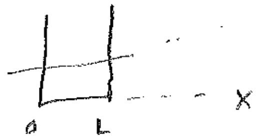
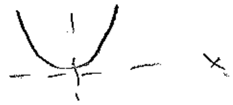
Particle in potential $V(x)$

Box



Harm. osc

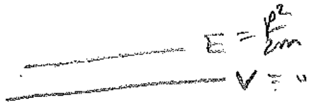


} finite allowed region (bound particle) ⇒ discrete energy levels

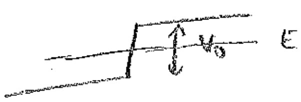
$E_n = \frac{(\hbar \pi n)^2}{2mL^2}$

$E_n = \hbar\omega(n + \frac{1}{2})$

Free
$V(x) = 0$

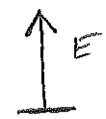


Step

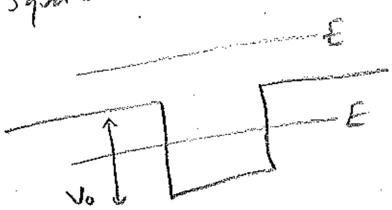


Barrier

} (semi)infinite allowed region ⇒ continuum energy levels
"free" particle (can escape to $\pm\infty$) $(E > 0)$

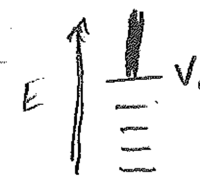


Square well potential

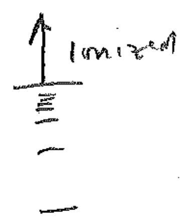


if $E < V_0$, finite allowed ⇒ discrete level

if $E > V_0$, infinite allowed ⇒ continuum

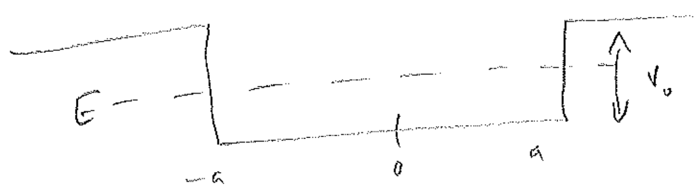


(eg hydrogen:



)

Square well potential



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

Assume $E<V_0$.

$\boxed{\text{Region } x>a}$ $\quad u(x) = \underbrace{\cancel{Ce^{\alpha x}}}_{\to 0} + De^{-\alpha x} \qquad \alpha = \dfrac{\sqrt{2m(V_0-E)}}{\hbar}$

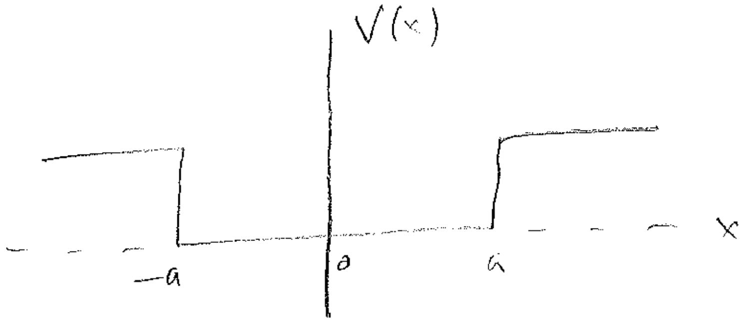
$\boxed{\text{Region } x<-a}$ $\quad u(x) = Fe^{\alpha x} + \cancel{Ge^{-\alpha x}}$

$\boxed{\text{Region: } |x|<a}$ $\quad u(x) = Ae^{ikx} + Be^{-ikx} \qquad k = \dfrac{\sqrt{2mE}}{\hbar}$

Can also write

$= A\cos kx + iA\sin kx + B\cos kx - iB\sin kx$

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



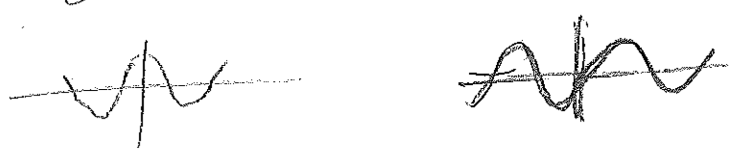
Observe that potential energy is symmetric under reflection $x \to -x$

$$V(-x) = V(x)$$

It is an <u>even</u> function

An <u>odd</u> function is antisymmetric, i.e. $f(-x) = -f(x)$.

