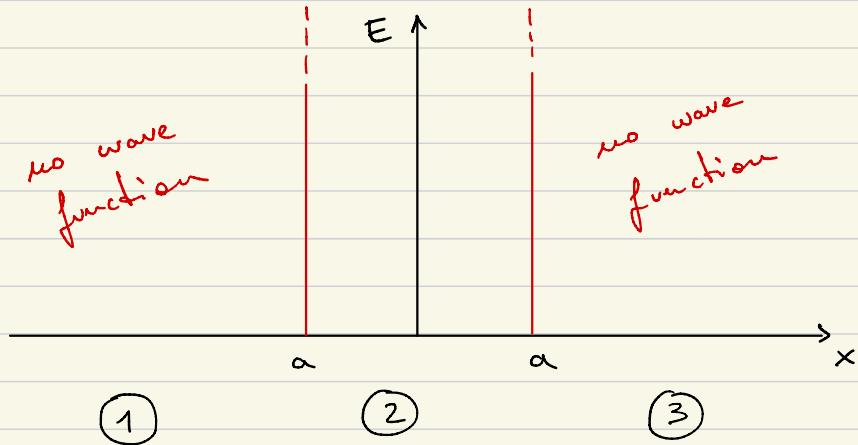


Quantum mechanics I : tutorial solutions

2020.10.22

/ self-study pack 2

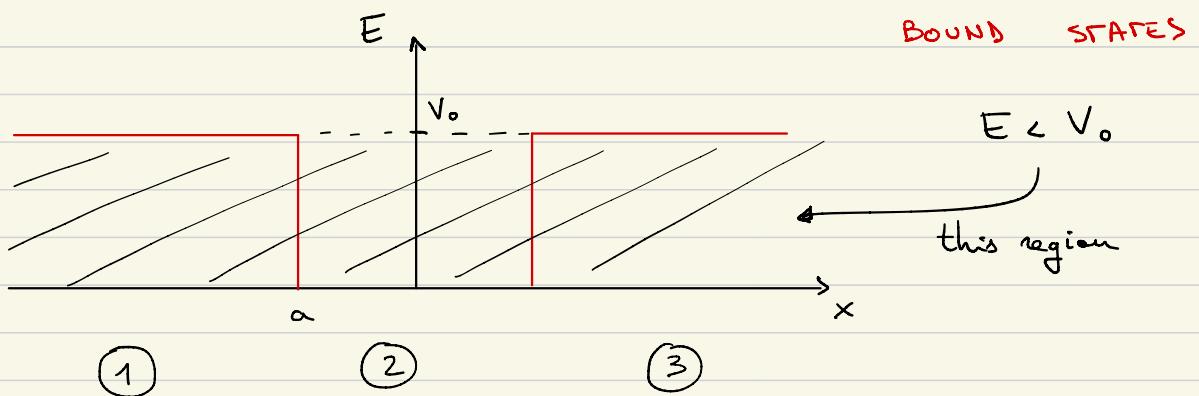
- We have seen that, the wave function of a particle in an infinite square well is,

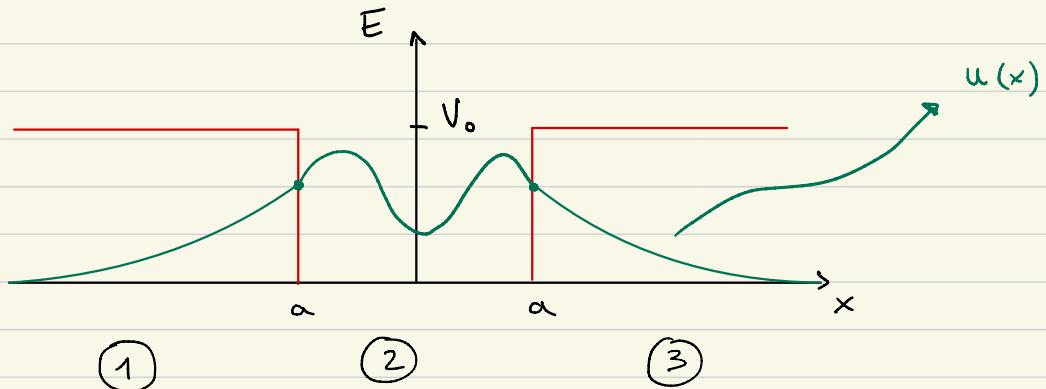


wave function $\psi(x) = \cos(kx)$ (or $\sin(kx)$)

while the energy levels are $E_n = \frac{\hbar^2 n^2 \pi^2}{8 m a^2}$

- Now, we look at the **BOUND STATES** in the **FINITE** square well.





