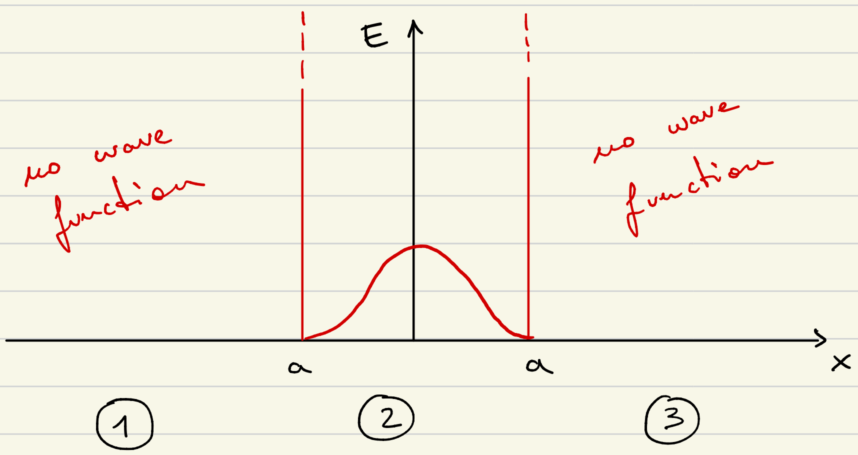
Quantum mechanics I : tutorial solutions

2021.10.14 / self-study pack 2

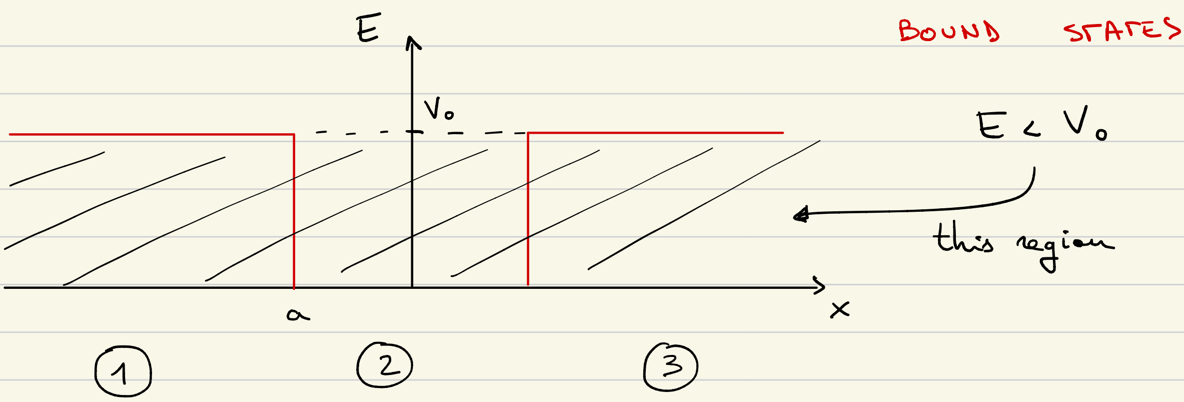
- We have seen that the wave function of a particle in an infinite square well is,

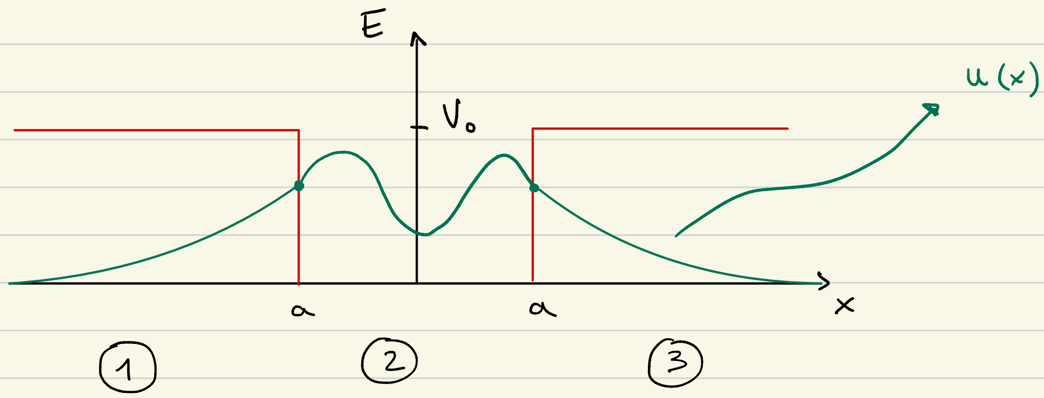


wave function $\psi(x) = \cos(kx)$ (or $\sin(kx)$)

