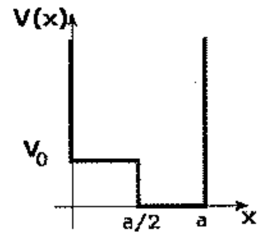
3 2015

Problem 3: Double Step Potential

Consider a single particle of mass m in a one dimensional well of width a and a potential, $V(x)$, given by:

$$V(x) = \begin{cases} \infty, & x < 0 \\ V_0, & 0 < x < \frac{a}{2} \\ 0, & \frac{a}{2} < x < a \\ \infty, & x > a \end{cases} \tag{1}$$



In this question, you will consider the special cases where this potential well has a bound state at the energy $E = V_0$. There are only certain values of V_0 and a where this will happen.

In this problem, use the constant

$$k = \sqrt{\frac{2mV_0}{\hbar^2}} \tag{2}$$

(a) [2 pts] For the energy $E = V_0$ in this potential, determine the general eigenfunction solutions to the time-independent Schrödinger equation in all regions of x. Show your work.

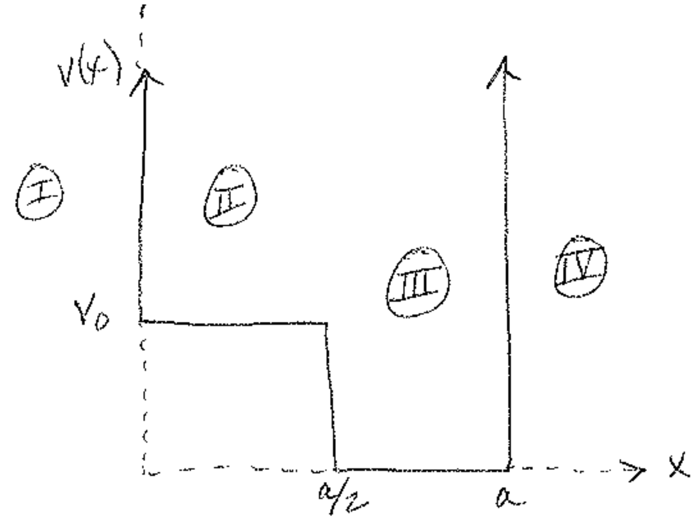
(b) [3 pts] Apply boundary conditions to determine relationships between the constants you introduced in writing the wave functions in part (a).

(c) [2 pts] From your results above, derive a transcendental equation that gives the values of V_0 where there is an energy eigenstate with $E = V_0$, for a fixed well width a. This equation will have the form $z = f(z)$ with $z = k\frac{a}{2}$. Plot this function and determine a relationship between the first energy V_0 that satisfies this equation and the bound state energies of a square well of width a.

(d) [2 pts] Qualitatively sketch the wave function that corresponds to the smallest value of V_0 that satisfies the transcendental equation from part (c), for a fixed value of a.

(e) [1 pt] Finally, consider the case where the width of the well is fixed but the potential step, V_0, can be changed. There are an infinite number of possible values of V_0 where the well contains an energy eigenstate with $E = V_0$. Describe, qualitatively, the changes in the wavefunctions of these eigenstates as V_0 gets larger.

(a)



We must have

$$\psi_{I}(x) = 0$$
$$\psi_{IV}(x) = 0$$

in regions (I) and (IV) since the potential is infinite. In region (III), we have $V=0$ so our Schrödinger equation is

$$-\frac{\hbar^2}{2m}\frac{d^2\psi_{III}}{dx^2} = E\psi_{III}$$

$$\frac{d^2\psi_{III}}{dx^2} = -\frac{2mE}{\hbar^2}\psi_{III}.$$

We have $E=V_0$, so letting

$$k = \frac{\sqrt{2mV_0}}{\hbar},$$

we have

$$\frac{d^2\psi_{III}}{dx^2} = -k^2\psi_{III}.$$

The general solution is then

$$\psi_{III}(x) = Ce^{ikx} + De^{-ikx}.$$

(a), cont'd...

In region (II), we have

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V_0\right]\psi_{II} = E\psi_{II}$$

$$-\frac{\hbar^2}{2m}\frac{d^2\psi_{II}}{dx^2} = (E - V_0)\psi_{II}.$$

But $E = V_0$, so we simply have

$$\frac{d^2\psi_{II}}{dx^2} = 0.$$

The general solution is then

$$\psi_{II}(x) = Ax + B.$$

Overall, our general eigenfunction solutions are

$$\boxed{\psi(x) = \begin{cases} 0 & , \quad x < 0 \\ Ax + B & , \quad 0 < x < \frac{a}{2} \\ Ce^{ikx} + De^{-ikx} & , \quad \frac{a}{2} < x < a \\ 0 & , \quad x > a \end{cases}}.$$

(b)