$$u_1(x) = C e^{q|x|} \quad u_3(x) = D e^{-q|x|}$$

watch out the sign of the exp.
 → the w.f. has to decay

$$u(x) = \begin{cases} u_1(x) = C e^{q|x|}, & x \leq -a \\ u_2(x) = A \cos(kx) + B \sin(kx), & -a < x \leq a \\ u_3(x) = D e^{-q|x|}, & x > a \end{cases}$$

1) We study the symmetric solution ($\cos(kx)$).

We need the derivative $\frac{du(x)}{dx}$ to study the boundary conditions in $x = -a, x = a$

in $x = a$:

$$u_3(a) = D e^{-qa} = A \cos(ka) = u_2(a)$$

$$u'_3(a) = -q D e^{-qa} = -k A \sin(ka) = u'_2(a)$$

fixing $A = 1$ we have

$$\left\{ \begin{array}{l} D = e^{qa} \cos(ka) \\ -q D e^{-qa} = -k \sin(ka) \end{array} \right.$$

$$\left\{ \begin{array}{l} D = e^{qa} \cos(ka) \\ -q \cancel{e^{qa}} \cos(ka) \cancel{e^{-qa}} = -k \sin(ka) \end{array} \right.$$

$$\Rightarrow q = k \tan(ka)$$

2) For the ANTI-SYMMETRIC solution ($\sin(kx)$) we have,

in $x = a$:

$$u_3(a) = D e^{-qa} = A \sin(ka) = u_2(a)$$

$$u'_3(a) = -q D e^{-qa} = kA \cos(ka) = u'_2(a)$$

fixing $A = 1$,

$$\left\{ \begin{array}{l} D = e^{qa} \sin(ka) \\ -q D e^{-qa} = k \cos(ka) \end{array} \right.$$

$$\left\{ \begin{array}{l} D = e^{qa} \sin(ka) \\ -q \cancel{e^{qa}} \sin(ka) \cancel{e^{-qa}} = k \cos(ka) \end{array} \right.$$

$$\Rightarrow -q = k \cot(ka)$$

3)

the boundary conditions impose the wave function to satisfy,

for a SYMMETRIC SOLUTION : $q = k \tan(ka)$

for an ANTI-SYMMETRIC SOLUTION : $q = -k \cot(ka)$

Using the existing relation between k & q , we can look for legitimate solutions.

