Quantum mechanics I : tutorial solutions

2021.10.21 / exercises week 3

1. In lectures we solved the particle-in-a-box (infinite square well) problem using the potential:

$$V(x) = \begin{cases} 0 & (-a \le x \le a) \\ \infty & \text{elsewhere} \end{cases}$$

(a) Write down the eigenfunctions and eigenvalues for the potential:

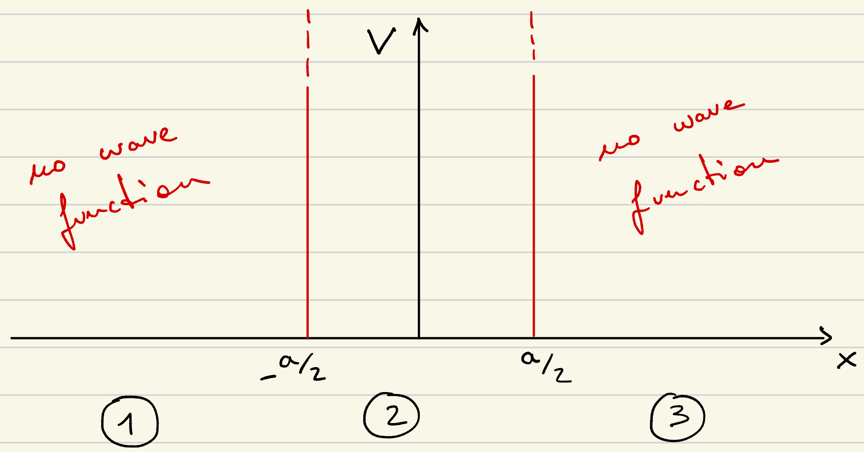
$$V(x) = \begin{cases} 0 & (-a/2 \le x \le a/2) \\ \infty & \text{elsewhere} \end{cases}.$$

(b) Now solve the equivalent problem for the potential:

$$V(x) = \begin{cases} 0 & (0 \le x \le a) \\ \infty & \text{elsewhere} \end{cases}$$

In particular show that the energy eigenvalues are the same as for one of the problems above (which one?), and that the wave functions have the same shape (though not the same functional forms) as for that problem.

(a)



The wave function is

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

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

(where does this value of k comes from? Remember we are dealing with a free particle)

from time-ind. Schr. eq.

$$E\,u(x) = \frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}u(x) + V(x)\,u(x)$$

boundary conditions,

$$x = a/2 \qquad u(a/2) = 0 = A\cos\frac{ka}{2} + B\sin\frac{ka}{2}$$

$$x = -\frac{a}{2} \qquad u\left(-\frac{a}{2}\right) = 0 = A\cos\frac{ka}{2} - B\sin\frac{ka}{2}$$

Here either A or B are 0 for a sol. to exist.

$$\text{if} \quad A = 0 \qquad u\left(\frac{a}{2}\right) = B\sin\frac{ka}{2}$$

$$\text{if} \quad B = 0 \qquad u\left(\frac{a}{2}\right) = A\cos\frac{ka}{2}$$

we know that $u\left(-\frac{a}{2}\right) = u\left(\frac{a}{2}\right) = 0$, this means

