$ since $\cos(0)=1$.
To enforce $\psi(L)=0$, $A\sin(kL)=0$ without $A=0$ (else zero vector)
which means $kL = n\pi$, or
$$k_n = n\pi/L$$
where $n \neq 0$ (else zero vector again) and $-n$ gives no new info that n doesn't give ($\sin(-x) = -\sin(x)$ ...) so, $n \in \mathbb{N}$.
↳ square mod is the same!

What is A? want $\langle\psi_n|\psi_n\rangle = 1$, so:

$$1 = \int_0^L A_n^2 \sin^2\left(\frac{n\pi}{L}x\right)dx = A_n^2\left[\frac{1}{2}\left(x - \frac{L}{2n\pi}\sin\left(\frac{2n\pi}{L}x\right)\right)\right]_0^L$$

$$1 = A_n^2\frac{L}{2} \rightarrow A_n = \sqrt{\frac{L}{2}}$$

Can also find E_n: $k_n = \frac{n\pi}{L} = \sqrt{\frac{2mE_n}{\hbar^2}} \rightarrow E_n = \frac{\hbar^2\pi^2}{2mL^2}n^2$
which means E_n increases quadratically with n.
Also, $\psi(x)$:



- the number of nodes increases linearly with n
- states are alternatingly even or odd, also non-degenerate.

(if we centered box @ $x=0$, $[\hat{H},\hat{\Pi}]=0$, even/odd as in finite well!)

Because non-degenerate, $\hat{H} = \sum_{\lambda \in \sigma(\hat{H})} \lambda \hat{P}_\lambda = \sum_{n=1}^{\infty} E_i |\psi_n\rangle\langle\psi_n|$

and $\hat{U}(t) = e^{-i\hat{H}t/\hbar} = \sum_{n=1}^{\infty} e^{iE_nt/\hbar} |\psi_n\rangle\langle\psi_n|$

which has phase factor $e^{iE_nt/\hbar}$ that is sometimes 1 for some values of t!!

$$\frac{E_nT}{\hbar} = \frac{\pi\hbar}{4mL^2} T\,(2\pi n^2) \longrightarrow \text{for } T = \frac{4mL^2}{\pi\hbar},\ \frac{E_nT}{\hbar} = 2\pi n^2$$

so:

$$\hat{U}(\overset{T}{t}) = \sum_{n=1}^{\infty} e^{i2\pi n^2} |\psi_n\rangle\langle\psi_n| = \sum_{n=1}^{\infty} |\psi_n\rangle\langle\psi_n| = \hat{1}$$

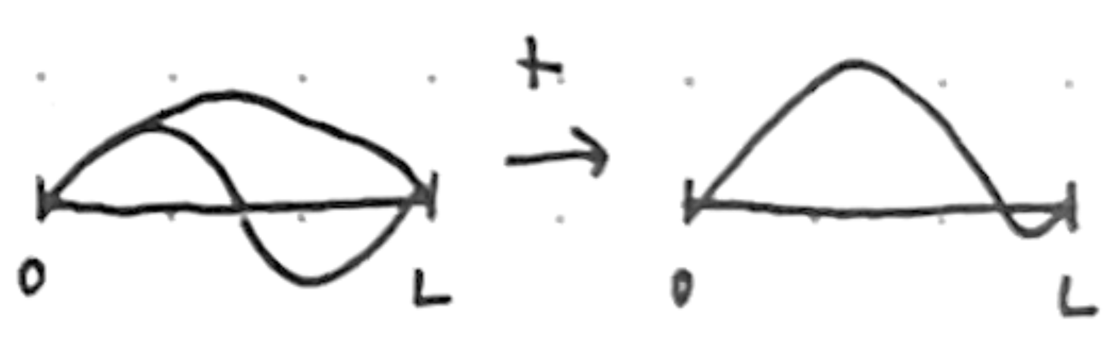
(in the basis of $\hat{H}$'s eigenfunctions)

This means at very special times T, the evolved $\psi(x)$ looks just like the original $\psi(x)$: "revival"

There are infinitey many n's, so infinitely many T's.)