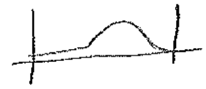
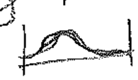
eg $\cos x$ is even $\sin$ is odd



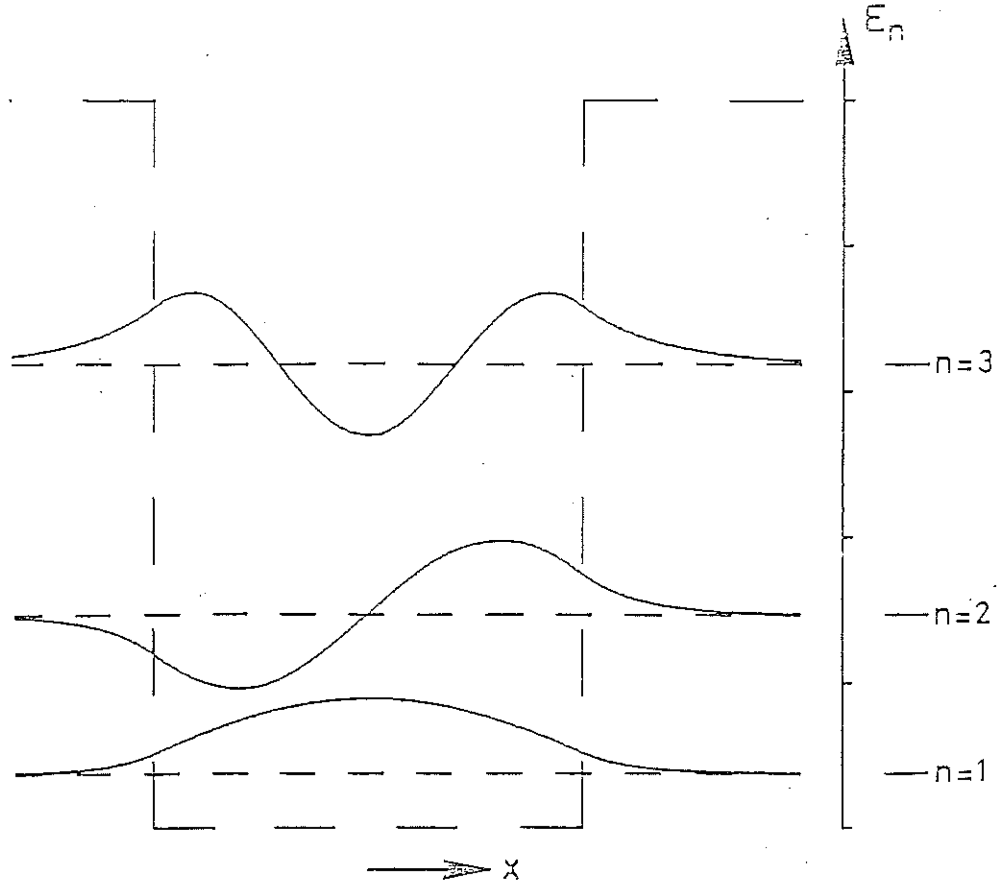
General result: whenever the potential is symmetric, the nondegenerate solutions of the t.i.S.e are

either even $u(-x) = u(x)$
or odd $u(-x) = -u(x)$

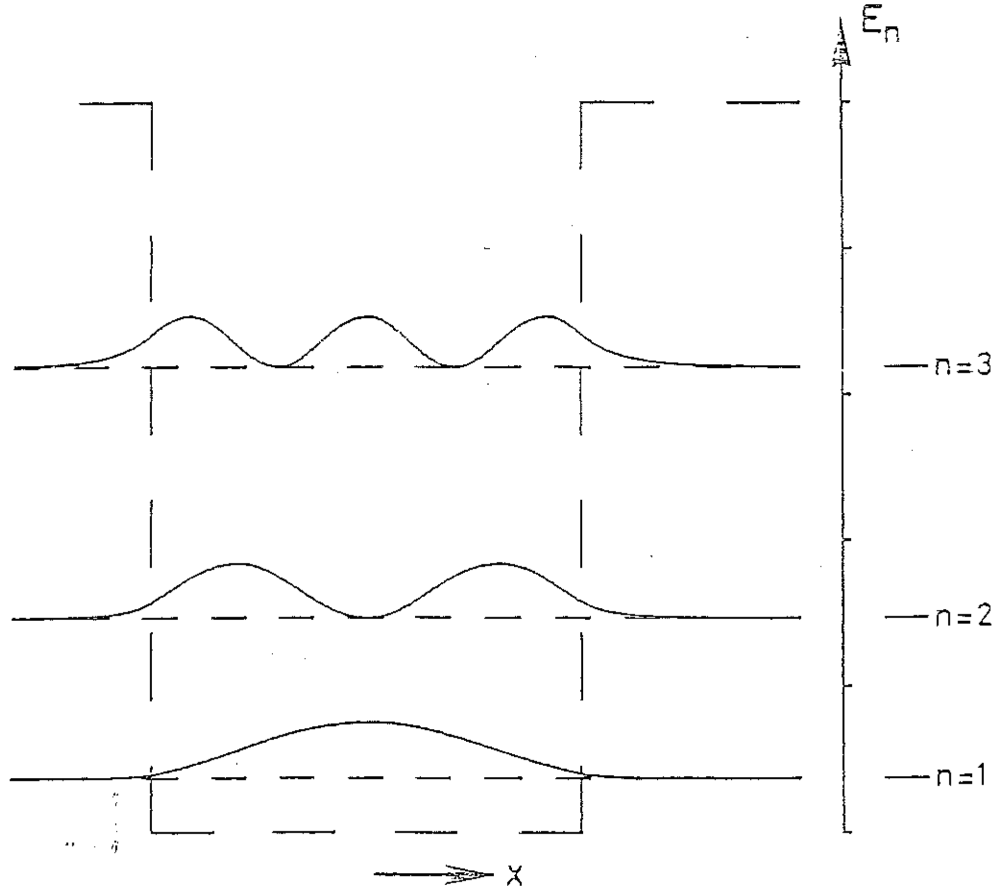
[show examples: particle in box, harmonic oscillator]