$$k = \frac{n\pi}{a}$$

such that for

$$n \text{ odd:} \qquad u(x) = A\cos(kx)$$

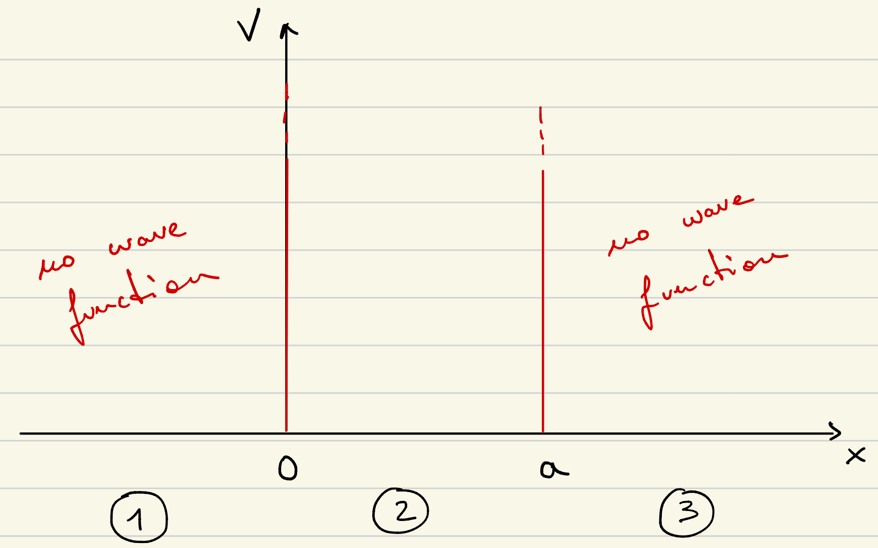
$$n \text{ even:} \qquad u(x) = B\sin(kx)$$

do these satisfy the boundary conditions?

→ BOUNDARY CONDITIONS translate in QUANTISATION

$$E = \frac{\hbar k^2}{2m} = \frac{\hbar^2 n^2\pi^2}{2ma^2}$$

(b)



wave f^n

$$u(x) = A\cos(kx) + B\sin(kx)$$

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

boundary conditions

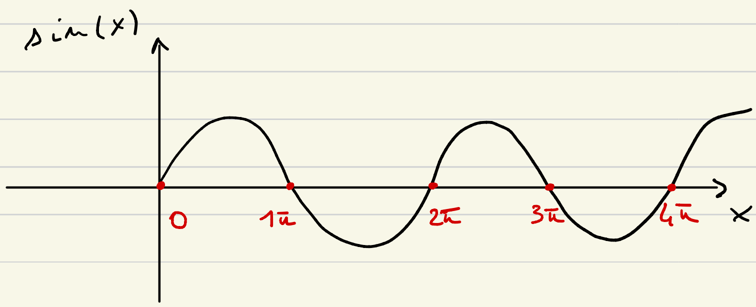
$$\begin{cases} u(0) = 0 = A \\ u(a) = 0 = A\cos(ka) + B\sin(ka) \end{cases}$$

therefore $\quad u(x) = B\sin(kx)$

with $\quad k = \frac{n\pi}{a}$ to satisfy the condition

$$u(a) = 0 = B\sin\left(\frac{n\pi}{a}a\right)$$

$$= B\sin(n\pi) \qquad \forall n.$$



the energy levels are

$$E = \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2 n^2 \pi^2}{2ma}$$

same result as in point (a).

RECAP

(a)

wave function:

n odd, $\qquad u(x) = A \cos(kx)$

n even, $\qquad u(x) = B \sin(kx)$

where $k = \frac{n\pi}{a}$

energies:

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

(b)

wave function:

$$u(x) = B \sin(kx)$$

where $k = \frac{n\pi}{a}$

energies:

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

2. For the ground state of the problem in 1(b) above:

(a) Normalize the wave function.

(b) Find the probabilities for locating the particle (i) closer to the edge than to the centre of the well (i.e. $0 < x < a/4$ or $3a/4 < x < a$) and (ii) closer to the centre than the edge (i.e. $a/4 < x < 3a/4$). How do your results compare with the classical prediction?

(c) Calculate the expectation value of p_x and of p_x^2.

(d) A reasonable estimate of the uncertainty in p_x is $\sqrt{\langle p_x^2 \rangle}$. Combine this with a reasonable estimate of the position uncertainty and show that the uncertainty principle you obtain is $\Delta x \Delta p_x \geq C$ where C is a constant of the order of $\hbar$.