We must have $\psi(0) = 0$, so

$$\psi(0) = A(0) + B = 0,$$

which implies we must have $B = 0$. We also know $\psi(a) = 0$, so

$$\psi(a) = Ce^{ika} + De^{-ika} = 0$$
$$Ce^{2ika} + D = 0$$
$$D = -Ce^{2ika}.$$

We must also have

$$\psi_{II}(a/2) = \psi_{III}(a/2),$$

so since

$$\psi_{II}(x) = Ax$$
$$\psi_{III}(x) = C\left(e^{ikx} - e^{2ika}e^{-ikx}\right),$$

we have

$$A(a/2) = C\left(e^{ika/2} - e^{2ika}e^{-ika/2}\right)$$
$$\frac{Aa}{2} = C\left(e^{ika/2} - e^{3ika/2}\right),$$

or

$$A = \frac{2C}{a}\left(e^{ika/2} - e^{3ika/2}\right).$$

(b), cont'd...

We must also have

$$\left.\frac{d\psi_{II}}{dx}\right|_{x=a/2} = \left.\frac{d\psi_{III}}{dx}\right|_{x=a/2} ,$$

so

$$\frac{d\psi_{II}}{dx} = A$$

$$\frac{d\psi_{III}}{dx} = ikC\left(e^{ikx} + e^{2ika}e^{-ikx}\right)$$

and

$$A = ikC\left(e^{ika/2} + e^{2ika}e^{-ika/2}\right) = ikC\left(e^{ika/2} + e^{3ika/2}\right)$$

In summary:

(1) $A = \frac{2C}{a}\left(e^{ika/2} - e^{3ika/2}\right)$

(2) $A = ikC\left(e^{ika/2} + e^{3ika/2}\right)$

(3) $B = 0$

(4) $D = -Ce^{2ika}$

(c)

Setting ① and ② equal to one another, we have

$$\frac{2C}{a}\left(e^{ika/2} - e^{3ika/2}\right) = ikC\left(e^{ika/2} + e^{3ika/2}\right)$$

and rearranging,

$$k\frac{a}{2} = \frac{-i\left(e^{ika/2} - e^{3ika/2}\right)}{\left(e^{ika/2} + e^{3ika/2}\right)}$$

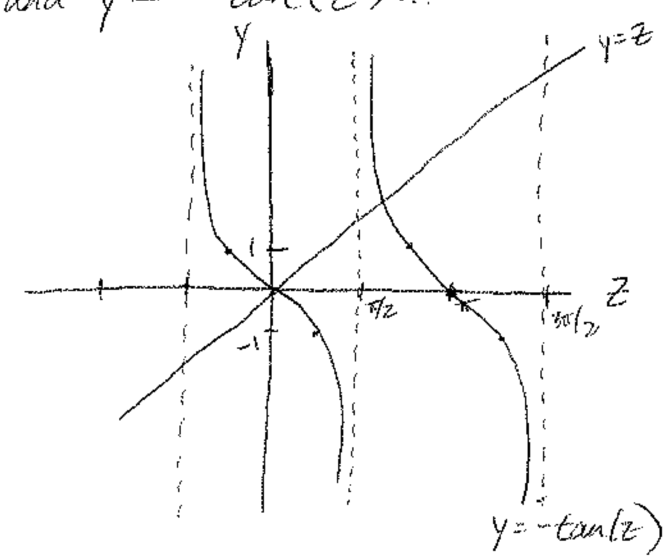
$$k\frac{a}{2} = -i\left(-i\tan(ka/2)\right)$$

$$k\frac{a}{2} = -\tan(ka/2).$$

Let $z = k\frac{a}{2}$. Then our transcendental equation is

$$\boxed{z = -\tan(z)}.$$

Plotting $y=z$ and $y=-\tan(z)$...



(c), cont'd...

We can see that our solutions occur where

$$z \gtrsim n\frac{\pi}{2}$$

where $n = 1, 3, 5, \ldots$ The first energy that satisfies this equation occurs for $n = 1$. Then

$$\frac{a}{2}\frac{\sqrt{2mV_0}}{\hbar} \approx n\frac{\pi}{2}$$

$$\sqrt{2mV_0} \approx \frac{n\pi\hbar}{a}$$

$$2mV_0 \approx \frac{n^2\pi^2\hbar^2}{a^2}$$

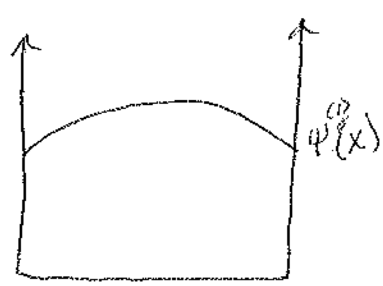
$$\boxed{V_0 \approx \frac{n^2\pi^2\hbar^2}{2ma^2}}$$

is our general expression and

$$\boxed{V_0^{(1)} \approx \frac{\pi^2\hbar^2}{2ma^2}}$$

(d)

The wavefunction should look like



(e) As V_0 gets larger, I would expect the wavefunctions to all converge to zero, where $V \to \infty$ implies $\psi \to 0$.