$$E = \frac{\hbar^2 k^2}{2m} \rightarrow k^2 = \frac{2mE}{\hbar^2}$$

$$2 q^2 = \frac{2m(V_0 - E)}{\hbar^2}$$

defining for convenience $k_0^2 = \frac{2mV_0}{\hbar^2}$
we have

$$q^2 = k_0^2 - k^2$$

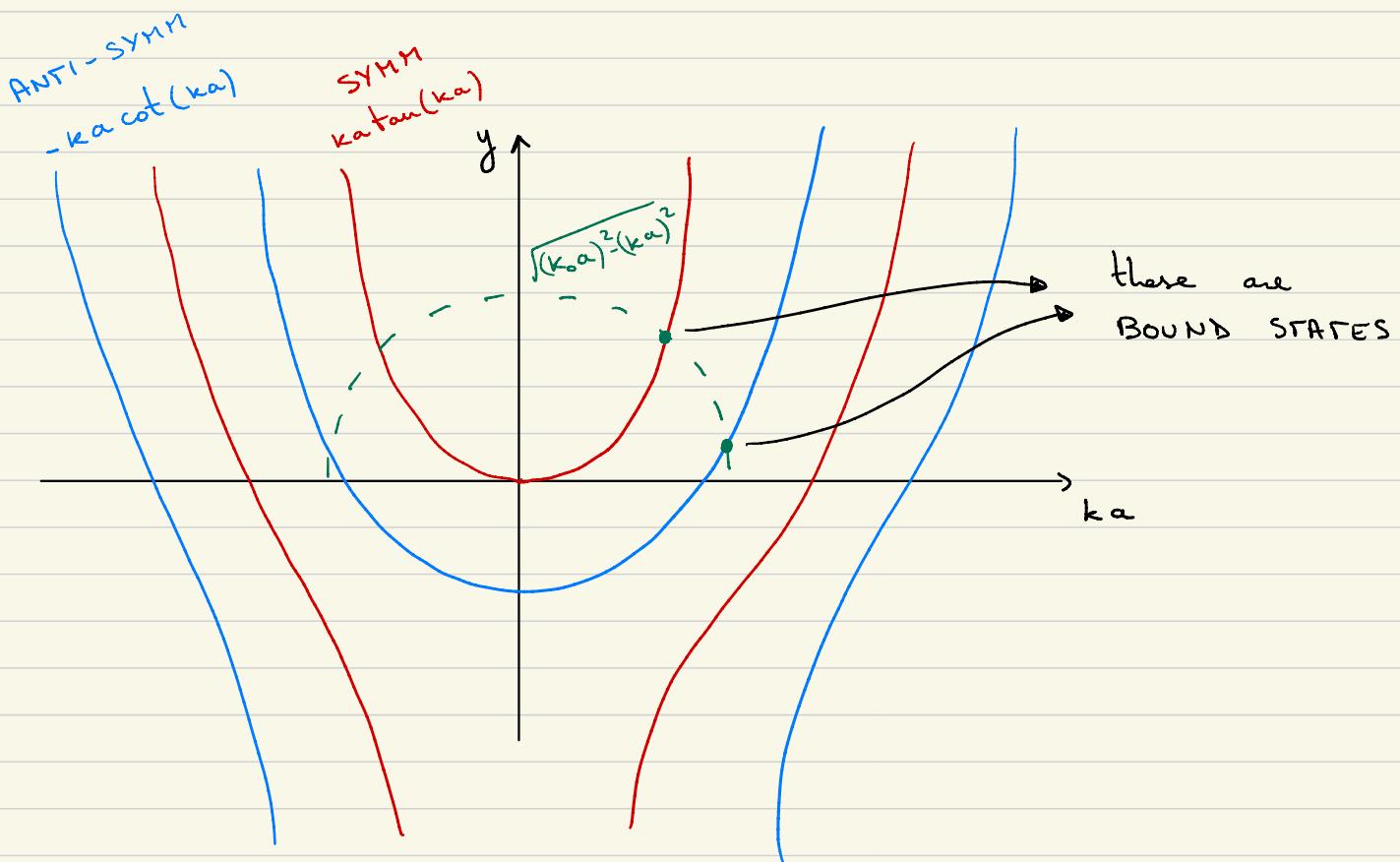
Now, we use $q = k \tan(ka)$ in this expression,

$$ka \tan(ka) = \sqrt{(k_0 a)^2 - (ka)^2}$$

→ note that
we multiplied
every term
by a

this expression gives the condition for having
 BOUND STATES!

See graph at : [HTTPS://www.desmos.com/calculator/lbfjb9ytkq](https://www.desmos.com/calculator/lbfjb9ytkq)