The g.s. of problem 1(b) is

$u(x) = B \sin(kx)$ with $k = \frac{n\pi}{a}$

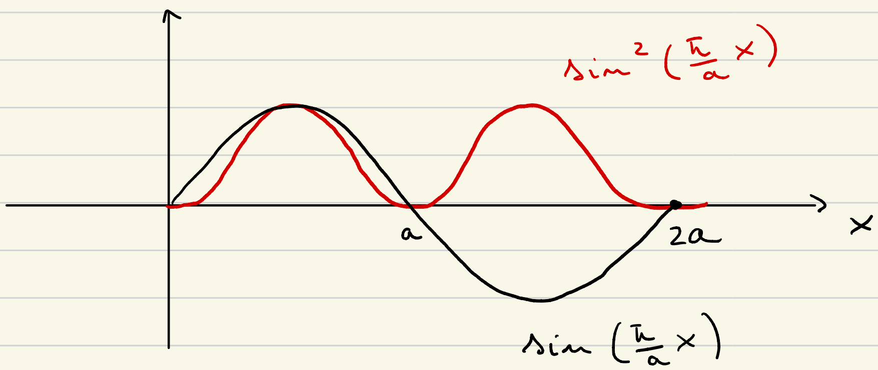
GROUND STATE $\longrightarrow$ $n = 1$

$k = \frac{\pi}{a}$ $\qquad u_{gs}(x) = B \sin\left(\frac{\pi}{a} x\right)$

a) normalise. The wf^n exists in the range $[0, a]$, therefore the integral of the probability density $|u(x)|^2$ has to be $= 1$ in these range

$$\int_0^a dx \; B^2 \sin^2\left(\frac{\pi}{a} x\right) = 1$$

Let's see what this $\int^{n}$ is



$$\int_0^a dx \left(\sin^2\left(\frac{\pi}{a}x\right) + \cos^2\left(\frac{\pi}{a}x\right)\right) = \int_0^a dx \; 1 = a$$

$$\rightarrow \int_0^a dx \, \sin^2\left(\frac{\pi}{a}x\right) = \frac{a}{2}$$

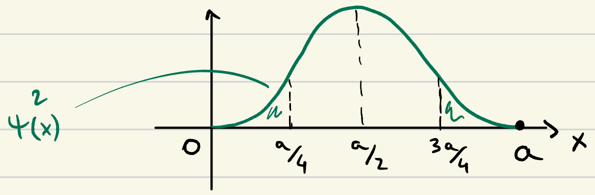
$$\int_0^a dx \; B^2 \sin^2\left(\frac{\pi}{a}x\right) = 1 = \frac{a}{2} B^2$$

$$B = \sqrt{\frac{2}{a}} \rightarrow u(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{\pi}{a}x\right)$$

Otherwise try to write the identity

$$\sin^2\left(\frac{\pi}{a}x\right) = \frac{1}{2} - \frac{1}{2}\cos\left(\frac{2\pi}{a}x\right)$$

where we used: $\sin^2(\theta) = \dfrac{1-\cos(2\theta)}{2}$



symmetry

b) $P\left(0 < x < \frac{a}{4} + \frac{3}{4} < x < a\right) = 2 \cdot \frac{2}{a} \int_0^{a/4} \sin^2\left(\frac{\pi}{a} x\right) dx$

this is why we have the "2" in front

$$= 2 \cdot \frac{2}{a} \int_0^{a/4} \left(\frac{1}{2} + \frac{\cos\left(\frac{2\pi}{a} x\right)}{2} \right) dx$$

$$= \dots$$

$$P\left(\frac{a}{4} < x < \frac{3}{4} a\right) = \frac{2}{a} \int_{a/4}^{3/4 a} \sin^2\left(\frac{\pi}{a} x\right) dx$$

$$= \dots$$

NB: Incomplete. I will try to upload the complete version asap. You are good w/ the material you have for the mid-term.