[Proof in words (optional):
Suppose eigenfunction is 
then  is also a solution w/ same E.
But nondegenerate so must be same.
only possible if even, or odd
(because $-u$ same as u)]

Will find all even eigenfns of square well in class
problem: find odd



E_n
n = 3
n = 2
n = 1
x



E_n
n = 3
n = 2
n = 1
x

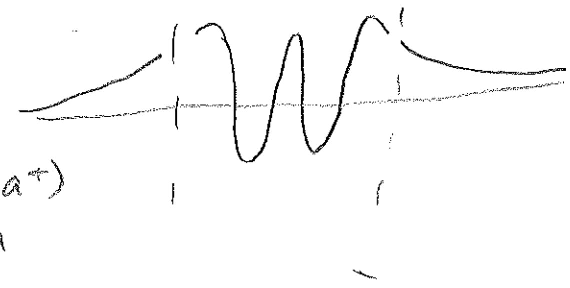
Consider even eigenfunctions of square well $\Rightarrow$ $A=B$, $D=F$ L4

even eigenfunctions

$$u(x) = \begin{cases} De^{\alpha x} & x<a \\ 2A\cos kx & -a<x<a \\ De^{-\alpha x} & x>a \end{cases}$$

where $k = \frac{+\sqrt{2mE}}{\hbar}$ and $\alpha = \frac{+\sqrt{2m(V_0-E)}}{\hbar}$

choose k positive!! must be positive.



Boundary conditions:

$$u(x\to a^-) = u(x\to a^+)$$

$$2A\cos ka = De^{-\alpha a}$$

$$\frac{du}{dx}(x\to a^-) = \frac{du}{dx}(x\to a^+)$$

$$-2Ak\sin(ka) = -\alpha De^{-\alpha a}$$

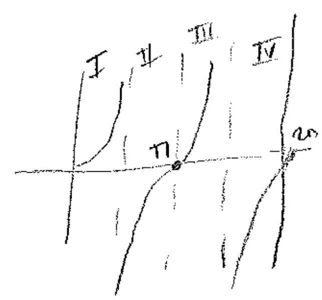
Divide again

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

$$k\tan(ka) = \alpha$$

Since $k, \alpha > 0$, $\tan(ka)$ must be positive $\Rightarrow$

$\Rightarrow ka$ must be in quadrants I or III



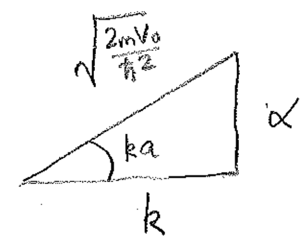
Condition for even eigenfunctions

$$k \tan(ka) = \alpha \qquad \text{where } k = \frac{\sqrt{2mE}}{\hbar}, \quad \alpha = \frac{\sqrt{2m(V_0 - E)}}{\hbar}$$

(take the positive square root)

$$k^2 \tan^2(ka) = \alpha^2 = \frac{2mV_0}{\hbar^2} - \frac{2mE}{\hbar^2} = \frac{2mV_0}{\hbar^2} - k^2$$

