

# Homework 2

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## Time dependent Shrodinger's equation

$$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} + V(x, t)\psi \quad (1)$$

Where:

- $V(x, t)$  is the potential.

In order to get the wave function  $\Psi(x, t)$ , we need to solve the Schrödinger equation (1). If  $V$  is independent of  $t$ , the Schrödinger equation can be solved by the method of separation of variables.

$$\Psi(x, t) = \psi(x)\varphi(t) \quad (2)$$

Where:

- $\psi$  is the function of  $x$  alone, and  $\varphi$  is the function of  $t$  alone.

For the separable solutions we have:

$$\frac{\partial \Psi}{\partial t} = \psi \frac{d\varphi}{dt}, \quad \frac{\partial^2 \Psi}{\partial x^2} = \frac{d^2 \psi}{dx^2} \varphi$$

Substitute the solutions back to equation (1). Now we have:

$$i\hbar \psi \frac{d\varphi}{dt} = -\frac{\hbar^2}{2m} \frac{d^2 \psi}{dx^2} \varphi + V(x)\psi \quad (3)$$

Dividing both sides by  $\psi\varphi$ :

$$i\hbar \frac{1}{\varphi(t)} \frac{d\varphi}{dt} = -\frac{\hbar^2}{2m} \frac{d^2 \psi}{dx^2} \frac{1}{\psi(x)} + V(x) \quad (4)$$

Now the right side is the function of  $t$ , and the left side is the function of  $x$ . Next, we set left side equal separation constant  $E$ :

$$i\hbar \frac{1}{\varphi(t)} \frac{d\varphi(t)}{dt} = E \quad \text{or} \quad \frac{d\varphi(t)}{dt} = -\frac{iE}{\hbar} \varphi(t) \quad (5)$$

and:

$$-\frac{\hbar^2}{2m} \frac{d^2 \psi}{dx^2} \frac{1}{\psi(x)} + V(x)\psi = E \quad \text{or} \quad -\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + V(x)\psi = E\psi \quad (6)$$

## Time independent Shrodinger's equation

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + V(x)\psi = E\psi \quad (7)$$

Notice that the potential  $V$  only depends on  $x$ .

## Hamiltonian

They are states of *definite total energy*. In classical mechanics, the total energy (kinetic + potential) is called the Hamiltonian.

$$H(x, p) = \frac{p^2}{2m} + V(x) \quad (8)$$

The corresponding Hamiltonian operator, obtained by the canonical substitution  $p \rightarrow -i\hbar \frac{\partial}{\partial x}$

$$\hat{H} = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \quad (9)$$

$$\Rightarrow \hat{H}\psi = E\psi \quad (10)$$

The general solution is the linear combination of separable solutions.

$$\Psi_1(x, t) = \psi_1(x)e^{-iE_1 \frac{t}{\hbar}}, \Psi_2(x, t) = \psi_2(x)e^{-iE_2 \frac{t}{\hbar}}, \dots$$

There is a different wave function for each allowed energy.

The general solution:

$$\Psi(x, t) = \sum_{n=1}^{\infty} c_n \psi_n(x) e^{-iE_n \frac{t}{\hbar}} \quad (11)$$

## The Infinite Square Well

Suppose the potential energy:

$$V(x) = \begin{cases} 0 & , 0 \leq x \leq a, \\ \infty & , \text{otherwise} \end{cases} \quad (12)$$

Inside the well,  $V = 0$ :

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

or

$$\frac{d^2\psi}{dx^2} = -k^2\psi$$

where:

$$k \equiv \frac{\sqrt{2mE}}{\hbar}$$

The possible values of E:

$$E_n = \frac{n^2 \pi^2 \hbar^2}{2ma^2} = \frac{\hbar^2 k_n^2}{2m} \quad (13)$$

The solution inside the well:

$$\psi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a}x\right) \quad (14)$$

### Problem 2.4

$$\langle x \rangle = \int x |\Psi(x, t)|^2 dx$$

In the  $n$ th Stationary State:

$$|\Psi(x, t)|^2 = \Psi^* \Psi = \psi^* e^{+iE \frac{t}{\hbar}} \psi e^{-iE \frac{t}{\hbar}} = |\psi(x)|^2$$

