Quantum Physics 1
Class 14

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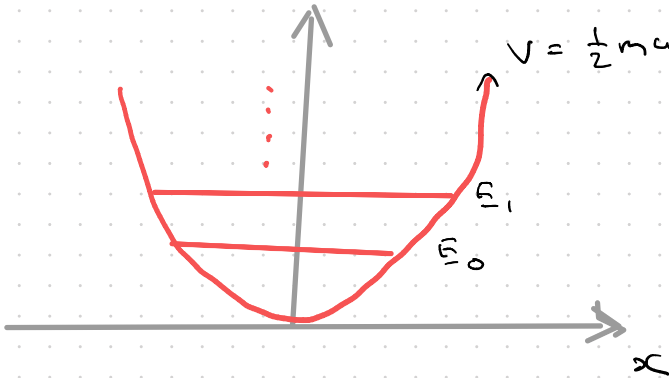
Finite Potential Well

Last Time:

Quantum Harmonic Oscillator:

$V = \frac{1}{2} m\omega^2 x^2 \sim \frac{1}{2} k x^2$



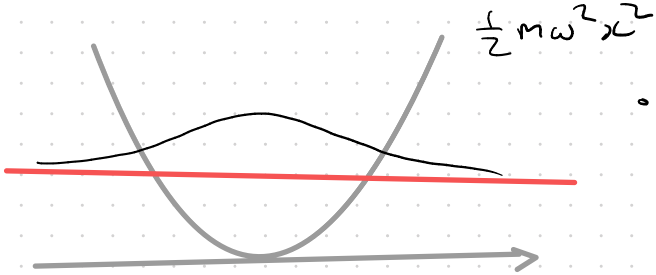
$$\left[-\frac{\hbar^2}{2M}\frac{d^2}{dx^2} + \underbrace{V(x)}_{\frac{1}{2} m\omega^2 x^2}\right]\varphi(x) = E\,\varphi(x)$$

w/ $$\varphi_n(x) = A_n \underbrace{H_n\left(\sqrt{\frac{m\omega}{\hbar}}\,x\right)}_{\text{Hermite Polynomial}} e^{-m\omega x^2/2\hbar}$$

& $$E_n = \left(n + \frac{1}{2}\right)\hbar\omega \quad ; \quad n = 0, 1, 2, 3, \dots$$

where $$\int \varphi^*_{n'}\,\varphi_n(x)\,dx = 0 \quad ; \quad n \neq n'$$

Recall the ground state:

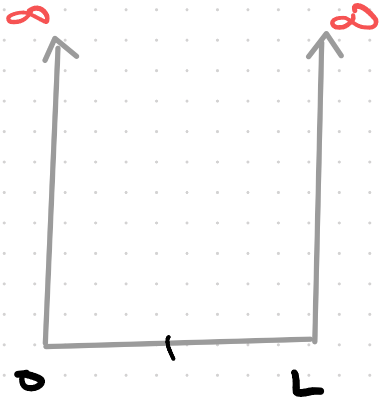


- probability density is not time dependent.
- $\Delta p \Delta x = \hbar/2$

Consider kinetic energy versus potential energy:

Kinetic Energy
$$\langle T \rangle = \langle \tfrac{1}{2}mv^2 \rangle$$
$$= \langle p^2/2m \rangle = \frac{1}{2m}\langle p^2 \rangle$$
$$= \frac{1}{2m}\left(\frac{m\omega\hbar}{2}\right) = \frac{\hbar\omega}{4}$$

Potential Energy
$$\langle V \rangle = \langle \tfrac{1}{2}m\omega^2x^2 \rangle$$
$$= \frac{1}{2}m\omega^2\left[\frac{1}{2\pi}\cdot\frac{1}{\left(\frac{m\omega}{\pi\hbar}\right)}\right]$$
$$= \frac{\hbar\omega}{4}$$



Recall for infinite square well

$$E_n = \frac{n^2 \pi^2 \hbar^2}{2mL^2} \;; \quad \varphi_n = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right)$$

? Is $-L/2 < x < L/2$

Should be equivalent!