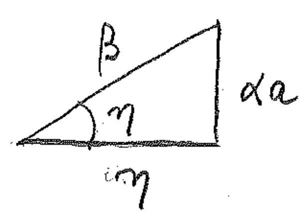
$$k^2 \underbrace{(\tan^2(ka) + 1)}_{\sec^2(ka) = \frac{1}{\cos^2(ka)}} = \frac{2mV_0}{\hbar^2}$$



$$\Rightarrow (ka)^2 \frac{\hbar^2}{2mV_0 a^2} = \cos^2(ka)$$

Define dimensionless variables: $\begin{cases} \eta = ka \\ \beta^2 = \frac{2mV_0 a^2}{\hbar^2} \end{cases}$

$$\eta^2 \frac{1}{\beta^2} = \cos^2 \eta$$



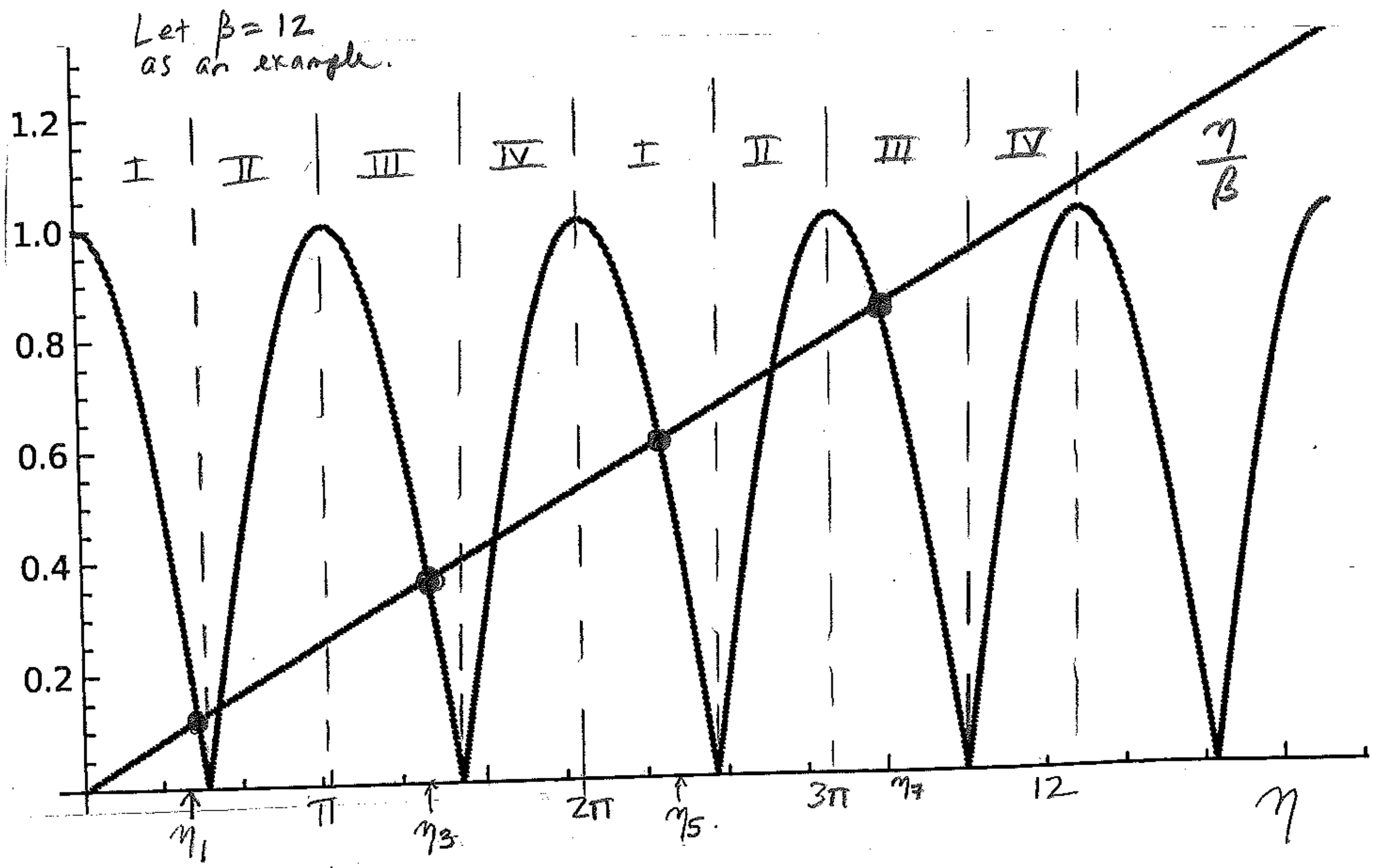
$$\frac{\eta}{\beta} = \pm \cos \eta$$

But $k > 0$, so $\eta > 0$, so. l.h.s must be positive

$$\frac{\eta}{\beta} = |\cos \eta|$$

How to solve the transcendental equation $\frac{\eta}{\beta} = |\cos \eta|$?