So we have:

$$\langle x \rangle = \int x |\psi_n(x)|^2 dx$$

from (14) we have:

$$\langle x \rangle = \int_0^a x \left( \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a}x\right) \right)^2 dx \quad (15)$$

$$= \frac{2}{a} \int_0^a x \left( \sin\left(\frac{n\pi}{a}x\right) \right)^2 dx \quad (16)$$

$$= \frac{2}{a} \int_0^a x \left( \frac{1 - \cos(\alpha x)}{2} \right) dx \quad \text{where} \quad \frac{2n\pi}{a} = \alpha \quad (17)$$

$$= \frac{2}{a} \left( \int_0^a \frac{x}{2} dx - \frac{1}{2} \int_0^a x \cos(\alpha x) dx \right) \quad (18)$$

$$= \frac{2}{a} \left[ \frac{x^2}{4} \right]_0^a = \frac{a}{2} \quad (19)$$

$$\langle x^2 \rangle = \int_0^a x^2 \left( \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a}x\right) \right)^2 dx \quad (20)$$

$$= \int_0^a x^2 \left( \frac{2}{a} \sin^2\left(\frac{n\pi}{a}x\right) \right) dx \quad \text{Let} \quad \frac{n\pi x}{a} = y : \quad (21)$$

$$= \int_0^{n\pi} \left( \frac{ay}{n\pi} \right)^2 \left( \frac{2}{a} \right) \sin^2(y) \left( \frac{a}{n\pi} \right) dy \quad (22)$$

$$= \left( \frac{a}{n\pi} \right)^3 \left( \frac{2}{a} \right) \int_0^{n\pi} y^2 \sin^2(y) dy \quad (23)$$

$$= \left( \frac{a}{n\pi} \right)^3 \left( \frac{2}{a} \right) \left\{ \left[ y^2 \left( \frac{y}{2} - \frac{\sin 2y}{4} \right) \right]_0^{n\pi} - \int_0^{n\pi} 2y \left( \frac{y}{2} - \frac{\sin 2y}{4} \right) dy \right\} \quad (24)$$

$$= \left( \frac{a}{n\pi} \right)^3 \left( \frac{2}{a} \right) \left( \frac{(n\pi)^3}{6} - \frac{n\pi}{4} \right) \quad (25)$$

$$= a^2 \left( \frac{1}{3} - \frac{1}{2(n\pi)^2} \right) \quad (26)$$

$$(27)$$

$$\langle \rho \rangle = m \frac{d\langle x \rangle}{dt} = 0 \quad \text{since } \langle x \rangle \text{ is a constant} \quad (28)$$

$$(29)$$

$$\langle \rho^2 \rangle = \int_0^a \psi_n^* \left( \frac{\hbar}{i} \frac{d}{dx} \right)^2 \psi_n dx \quad (30)$$

$$= -\hbar^2 \int_0^a \psi_n^* \frac{d^2 \psi_n}{dx^2} dx \quad (31)$$

$$\text{From equation (7)} \quad (32)$$

$$\langle \rho^2 \rangle = -\hbar^2 \int_0^a \psi_n^2 \left( \frac{-2mE_n}{\hbar^2} \right) \psi_n dx \quad (33)$$

$$= 2mE_n \int_0^a |\psi_n|^2 dx = 2mE_n \quad (34)$$

$$\text{From equation (13):} \quad (35)$$

$$\langle \rho^2 \rangle = 2m \frac{n^2 \pi^2 \hbar^2}{2ma^2} = \frac{n^2 \pi^2 \hbar^2}{a^2} \quad (36)$$

$$\sigma_x = \sqrt{\langle x^2 \rangle - \langle x \rangle^2} = \sqrt{a^2 \left( \frac{1}{3} - \frac{1}{2(n\pi)^2} \right) - \frac{a^2}{4}} = \sqrt{\frac{a^2}{12}} \quad (37)$$

$$\sigma_p = \sqrt{\langle \rho^2 \rangle - \langle \rho \rangle^2} = \sqrt{\frac{n^2 \pi^2 \hbar^2}{a^2} - 0} = \frac{n\pi\hbar}{a} \quad (38)$$

## Problem 2.5

$$\Psi(x, 0) = A [\psi_1(x) + \psi_2(x)]$$

(a) Normalize  $\Psi(x, 0)$

$$\begin{aligned} \int |\Psi(x, 0)|^2 dx &= 1 \\ \int A^2 [\psi_1(x) + \psi_2(x)]^2 dx &= 1 \\ A^2 \int (\psi_1(x) + \psi_2(x))^* (\psi_1(x) + \psi_2(x)) dx &= 1 \\ A^2 \int |\psi_1(x)|^2 + |\psi_2(x)|^2 + \psi_1^*(x)\psi_2(x) + \psi_2^*(x)\psi_1(x) dx &= 1 \\ A^2 [1 + 1 + 0 + 0] &= 1 \\ A &= \frac{1}{\sqrt{2}} \end{aligned}$$