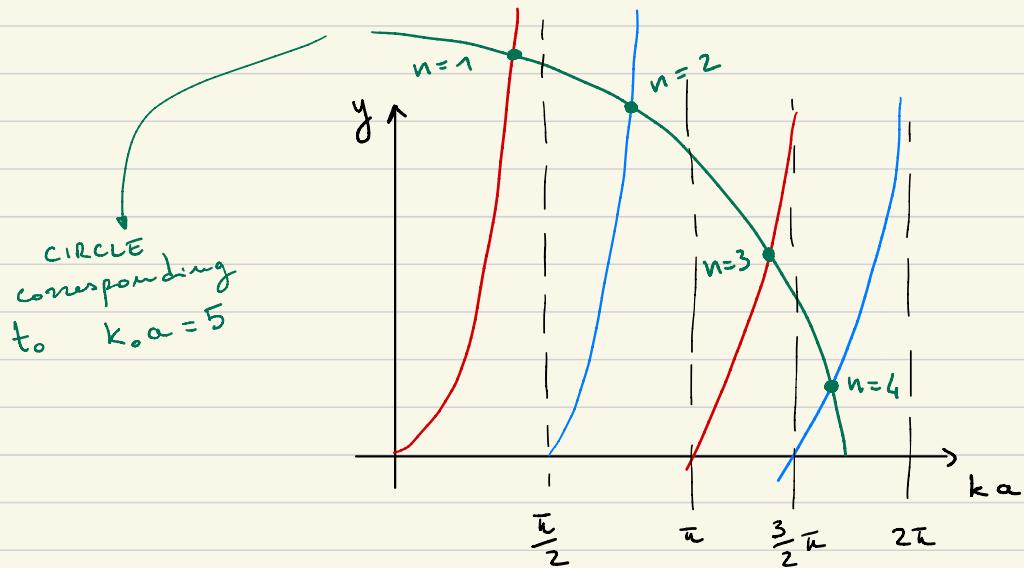


- Note that there are NO ANTI-SYMM solutions

$$\text{when } ka = \sqrt{\frac{2meE}{\hbar^2}} \quad a < \frac{\pi}{2}$$

- Always at least 1 SYMMETRIC solution

4) 5) 6) Numerical method (Bisection)



we look for $n=1$ solution

We see that the solution is between $0 < ka < \frac{\pi}{2}$

the 2 intersecting functions are

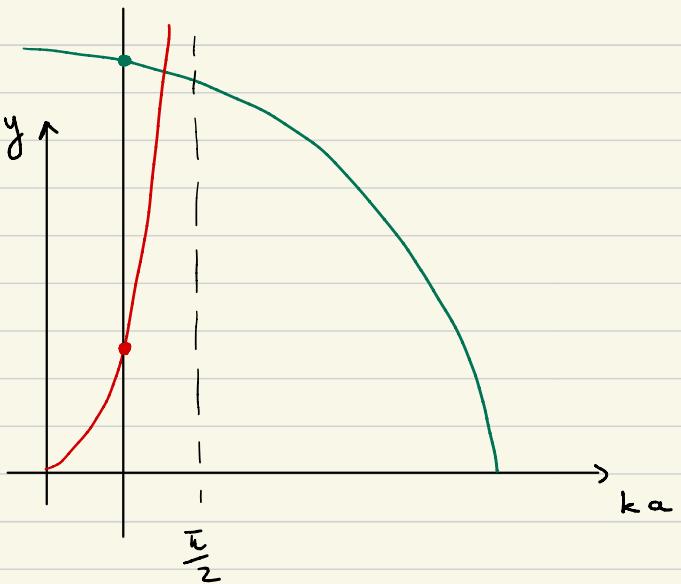
$$y = ka \tan(ka) \quad \text{and} \quad y = \sqrt{(k_0 a)^2 - (ka)^2}$$

the value midway between 0 and $\frac{\pi}{2}$ is $\frac{\pi}{4}$.

We substitute this value in the 2 functions.

$$y = \frac{\pi}{4} \tan\left(\frac{\pi}{4}\right) = \frac{\pi}{4} \approx 0.79$$

$$y = \sqrt{\left(5\right)^2 - \left(\frac{\pi}{4}\right)^2} \approx 4.94$$



we clearly see from the graph that the solution has to be at a larger value of ka .

We repeat the same process,

- $\frac{\pi}{4} < ka < \frac{\pi}{2}$, midway $ka = \frac{3}{8}\pi$

$$y = \frac{3}{8}\pi \tan\left(\frac{3}{8}\pi\right) \approx 2.84$$

$$y = \sqrt{(5)^2 - \left(\frac{3}{8}\pi\right)^2} \approx 4.86$$

- $\frac{3}{8}\pi < ka < \frac{\pi}{2}$, midway $ka = \frac{7}{16}\pi$

$$y = \frac{7}{16}\pi \tan\left(\frac{7}{16}\pi\right) \approx 6.90$$

$$y = \sqrt{(5)^2 - \left(\frac{7}{16}\pi\right)^2} \approx 4.81$$

- Here, $y \approx 6.90$ (\tan) is too large, hence we invert the limits.