Consider:

$$-\frac{L}{2} < x < \frac{L}{2} \;; \quad \frac{d^2\varphi(x)}{dx^2} = -k^2 \varphi(x) \;, \quad k = \frac{\sqrt{2mE}}{\hbar}$$

$$\ \& \quad \varphi(x) = Ae^{ikx} + Be^{-ikx}$$

$$= A\left[\cos kx + i \sin kx\right] + B\left[\cos kx - i \sin kx\right]$$

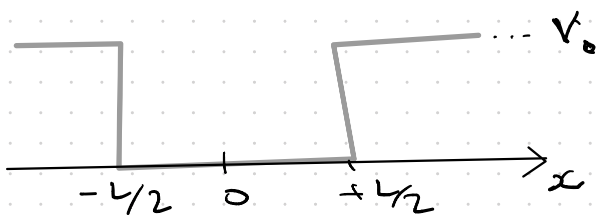
$$= (A+B) \cos kx + (A-B)\, i \sin kx$$

Where $-\frac{L}{2} < x < \frac{L}{2}$;

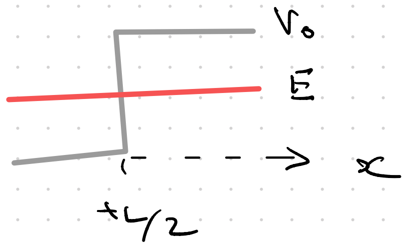
$$-\frac{\hbar^2}{2m} \frac{\partial^2 \varphi}{\partial x^2} = E\varphi \;; \quad E > 0 \,, \quad k > 0$$

w/ $k = \sqrt{2mE}/\hbar$

Now, consider the finite Square Well:



For $x > +\frac{L}{2}$



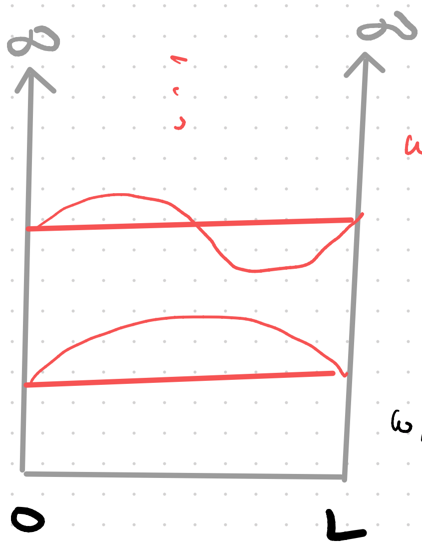
$$-\frac{\hbar^2}{2m}\frac{d^2\varphi}{dx^2} = \underbrace{-(E-V_0)}_{-k'}\varphi(x)$$

$$\Rightarrow -\frac{\hbar^2}{2m}\frac{d^2\varphi}{dx^2} = -k'\varphi(x)$$

- What are the eigenfunctions?
- What are the eigenvalues?

Consider again the ∞ square well:

(1)



w/t $\frac{d^2\varphi(x)}{dx^2} = -k^2\varphi(x)$

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

w/t ansatz:

$\varphi(x) = Ae^{ikx} + Be^{-ikx}$

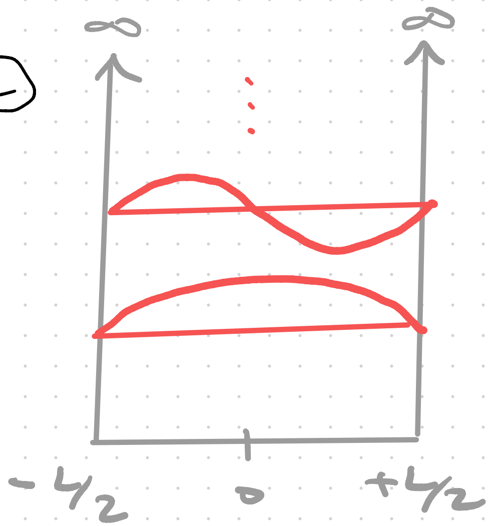
B.C.: w/t $\varphi(x=0) = \varphi(x=L) = 0$

yields: $A = -B$; $k_n = \frac{n\pi}{L}$

& $\varphi_n(x) \sim \sin\left(\frac{n\pi x}{L}\right)$;

$$E_n \sim \frac{n^2\pi^2\hbar^2}{2mL^2}$$

2



$$\varphi(x) = Ae^{ikx} + Be^{-ikx}$$

$$= A[\cos kx + i\sin kx]$$

$$+ B[\cos kx - i\sin kx]$$

$$= (A+B)\cos kx +$$

$$(A-B)\, i\sin kx$$

In-class 14-1

Boundary Conditions:

@ $x = +L/2$:

$$\varphi\left(\tfrac{L}{2}\right) = (A+B)\cos k\tfrac{L}{2} + (A-B)\, i\sin k\tfrac{L}{2} = 0$$

will only hold if $A+B=0$ or $A-B=0$

(i) $A + B = 0$:

$$\sin k\frac{L}{2} = 0 \Rightarrow \frac{kL}{2} = \pi, 2\pi, 3\pi, \ldots$$

$$\therefore \quad k = \frac{1}{L}(2\pi, 4\pi, 6\pi, \ldots)$$

$$k_n = \frac{n\pi}{L}\,; \quad n = 2, 4, 6, \ldots$$

[Even #]

(ii) $A - B = 0$:

$$\cos k\frac{L}{2} = 0 \Rightarrow \frac{kL}{2} = \frac{\pi}{2}, \frac{3\pi}{2}, \frac{5\pi}{2}, \ldots$$

$$k = \frac{1}{L}(\pi, 3\pi, 5\pi, \ldots)$$

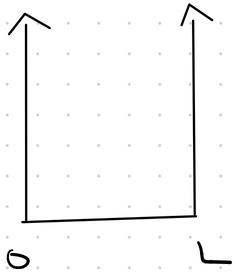
$$k = \frac{n\pi}{L}\,; \quad n = 1, 3, 5, \ldots$$

[ODD #]

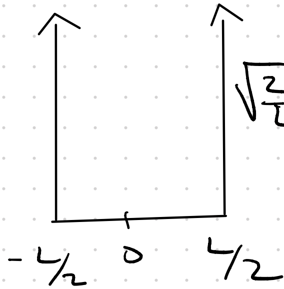
Summary:

$$\varphi_n(x) = \begin{cases} \left.\begin{array}{ll} \sqrt{\frac{2}{L}}\cos\frac{n\pi}{L}x, & n = 1, 3, 5, \ldots \\ \sqrt{\frac{2}{L}}\sin\frac{n\pi}{L}x\,; & n = 2, 4, 6, \ldots \end{array}\right\} & -\frac{L}{2} \le x \le \frac{L}{2} \\ 0 & , \text{elsewhere} \end{cases}$$

Compare ground state for two cases:



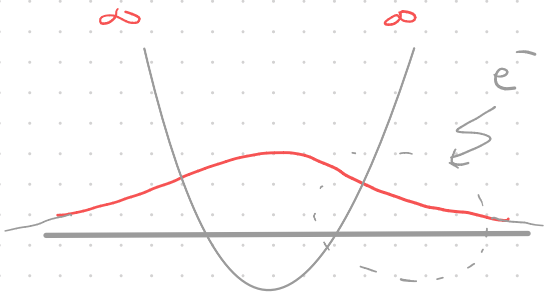
$\sqrt{\frac{2}{L}} \sin \frac{\pi x}{L}$



$\sqrt{\frac{2}{L}} \cos \frac{\pi x}{L}$

$$E_n = \frac{n^2 \pi^2 \hbar^2}{2mL^2}$$

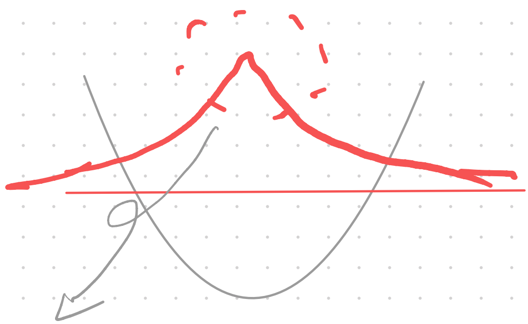
Recall: Harmonic oscillator



e^{-ax^2}

Need to choose e^{-ax^2} as the ground state.

- consider using e^{-ax}?