(b) From (11):

$$\Psi(x, t) = \sum_{n=1}^{\infty} c_n \psi_n(x) e^{-iE_n \frac{t}{\hbar}}$$

when  $t = 0$ :

$$\frac{1}{\sqrt{2}} (\psi_1(x) + \psi_2(x)) = \sum_{n=1}^{\infty} c_n \psi_n(x)$$

Now we have  $c_1 = c_2 = \frac{1}{\sqrt{2}}$

$$\Psi(x, t) = \frac{1}{\sqrt{2}} \left[ \psi_1(x) e^{-iE_1 \frac{t}{\hbar}} + \psi_2(x) e^{-iE_2 \frac{t}{\hbar}} \right] \quad (39)$$

$$= \frac{1}{\sqrt{2}} \left[ \psi_1(x) e^{-i \frac{\pi^2 \hbar}{2ma^2} t} + \psi_2(x) e^{-i \frac{4\pi^2 \hbar}{2ma^2} t} \right] \quad (40)$$

$$= \frac{1}{\sqrt{2}} \left( \sqrt{\frac{2}{a}} \sin\left(\frac{\pi x}{a}\right) e^{-i\omega t} + \sqrt{\frac{2}{a}} \sin\left(\frac{2\pi x}{a}\right) e^{-i4\omega t} \right) \quad (41)$$

$$= \frac{1}{\sqrt{a}} \left( \sin\left(\frac{\pi x}{a}\right) e^{-i\omega t} + \sin\left(\frac{2\pi x}{a}\right) e^{-i4\omega t} \right) \quad (42)$$

$$\Psi^*(x, t) \cdot \Psi(x, t) = \frac{1}{a} \left( \sin\left(\frac{\pi x}{a}\right) e^{i\omega t} + \sin\left(\frac{2\pi x}{a}\right) e^{i4\omega t} \right) \cdot \left( \sin\left(\frac{\pi x}{a}\right) e^{-i\omega t} + \sin\left(\frac{2\pi x}{a}\right) e^{-i4\omega t} \right) \quad (43)$$

$$= \frac{1}{a} \left( \sin^2\left(\frac{\pi x}{a}\right) + \sin^2\left(\frac{2\pi x}{a}\right) + \sin\left(\frac{\pi x}{a}\right) \sin\left(\frac{2\pi x}{a}\right) (e^{i3\omega t} + e^{-i3\omega t}) \right) \quad (44)$$

$$= \frac{1}{a} \left( \sin^2\left(\frac{\pi x}{a}\right) + \sin^2\left(\frac{2\pi x}{a}\right) + 2 \sin\left(\frac{\pi x}{a}\right) \sin\left(\frac{2\pi x}{a}\right) \cos(3\omega t) \right) \quad (45)$$

(c)

$$\langle x \rangle = \int_0^a x |\Psi(x, t)|^2 dx \quad (46)$$

$$= \int_0^a x \frac{1}{a} \left( \sin^2\left(\frac{\pi x}{a}\right) + \sin^2\left(\frac{2\pi x}{a}\right) + 2 \sin\left(\frac{\pi x}{a}\right) \sin\left(\frac{2\pi x}{a}\right) \cos(3\omega t) \right) dx \quad (47)$$

$$= \frac{1}{a} \cos(3\omega t) \left( \int_0^a x \sin^2\left(\frac{\pi x}{a}\right) dx + \int_0^a x \sin^2\left(\frac{2\pi x}{a}\right) dx + 2 \int_0^a x \sin\left(\frac{\pi x}{a}\right) \sin\left(\frac{2\pi x}{a}\right) dx \right) \quad (48)$$

$$= \frac{1}{a} \cos(3\omega t) \left( \frac{a^2}{4} + \frac{a^2}{4} + 2 \left( \frac{-8a^2}{9\pi^2} \right) \right) \quad (49)$$