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

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





$$u_1(x) = C e^{qx} \qquad\qquad u_2(x) = A\cos(kx) + B\sin(kx) \qquad\qquad u_3(x) = D e^{-qx}$$

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

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

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 $x = a$:

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

$$\underbrace{u_3'(a) = -qDe^{-qa}}_{} \underset{=}{} \underbrace{-kA\sin(ka) = u_2'(a)}_{}$$

fixing $A = 1$ we have

$$\begin{cases} D = e^{qa} \cos(ka) \\ -q D e^{-qa} = -k \sin(ka) \end{cases}$$

$$\begin{cases} D = e^{qa} \cos(ka) \\ -q \cancel{e^{qa}} \cos(ka) \cancel{e^{-qa}} = -k \sin(ka) \end{cases}$$

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

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 $A = 1$,

$$\begin{cases} D = e^{qa} \sin(ka) \\ -q D e^{-qa} = k \cos(ka) \end{cases}$$

$$\begin{cases} D = e^{qa} \sin(ka) \\ -q \cancel{e^{qa}} \sin(ka) \cancel{e^{-qa}} = k \cos(ka) \end{cases}$$

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

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.

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

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

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

we have

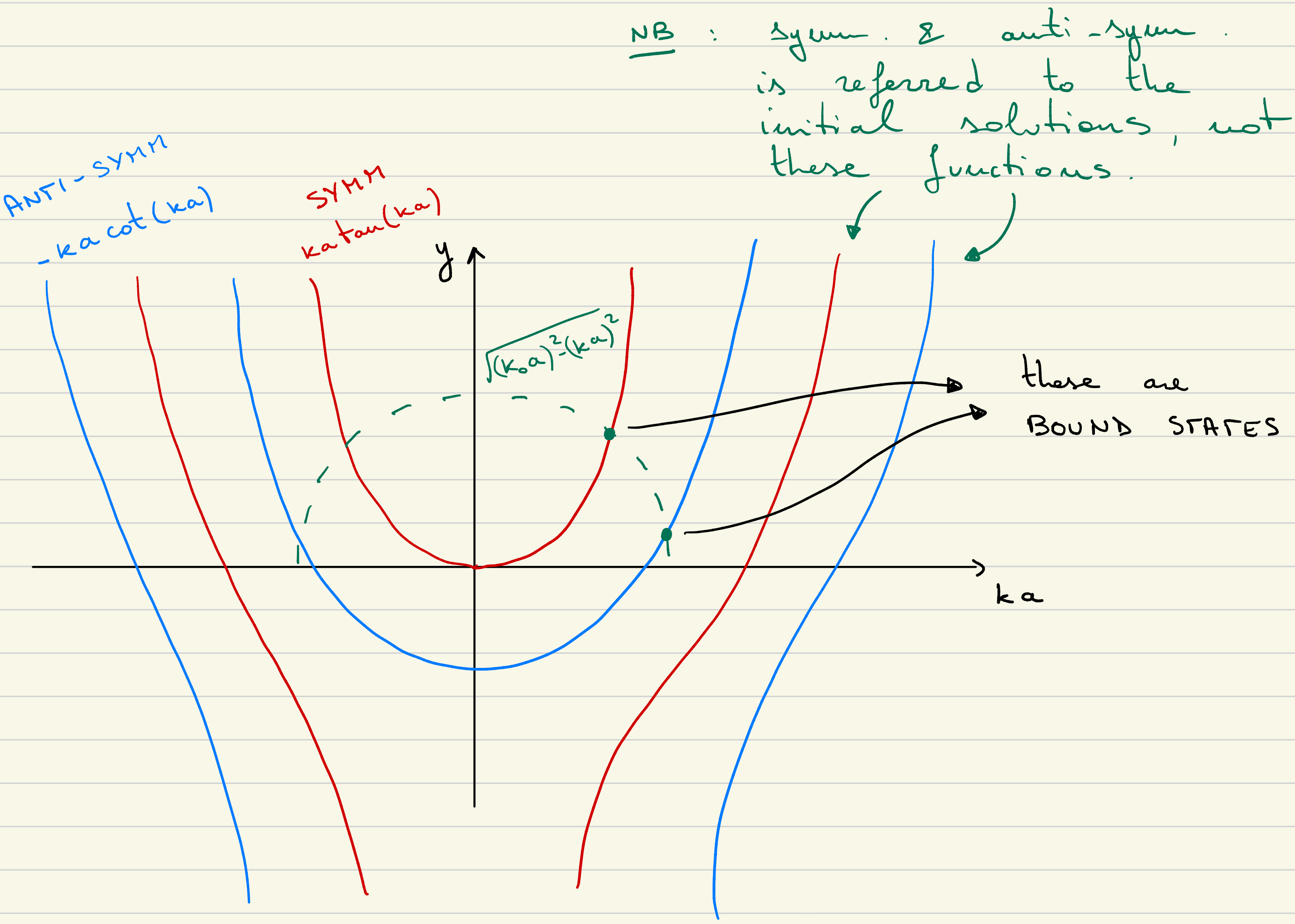
$$q^2 = k_0^2 - k^2$$

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 !