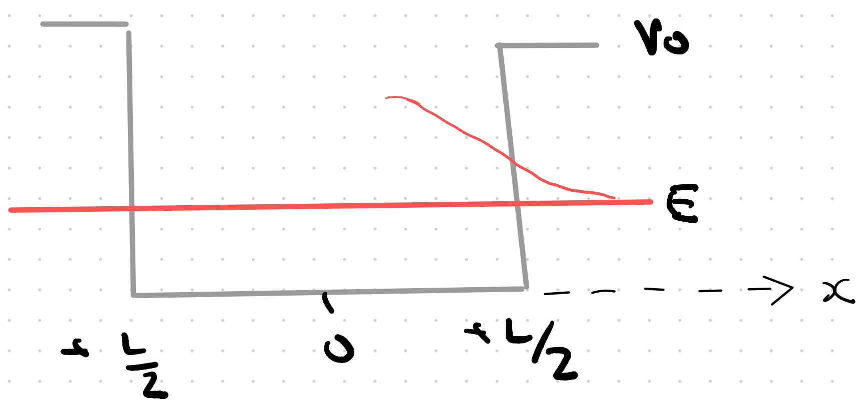
BAD: Discontinuous

1. Discontinuous
2. won't satisfy

$$-\frac{\hbar^2}{2m}\frac{\partial^2 \varphi}{\partial x^2} + \frac{1}{2}k_0 x^2 \varphi = E\varphi$$

Let's use these ideas for the finite square well:

So far we have:



consider the solution

for $-\frac{L}{2} < x < \frac{L}{2}$: $Ae^{ikx} + Be^{-ikx}$

Boundary conditions ?

at $x = \frac{L}{2}$, need ψ to be continuous.

① e^{ikx} for $x > \frac{L}{2}$ does not work though could be continuous.

② Decay solution ? e^{-ax^2} would not satisfy ψ' continuity condition.

③ e^{-ax^2} does not work b/c $V(x)$ has no x dependence here.

How can we stitch the appropriate solutions for:

connect I, II, III regions ?

Consider $E > 0$, $E < V_0$

II $-\frac{L}{2} < x < \frac{L}{2}$; $\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi$

$$\Rightarrow \frac{d^2}{dx^2}\psi = -k^2\psi \; ; \; k = \sqrt{2mE}/\hbar$$

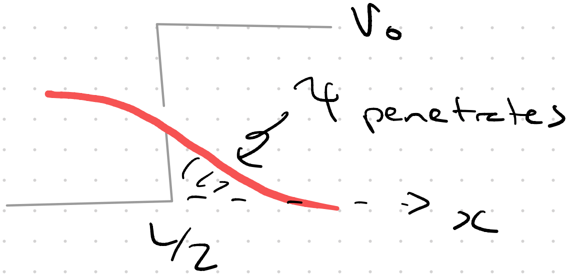
$E > 0$; $k > 0$

we found general solution:

$$\varphi = Ae^{ikx} + Be^{-ikx}$$

$$\Rightarrow (A+B)\cos kx + (A-B)\, i \sin kx$$

III $x > L/2$



$$-\frac{\hbar^2}{2m}\frac{d^2\varphi}{dx^2} + V_0\varphi = E\varphi$$

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

$$= -k'^2\varphi(x)$$

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

$$= i\,\frac{\sqrt{2m(V_0 - E)}}{\hbar}$$

$$= i k_1$$

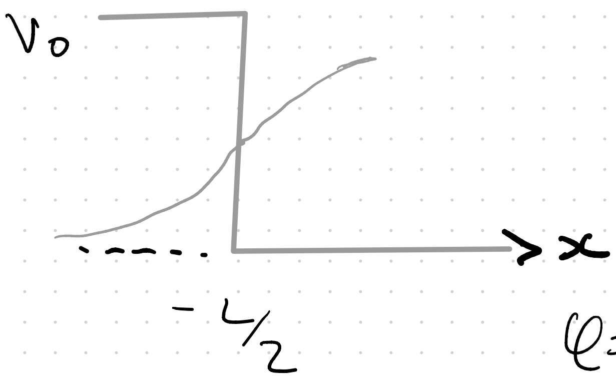
Now, $\psi = Ce^{ik'x} + De^{-ik'x}$

$$= Ce^{-k_1 x} + De^{+k_1 x}$$

To eliminate unphysical solutions as $x \to \infty \Rightarrow D = 0$

$\therefore \psi = Ce^{-k_1 x}$ remains.

(I) : $x < -L/2$



Now,

$$\psi = \cancel{C}e^{-k_1 x} + De^{+k_1 x}$$

$C \to 0$

$$\psi = De^{+k_1 x}$$

where $x < -L/2$

Consider: the even function solution (n is odd #), $A = B$.

$$\Rightarrow \quad -\frac{L}{2} < x < \frac{L}{2} \Rightarrow 2A\cos kx$$

$$x > \frac{L}{2} \Rightarrow Ce^{-k_1 x}$$

$$x < -\frac{L}{2} \Rightarrow De^{+k_1 x}$$

$\boxed{\text{In-class 14.2}}$

Boundary Conditions:

$\varphi(x)$ continuous at $x = +L/2$:

$$2A\cos k\frac{L}{2} = De^{-k_1 L/2} \quad \ldots (1)$$

$\varphi'(x)$ continuous at $x = +L/2$:

$$-2(k)A\sin kL/2 = -k_1 De^{-k_1 L/2} \quad \ldots (2)$$

Eliminate D: ②/① $\Rightarrow$ $k\tan\left(\frac{kL}{2}\right) = \kappa_1$

$$\tan\frac{kL}{2} = \frac{\kappa_1}{k} = \frac{\kappa_1 (L/2)}{k (L/2)} \quad ; \quad k = \frac{\sqrt{2mE}}{\hbar}$$

Define: $\xi = \frac{kL}{2}$; $\xi_0 = \frac{L}{\hbar}\sqrt{\frac{mV_0}{2}}$; $\kappa_1 = \frac{\sqrt{2m(V_0 - E)}}{\hbar}$

$$\therefore \tan\xi = \frac{\sqrt{\xi_0^2 - \xi^2}}{\xi} \quad \& \quad \sqrt{\xi_0^2 - \xi^2} = \kappa_1 \frac{L}{2}$$

$\boxed{\text{In-class 14.3}}$

How do we solve $\tan\xi = \frac{\sqrt{\xi_0^2 - \xi^2}}{\xi}$ to get a solution for E?

Odd n, or 'Even' function

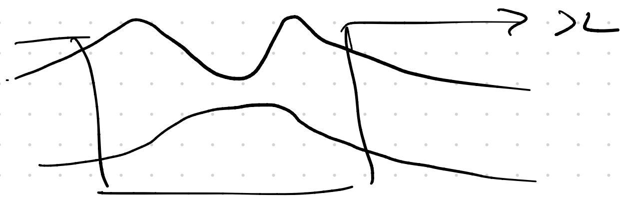
① No analytical solution for E

(2) ξ contains E as a function of V_0

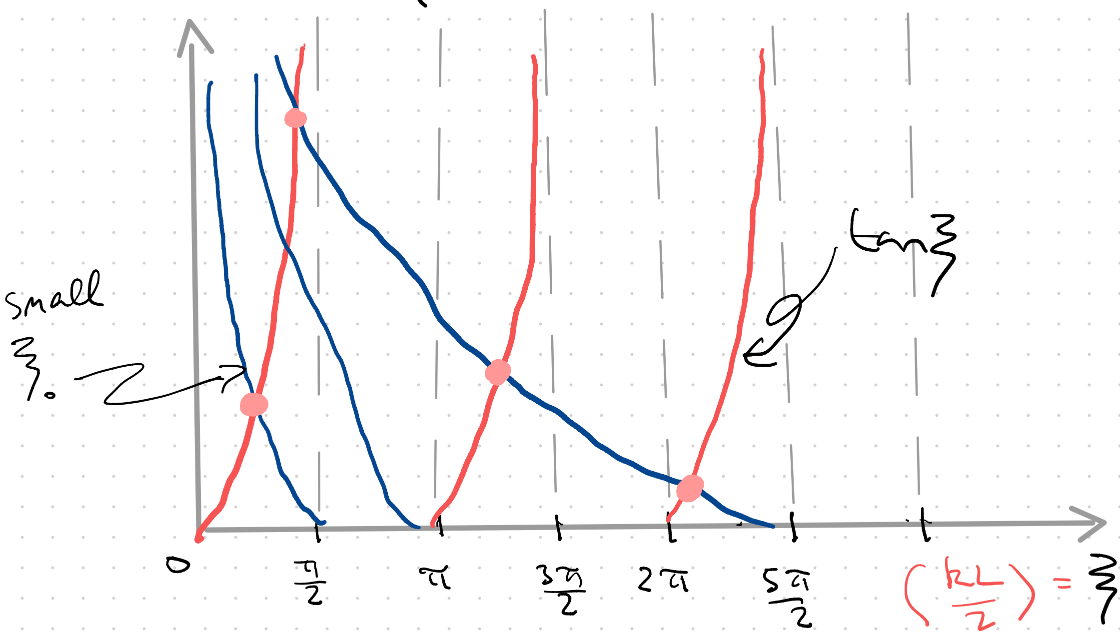
(3) Can use calculator / numerical solver.

(4) Graphical solution is possible!