(d)

$$\langle p \rangle = m \frac{d\langle x \rangle}{dt} \quad (50)$$

$$= m \frac{16aw \sin(3tw)}{3\pi^2} \quad (51)$$

(e)

$$\langle H \rangle = \sum_{n=1}^{\infty} |c_n|^2 E_n$$

we have  $c_1 = c_2 = \frac{1}{\sqrt{2}}$

$$\langle H \rangle = \frac{1}{2} E_1 + \frac{1}{2} E_2 = \frac{5\pi^2 \hbar^2}{4ma^2}$$

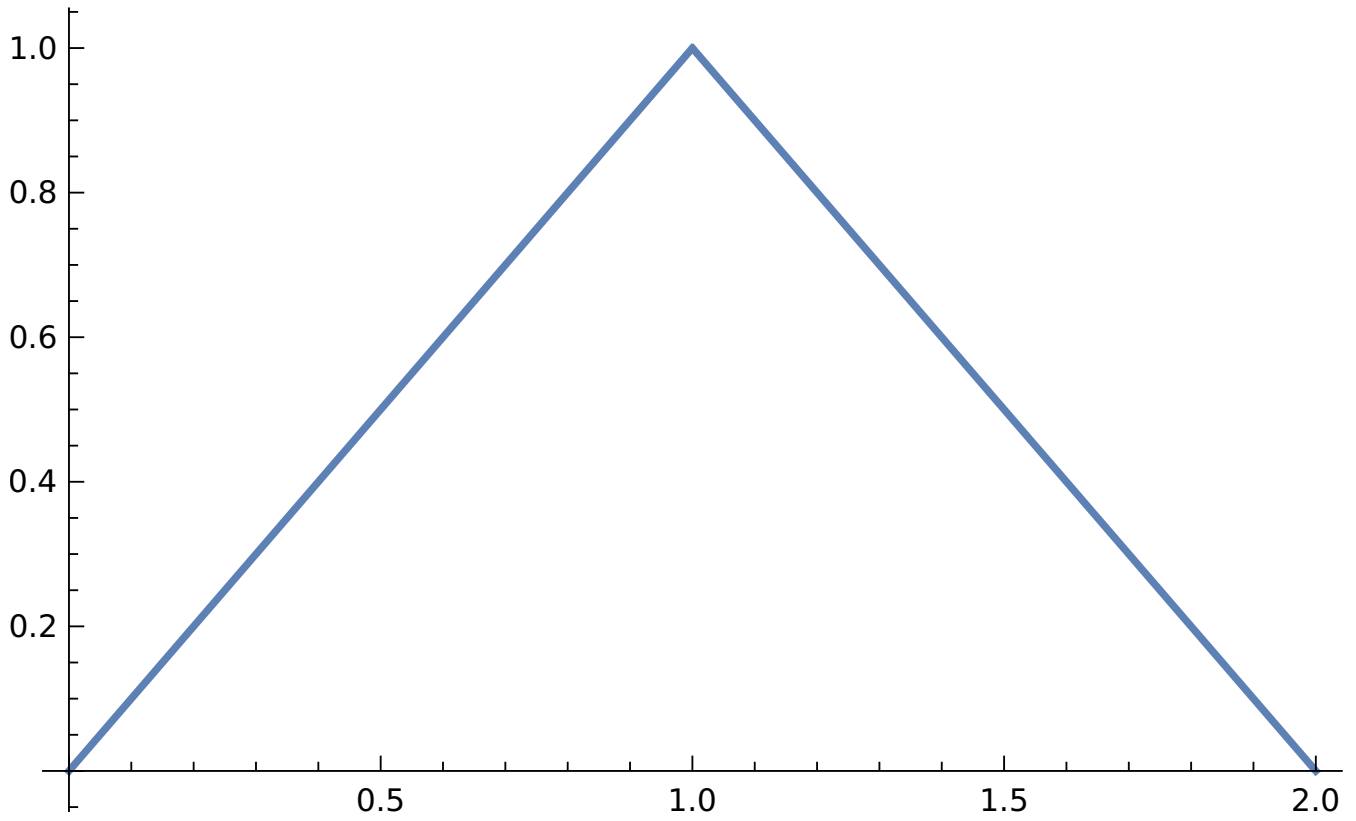


Figure 1:  $A = 1$  and  $a = 2$

### Problem 2.7

(a)

$$\int_{-\infty}^{\infty} |\Psi(x, 0)|^2 dx = 1$$

$$\int_0^{\frac{a}{2}} (Ax)^2 dx + \int_{\frac{a}{2}}^a (A(a-x)^2) dx = 1 \quad (52)$$