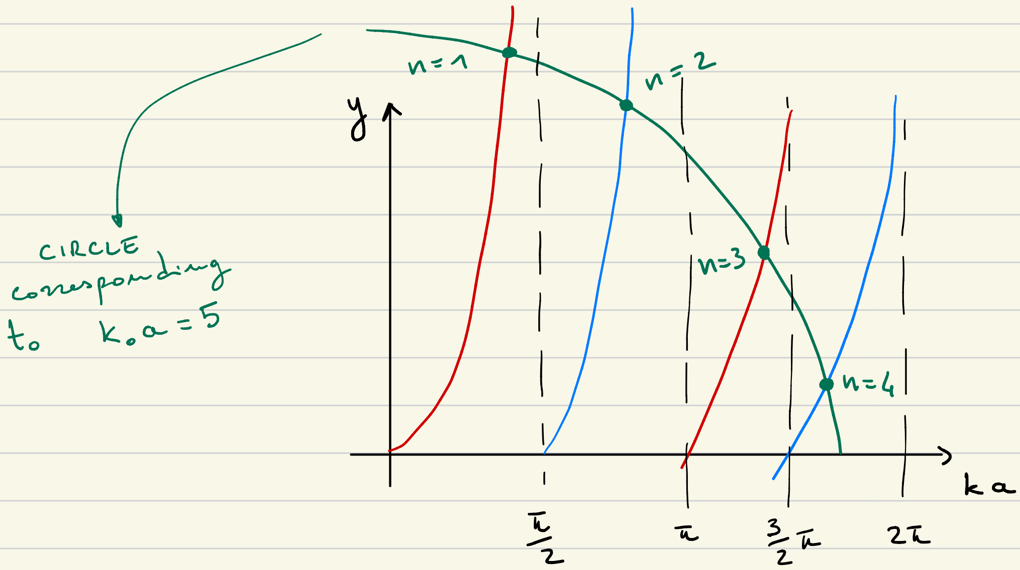
See graph at : HTTPS://www.desmos.com/calculator/lbfjb9ytkq



- Note that there are NO ANTI-SYMM solutions when $ka = \sqrt{\frac{2mE}{\hbar^2}}\, a < \frac{\pi}{2}$

- 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

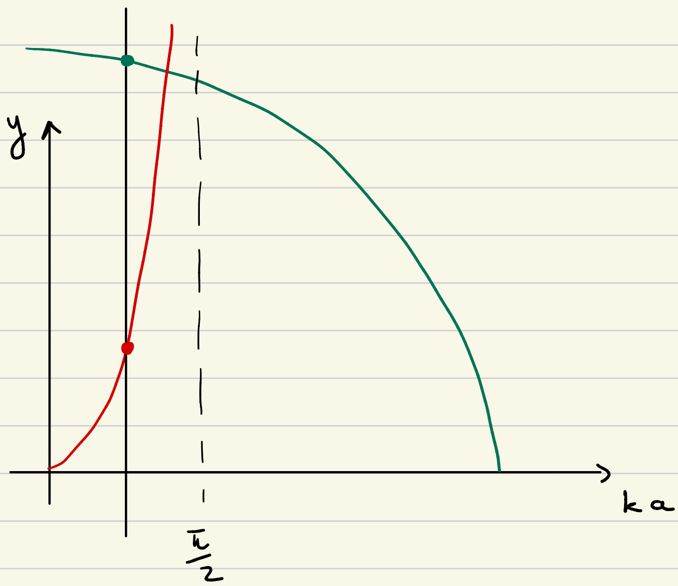
$$y = ka \tan(ka) \quad \text{and} \quad y = \sqrt{(k_o a)^2 - (ka)^2}$$

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

We substitute this value in the 2 functions.