Dynamics!

$|\psi(t=0)\rangle = \frac{1}{\sqrt{2}}(|\psi_1\rangle + |\psi_2\rangle)$

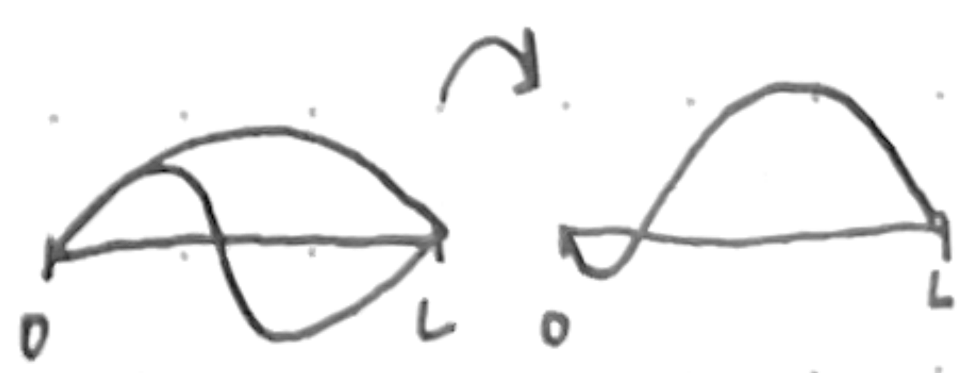


is skewed to the left, meaning particle is more likely to be found on the LHS of the box. Also the wavefcn is no longer even or odd.

After evolution:

$|\psi(t)\rangle = \frac{1}{\sqrt{2}} e^{-iE_nt/\hbar}(|\psi_1\rangle + e^{-i\omega_{21}t}|\psi_2\rangle)$

$|\psi(\frac{\pi}{\omega_{21}})\rangle = \frac{1}{\sqrt{2}} e^{-iE_nt/\hbar}(|\psi_1\rangle - |\psi_2\rangle)$



now the particle is more likely on the RHS.

(Makes sense if particle bounces back and forth in box)

$$\langle \hat{x} \rangle_{\psi(t)} = \frac{1}{2}\left(\langle \psi_1| + e^{i\omega_{21}t}\langle \psi_2|\right)\hat{x}\left(|\psi_1\rangle + e^{-i\omega_{21}t}|\psi_2\rangle\right)$$

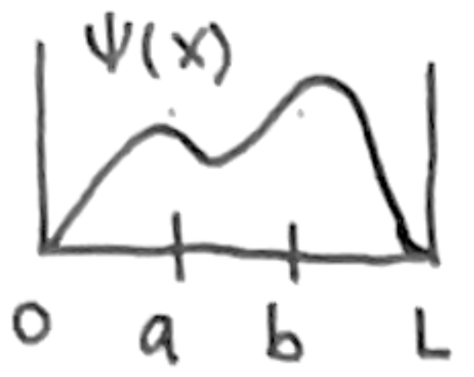
$$= \frac{1}{2}\left(\frac{L}{2} + \frac{L}{2} + e^{i\omega_{21}t}\langle \psi_2|\hat{x}|\psi_1\rangle + e^{-i\omega_{21}t}\langle \psi_1|\hat{x}|\psi_2\rangle\right)$$

$$= \frac{L}{2} + \langle \psi_2|\hat{x}|\psi_1\rangle \cos(\omega_{21}t)$$

where $\langle \psi_2|\hat{x}|\psi_1\rangle$ is matrix element: $\frac{2}{L}\int_0^L x \sin\left(\frac{\pi x}{L}\right)\sin\left(\frac{2\pi x}{L}\right) dx$

$\hat{H}^{-1}$ is also well-defined: $\hat{H}^{-1} = \sum_{n=1}^{\infty} \frac{1}{E_n}|\psi_n\rangle\langle\psi_n|$ and has the same eigenstates; the eigenvalues just converge like $1/n^2$, instead. So this is a compact operator, and the simplest case where you can demonstrate the spectral theorem.

