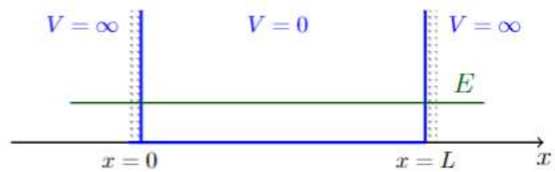
Deep Dive #10 - Quantum Mechanics

Its a good day to be a physics major!

$$-\frac{\hbar^2}{2m}\psi''(x) = E\,\psi(x),$$

$$\psi(0) = 0, \qquad \psi(L) = 0.$$



Question 1:

(1a) *(20 points)* Find all the eigenvalues and eigenfunctions in the problem above.

$$\Psi''(x) + \frac{2mE}{\hbar^2}\Psi(x) = 0$$
$$\lambda = \frac{2mE}{\hbar^2}$$

Can energy be negative? In this situation that would yield an exponential Ψ function which cannot be zero at two points. For $E = 0$ this is trivial, so we'll consider $E > 0$

The characteristic polynomial is

$$r^2 + \frac{2mE}{\hbar^2} = 0$$
$$r = \pm i\frac{\sqrt{2mE}}{\hbar}$$

This yields

$$\Psi(x) = c_+\cos(\frac{\sqrt{2mE}}{\hbar}x) + c_-\sin(\frac{\sqrt{2mE}}{\hbar}x)$$
$$\Psi(0) = 0 \implies 0 = c_+\cos(0) \implies c_+ = 0$$
$$\Psi(L) = 0 \implies 0 = c_-\sin(\frac{\sqrt{2mE}}{\hbar}L)$$

With $c \neq 0$, we have $\sin(n\pi) = 0$ this gives us

$$\frac{\sqrt{2mE}}{\hbar}L = n\pi$$
$$\frac{\sqrt{2mE}}{\hbar} = \frac{n\pi}{L}$$
$$\frac{2mE}{\hbar^2} = \left(\frac{n\pi}{L}\right)^2$$

Thus all eigenvalues are $\left(\frac{n\pi}{L}\right)^2$, and the allowed energies are

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

and the eigenfunctions are

$$y_n(x) = \sin(\sqrt{\lambda_n}x) = \sin(\frac{n\pi}{L}x)$$

for $c_- = 1$ (eigenfunctions can be scaled)

(1b)

$$L = a = 3$$
$$\alpha = 1, 2, 3, \ldots, n \implies \lambda_n = \left(\frac{\pi}{3}\right)^2, \left(\frac{2\pi}{3}\right)^2, \left(\frac{3\pi}{3}\right)^2, \ldots \left(\frac{n\pi}{L}\right)^2$$

(2a) *(20 points)* Split the solution function ψ as follows,

$$\psi(x) = \begin{cases} \psi_1(x) & \text{for} \quad 0 \leqslant x \leqslant a, \\ \psi_2(x) & \text{for} \qquad x \geqslant a, \end{cases}$$

Show that if you split the Schrödinger differential equation in the same way you can write it as

$$\begin{aligned} \psi_1'' &= -k^2\,\psi_1, & 0 \leqslant x \leqslant a, \\ \psi_2'' &= \kappa^2\,\psi_2, & x \geqslant a, \end{aligned}$$

where k and κ are appropriate positive constants given in terms of m, $\hbar$, V_0, and $|E|$. Find the formulas for $k > 0$ and $\kappa > 0$ in terms of the mass m, Planck constant $\hbar$, potential $V_0 > 0$, and energy $|E| > 0$. Also find one the boundary condition for ψ_1 and one boundary condition for ψ_2, obtained from the boundary conditions on ψ at $x = 0$ and at $x \to \infty$.

For $x < a, E - V > 0$ and we are in the well. For $x > a, E - V < 0$ we are outside the well, classically impossible.