$$\frac{3}{8}\pi < ka < \frac{7}{16}\pi \quad , \quad \text{midway} \quad ka = \frac{13}{32}\pi$$

$$y = \frac{13}{32}\pi \tan\left(\frac{13}{32}\pi\right) \approx 4.21$$

$$y = \sqrt{(5)^2 - \left(\frac{13}{32}\pi\right)^2} \approx 4.83$$

- $\frac{13}{32}\pi < ka < \frac{7}{16}\pi \quad , \quad \text{midway} \quad ka = \frac{27}{64}\pi$

$$y = \frac{27}{64}\pi \tan\left(\frac{27}{64}\pi\right) \approx 5.29$$

$$y = \sqrt{(5)^2 - \left(\frac{27}{64}\pi\right)^2} \approx 4.82$$

- $\frac{13}{32}\pi < ka < \frac{27}{64}\pi \quad , \quad \text{midway} \quad ka = \frac{53}{128}\pi$

$$y = \frac{53}{128}\pi \tan\left(\frac{53}{128}\pi\right) \approx 4.70$$

$$y = \sqrt{(5)^2 - \left(\frac{53}{128}\pi\right)^2} \approx 4.83$$

Once you find the precision needed, you take the last midway value of $ka \approx \frac{53}{128}\pi$

NB : to find $\frac{E}{V_0}$, recall the definitions of k and k_0 .

$$k = \sqrt{\frac{2mE}{\hbar^2}}, \quad k_0 = \sqrt{\frac{2mV_0}{\hbar^2}}$$

therefore, $\frac{E}{V_0} = \frac{k^2}{k_0^2} = \frac{k^2 a^2}{k_0^2 a^2}$

we obtain the following table :

n	ka	E/V_0
$y = k a \tan(ka)$	1	0.067
$y = -k a \cot(ka)$	2	0.27
	3	0.59
	4	0.96

C.F.

Rae A.I.M. "q. mechanics"
section 2.5



(the green values come from Rae's book)

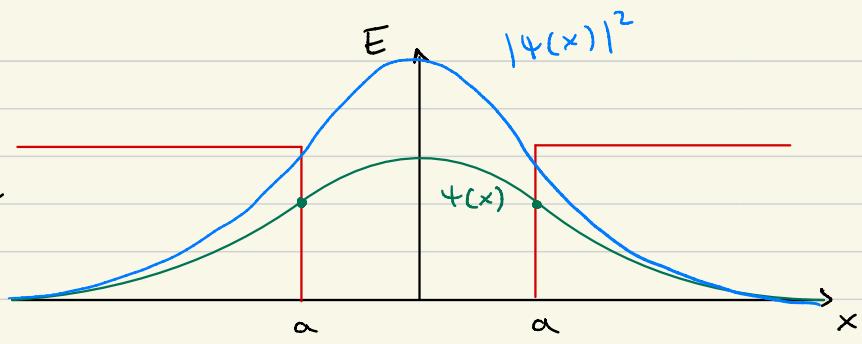
7) Sketch the w.f.

In the case of SYMMETRIC solution we have

$$u(x) = \begin{cases} u_1(x) = C e^{qx}, & x \leq -a \\ u_2(x) = A \cos(kx), & -a < x \leq a \\ u_3(x) = D e^{-qx}, & x > a \end{cases}$$

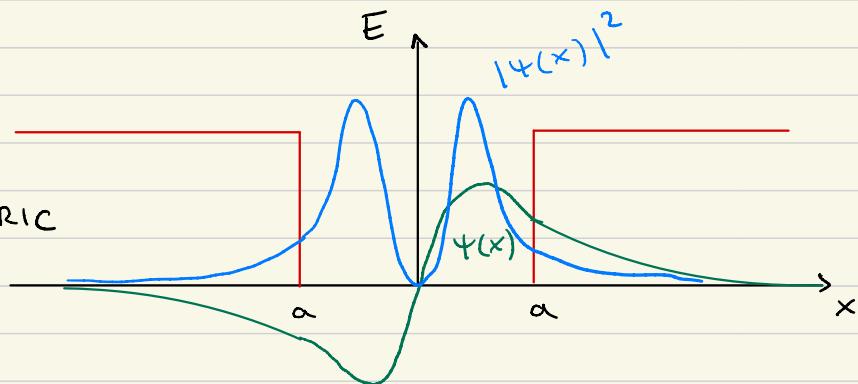
$n = 1$

SYMMETRIC



$n = 2$

ANTI-SYMMETRIC



$n = 3$

SYMMETRIC