$$\frac{a^3}{12} A^2 = 1 \quad (53)$$

$$A = \sqrt{\frac{12}{a^3}} \quad (54)$$

(b)

$$\Psi(x, t) = \sum_{n=1}^{\infty} c_n \psi_n(x) e^{-iE_n \frac{t}{\hbar}}$$

when  $t = 0$

$$\Psi(x, 0) = \sum_{n=1}^{\infty} c_n \psi_n(x)$$

$$\int \sum_{n=1}^{\infty} c_n \psi_n(x) \psi_m(x) dx = \int \Psi(x, 0) \psi_m(x) dx = \delta_{mn} \quad (55)$$

$$(56)$$

$$c_m = \int_0^a \Psi(x, 0) \psi_m(x) dx \quad (57)$$

$$= \int_0^{\frac{a}{2}} A x \psi_m(x) dx + \int_{\frac{a}{2}}^a A(a-x) \psi_m(x) dx \quad (58)$$

$$= A \sqrt{\frac{2}{a}} \int_0^{\frac{a}{2}} x \sin\left(\frac{m\pi x}{a}\right) dx + A \int_{\frac{a}{2}}^a (a-x) \sin\left(\frac{m\pi x}{a}\right) dx \quad (59)$$

$$= A \sqrt{\frac{2}{a}} \left( \frac{a \left( -\frac{1}{2} a m \pi \cos\left(\frac{m\pi}{2}\right) + a \sin\left(\frac{m\pi}{2}\right) \right)}{m^2 \pi^2} \right) + A \left( \frac{a^2 \left( m \pi \cos\left(\frac{m\pi}{2}\right) + 2 \sin\left(\frac{m\pi}{2}\right) - 2 \sin(m\pi) \right)}{2 m^2 \pi^2} \right) \quad (60)$$

$$= \frac{4\sqrt{6}}{m^2 \pi^2} (-1)^{\frac{m-1}{2}} \quad (61)$$

$$\Psi(x, t) = \frac{4\sqrt{6}}{\pi^2} \sum_{n=1}^{\infty} \frac{1}{n^2} \psi_n(x) e^{-i E_n \frac{t}{\hbar}} (-1)^{\frac{n-1}{2}}$$

(c) The probability of  $E_n$  is equal to  $|c_n|^2$ . We have:

$$c_n = \frac{4\sqrt{6}}{n^2 \pi^2} \quad \text{with } n = 1, 3, 5, \dots$$

$$|c_1|^2 = \left( \frac{4\sqrt{6}}{\pi^2} \right)^2$$

(d) The expectation value of the energy:

$$\langle H \rangle = \sum_{n=1}^{\infty} |c_n|^2 E_n \quad (62)$$

$$= \sum_{n=1,3,5,\dots}^{\infty} \left( \frac{4\sqrt{6}}{n^2 \pi^2} \right)^2 \frac{n^2 \pi^2 \hbar^2}{2ma^2} \quad (63)$$

$$= \frac{48\hbar^2}{\pi^2 ma^2} \sum_{n=1,3,5,\dots}^{\infty} \frac{1}{n^2} \quad (64)$$

### Problem 2.8

Normalizing  $\Psi(x, 0)$ :

$$\int_0^a |\Psi(x, 0)|^2 dx = 1 \quad (65)$$

$$\int_0^{\frac{a}{2}} |A|^2 dx = 1 \quad (66)$$

$$\Rightarrow A = \sqrt{\frac{2}{a}} \quad (67)$$

$$\Psi(x, t) = \sum_{n=1}^{\infty} c_n \psi_n(x) e^{-iE_n \frac{t}{\hbar}}$$

Because  $\frac{\pi^2 \hbar^2}{2ma^2} = E_1$ . So the probability of  $E_1$  is equal to  $|c_1|^2$ .

$$\int \psi_1(x) \Psi(x, 0) dx = \int \sum_{n=1}^{\infty} c_n \psi_n(x) \psi_1(x) dx = c_1 \quad (68)$$

$$c_1 = \frac{2}{a} \int_0^{\frac{a}{2}} \sin\left(\frac{\pi}{a}x\right) dx \quad (69)$$

$$= \frac{2}{a} \frac{a}{\pi} = \frac{2}{\pi} \quad (70)$$

$$\Rightarrow |c_1|^2 = \frac{4}{\pi^2} \quad (71)$$