Schrodigers equation can be split in the same way as $V(x)$

$$\psi''(x) = \begin{cases} \frac{2m}{\hbar^2}(-V_0 - E)\,\psi(x) & \text{for} \quad 0 \leq x \leq a \\ -\frac{2m}{\hbar^2}E\psi(x) & \text{for} \quad x \geq a \end{cases}$$

Remember that E<0 and can be represented correctly as E = -|E|

$$\psi''(x) = \begin{cases} -\frac{2m}{\hbar^2}(V_0 - |E|)\,\psi(x) & \text{for} \quad 0 \leq x \leq a \\ \frac{2m}{\hbar^2}|E|\psi(x) & \text{for} \quad x \geq a \end{cases}$$

This gets us our k-values

$$-k^2 = -\frac{2m}{\hbar^2}(V_0 - |E|)$$
$$\kappa^2 = \frac{2m}{\hbar^2}|E|$$

Also $\psi_1(0) = \psi_2(\infty) = 0$

2b

To be precise, there is one condition $E = -|E|$

The characteristic polynomial for ψ_1 yields

$$r_1^2 = -k^2$$
$$r_1 = \pm ik$$
$$\psi_1(x) = c_+ \cos(kx) + c_- \sin(kx)$$

And for ψ_2 yield

$$r_2^2 = \kappa^2$$
$$r_2 = \pm\kappa^2$$
$$\psi_2(x) = c_0 e^{\kappa x} + c_1 e^{-\kappa x}$$

From applying boundary condtions we see

$$\psi_1(0) = 0 \implies c_+ = 0$$
$$\psi_2(\infty) = 0 \implies c_0 = 0$$

There's another condition at $x = a$, but we get to that later

proportional to an exponential; let's call the proportionality factor d. The third part of the problem is to match the functions ψ_1 and ψ_2 found in (2b) at $x = 0$. Impose the matching conditions

$$\psi_1(a) = \psi_2(a), \qquad \psi_1'(a) = \psi_2'(a).$$

From these equations find a relation between k and κ and between the scaling factor for ψ_1, which we called it c, and the scaling factor for ψ_2, which we called it d, of the form

$$\frac{k}{\kappa} = -f(ka), \qquad d = c\, g(k,\kappa)\, e^{\kappa a},$$

Find the functions $f(ka)$ and $g(k,\kappa)$. These functions do not depend on c or d.

Lets do it.

$$\psi_1(a) = c\sin(k*a)$$
$$\psi_2(a) = de^{-\kappa a}$$
$$\psi_1'(a) = ck\cos(k*a)$$
$$\psi_2'(a) = -d\kappa e^{-\kappa * a}$$
$$\implies ck\cos(k*a) + d\kappa e^{-\kappa * a} = 0$$
$$\implies c\sin(k*a) - de^{-\kappa a} = 0$$
$$\kappa(c\sin(k*a) - de^{-\kappa a})$$

We can add the zeroes together

$$ck\cos(k*a) + d\kappa e^{-\kappa * a} + c\kappa\sin(k*a) - \kappa de^{-\kappa a} = 0$$
$$ck\cos(k*a) = -c\kappa\sin(k*a)$$
$$\frac{k}{\kappa} = -\frac{\sin(ka)}{\cos(ka)} - f(ka)$$

g is simple

$$de^{-\kappa a} = c\sin(k*a)$$
$$d = \frac{c\sin(k*a)}{e^{-\kappa a}} = c\sin(k*a)e^{\kappa a}$$
$$g(k) = \sin(k*a)$$

Wait, is it simple?

$$\implies ck\cos(k*a) + d\kappa e^{-\kappa * a} = 0$$
$$d\kappa e^{-\kappa * a} = -ck\cos(k*a)$$
$$d = c(-\frac{k}{\kappa}\cos(k*a))e^{\kappa a}$$
$$g(k, \kappa) = -\frac{k}{\kappa}\cos(k*a)$$

I'm not quite sure if the first formula is correct, but I'll leave it in anyways since I know the second one is what we were going for.

(3) there are two -9.2, -3.2, also trivially 0?