Analyze it graphically!



Solutions correspond to points where plots intersect.
Choose only intersections in quadrants I and III
(because $\tan \eta = \frac{\alpha a}{\eta} > 0$ for even eigenfunctions)

$$\left.\begin{aligned} \eta_1 &= 1.4497 \\ \eta_3 &= 4.3421 \\ \eta_5 &= 7.2095 \\ \eta_7 &= 10.609 \end{aligned}\right\} \text{Solutions for } \beta = 12$$

Energy eigenvalues:

Recall $k = \frac{\sqrt{2mE}}{\hbar} \Rightarrow E = \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2 \eta^2}{2ma^2} = \left(\frac{\eta}{\beta}\right)^2 V_0$

Since solutions exist only for $\eta \leq \beta$, the bound state energies obey $E < V_0$ (as expected)

For $\beta = 12$, there are 4 even bound state eigenfunctions with energies $E_i = \left(\frac{\eta_i}{\beta}\right)^2 V_0$

namely
$$E_1 = 0.01459\ V_0$$
$$E_3 = 0.13093\ V_0$$
$$E_5 = 0.36095\ V_0$$
$$E_7 = 0.69569\ V_0$$

There will also be some odd bound state eigenfunctions w/ energies E_2, E_4, etc.

Estimate the number of *even* bound state eigenfunctions.

There is one solution for every interval of π.

There are no solutions for $\eta > \beta$.

Therefore the *approximate* number of solutions is $\frac{\beta}{\pi}$

In the case of $\beta = 12$, $\frac{\beta}{\pi} = 3.82$

(of course the number of solutions must be an integer.)

Limiting cases:

Let $\beta \to \infty$, then $V_0 \to \infty$ (deep well = particle in box)

$$|\cos\eta| = \frac{\eta}{\beta} \longrightarrow 0$$

$$\cos\eta = 0 \quad \text{for} \quad \eta = \frac{\pi}{2},\ \frac{3\pi}{2},\ \frac{5\pi}{2},\ \frac{7\pi}{2}$$

$$\text{ie} \quad \eta_n = \frac{\pi}{2} n \quad \text{for} \quad n = \text{odd integer}$$

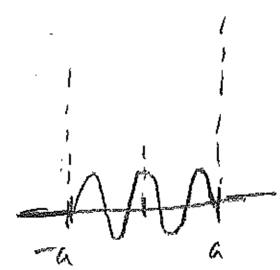
$$E_n = \frac{\hbar^2 \eta^2}{2ma^2} = \left(\frac{\hbar^2 \pi^2}{8ma^2}\right) n^2, \quad n = \text{odd}$$

$$k_n = \frac{\eta_n}{a} = \frac{\pi n}{2a}$$

$$\alpha_n = \frac{\sqrt{2m(V_0 - E_n)}}{\hbar} \longrightarrow \infty$$

Even eigenfunctions:

$$u = \begin{cases} De^{\alpha x} \longrightarrow 0 \\ 2A\cos ka \longrightarrow 2A\cos\left(\frac{\pi n x}{2a}\right) \\ De^{-\alpha x} \longrightarrow 0 \end{cases}$$

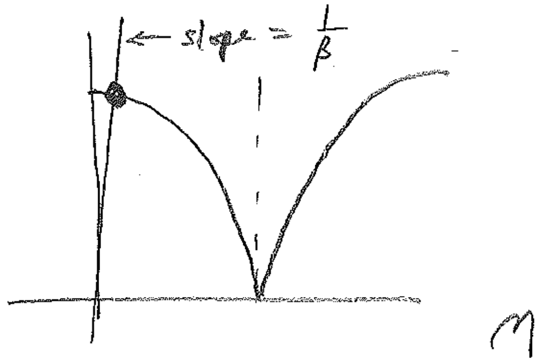


Note: for particle in a box of width $L = 2a$

expect energies $E = \dfrac{\hbar^2 \pi^2 n^2}{2mL^2} = \dfrac{\hbar^2 \pi n^2}{8ma^2}$. We've found the n = odd solutions

Limiting case

Let $\beta \to 0$, then $V_0 \to 0$ (shallow well)



There is only one intersection in quadrant I.

with $\frac{\eta}{\beta} = |\cos\eta| \approx 1 \quad \Rightarrow \eta_1 \approx \beta$

$$E_1 = \left(\frac{\eta_1}{\beta}\right)^2 V_0 \approx V_0 \quad \text{(almost unbound)}$$