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

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



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 $ka = \frac{3}{8}\pi$

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

we obtain the following table :

	n	ka	E/V_0
$y = ka\tan(ka)$	1	1.30	0.067
$y = -ka\cot(ka)$	2	2.59	0.27
	3	3.85	0.59
	4	4.90	0.96

C. F.

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

section 2.5

(the green values come from Rae 's book)

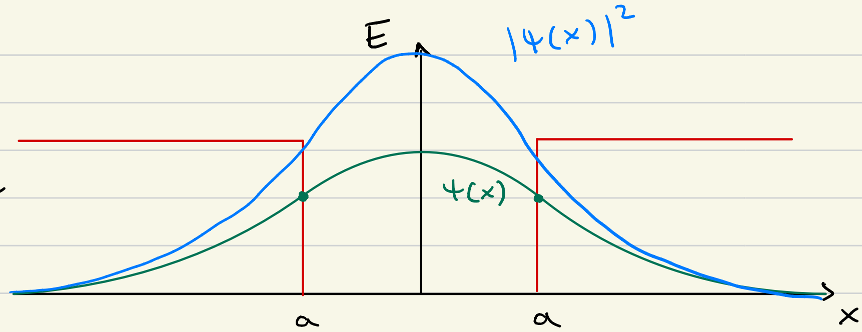
7) Sketch the w.f.

In the case of SYMMETRIC solution we have

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

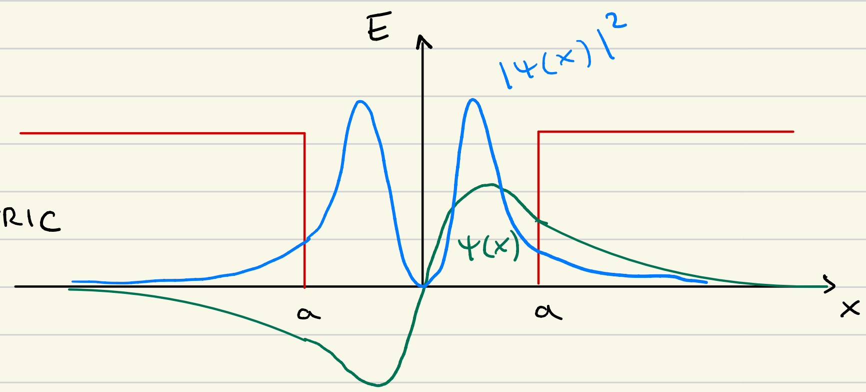
$n = 1$

SYMMETRIC



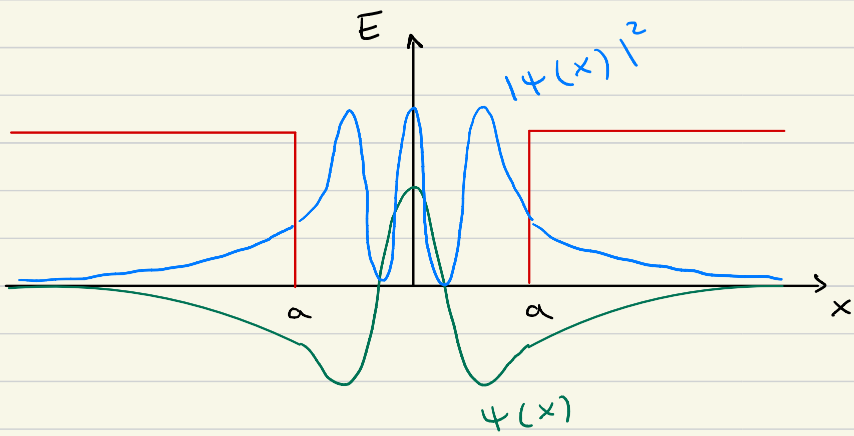
$n = 2$

ANTI-SYMMETRIC



$n = 3$

SYMMETRIC

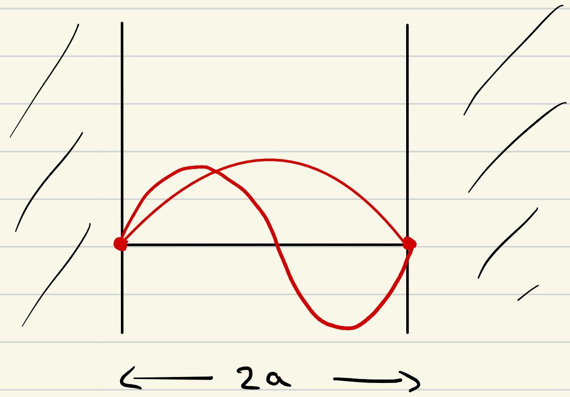


TIPS

A quick way to remember the INFINITE square well energy levels.

- free particle $E = \frac{p^2}{2m}$

- De Broglie $p = h/\lambda$



Since the wave function has to satisfy the boundary conditions, therefore being zero at the edges of the well, we have

$$2a = n\frac{\lambda}{2} \rightarrow \lambda = \frac{4a}{n}$$

$$E_n = \frac{h^2}{2m}\frac{n^2}{16a^2}, \qquad h = 2\pi\hbar$$

$$E_n = \frac{\hbar^2 n^2 \pi^2}{8ma^2}$$