(consider even states)

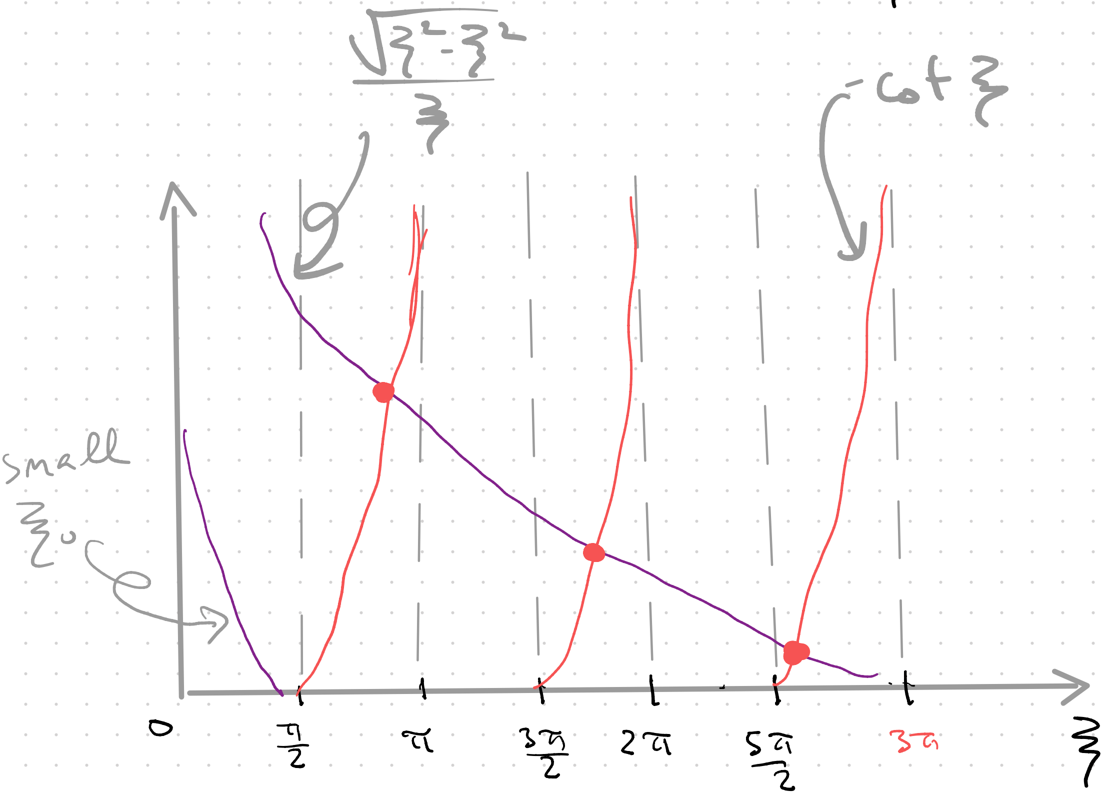


Plot: $\tan\xi$, $\dfrac{\sqrt{\xi_0^2-\xi^2}}{\xi}$, $\xi_0 = \dfrac{L}{\hbar}\sqrt{\dfrac{mV_0}{2}}$



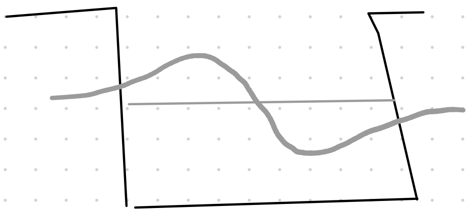
(5) Has discrete solutions

Above we considered $(A=B)$, even function.
Now let's consider $(A=-B)$, odd function.
We will obtain : $-\cot\xi = \dfrac{\sqrt{\xi_0^2-\xi^2}}{\xi}$



NB No solution for small ξ_0

odd states:



In-class 14.4

for $V_0 \to \infty$, $\xi_0 \to \infty$

$\tan\xi = \infty$; $\xi = \frac{\pi}{2}, \frac{3\pi}{2}, \frac{5\pi}{2}, \ldots$

$\frac{kL}{2} = \frac{\pi}{2}, \frac{3\pi}{2}, \ldots$

$\therefore kL = \pi, 3\pi, 5\pi, \ldots$

$= n\pi$; n is odd.

$\therefore\ k_n = \dfrac{n\pi}{L}$

or, $E_n = \dfrac{n^2\pi^2\hbar^2}{2mL^2}$

NB: Recover the Infinite square well soln (odd n).