Problems with particle in a box:



The probability of finding the particle between a and b for some $\psi(x)$, as described by the QM postulates, is:

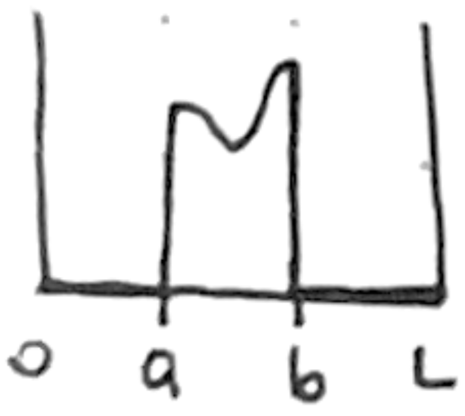
$\langle \psi|\hat{P}_{[a,b]}|\psi\rangle$ where $\hat{P}_{[a,b]} = \int_a^b dx\, |x\rangle\langle x|$, which is $\int_a^b |\psi(x)|^2 dx$

after measurement, the system is then in state:

$$|\psi\rangle \mapsto |\psi'\rangle = \hat{P}_{[a,b]}|\psi\rangle, \quad \psi'(x) = \langle x|\int_a^b dx'\,|x'\rangle\langle x'|\psi\rangle$$

$$\psi'(x) = \begin{cases} 0 & \text{if } x \notin [a,b] \\ \psi(x) & \text{if } x \in [a,b] \end{cases}$$

So it looks like:



Now the function is discontinuous and not in the domain of $\hat{H}$ anymore. We can still find $\langle \hat{H}\rangle$:

$$\frac{\langle \hat{H}\rangle_{\psi'}}{\langle \psi'|\psi'\rangle} = \frac{\sum_{n=0}^{\infty} E_n |\langle \psi_n|\psi'\rangle|^2}{\int_a^b |\psi|^2 dx} = \infty$$

because $E_n \propto n^2$ and that blows up faster than the other term decays. Thus, measurement appears to put the system into a state with infinite energy, which evidently is not possible.

We can still do $\hat{U}(t)|\psi'(t=0)\rangle$ since unitary operators are defined everywhere, but we cannot project into the position basis, so we're stuck.

second. $\langle x|\hat{p} = -i\hbar \frac{d}{dx} \langle x|$ is not an observable anymore. For some function ϕ and state ψ

$$\langle \phi|\hat{p}|\psi\rangle = \int_0^L -i\hbar\, \phi^* \frac{d}{dx} \psi\, dx = -i\hbar \left[\phi^*(x)\psi(x)\right]_0^L + i\hbar \int_0^L \frac{d}{dx}\phi^* \psi\, dx$$

(integration by parts)

$$= -i\hbar \left[\phi^*(x)\,\psi(x)\right]_0^L + \left(\int_0^L \psi^* \frac{d\phi}{dx}(-i\hbar)\right)^*$$

$$= -i\hbar \left[\phi^*(x)\,\psi(x)\right]_0^L + \langle\psi|\hat{p}|\phi\rangle^* = \langle\psi|\hat{p}|\phi\rangle^*$$

(since $\psi(0) = \psi(L) = 0$ for any $\psi(x)$ that can exist.)

The adjoint of $\hat{p}$ is defined, but the domain of $\hat{p}^\dagger \neq$ domain of $\hat{p}$. $\hat{p}$ takes $|\psi\rangle$ which is restricted on $[0, L]$. $\hat{p}^\dagger$ takes $|\phi\rangle$, which only needs to be continuous and integrable over $[0, L]$, it has no boundary condition.

Here, $\hat{p}$ is Hermitian but not self-adjoint!

Intuitively, $\langle x|p\rangle$ (eigenstates of $\hat{p}$ in pos. basis) are not possible in the infinite potential well; $e^{ipx/\hbar}/\sqrt{2\pi\hbar}$ is not 0 for $x = 0$ or $x = L$. So, we are never going to be in an eigenstate of momentum, and so we cannot measure momentum!!

$\hat{T}_{\Delta x}$ is also no longer unitary because it can shift wave functions out of the well; it is no longer surjective so it cannot be unitary.