Homework 2

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Time dependent Shrodinger's equation

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

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.

$$\Psi(x,t) = \psi(x)\varphi(t) \tag{2}$$

Where:

- ψ is the function of x alone, and φ is the function of t alone.

For the separable solutions we have:

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

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

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

Dividing both sides by $\psi\varphi$:

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

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

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

and:

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

Time independent Shrodinger's equation

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

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.

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

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

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

$$\Rightarrow \hat{H}\psi = E\psi \tag{10}$$

The general solution is the linear combination of separable solutions.

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

There is a different wave function for each allowed energy.

The general solution:

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

The Infinite Square Well

Suppose the potential energy:

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

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:

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

The solution inside the well:

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

Problem 2.4

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

In the nth 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:

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

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

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

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

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

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

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

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

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

$$= \left(\frac{a}{n\pi}\right)^3\left(\frac{2}{a}\right)\left\{\left[y^2\left(\frac{y}{2}-\frac{\sin 2y}{4}\right)\right]_0^{n\pi} - \int_0^{n\pi} 2y\left(\frac{y}{2}-\frac{sin2y}{4}\right)dy\right\} \tag{24}$$

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

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

$$\tag{27}$$

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

$$\tag{29}$$

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

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

From equation (7) (32)

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

$$= 2mE_n \int_0^a |\psi_n|^2 dx = 2mE_n \tag{34}$$

From equation (13) : (35)

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

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

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

Problem 2.5

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

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

$$\int |\Psi(x,0)|^2 dx = 1$$

$$\int A^2 \left[\psi_1(x) + \psi_2(x)\right]^2 dx = 1$$

$$A^2 \int \left(\psi_1(x) + \psi_2(x)\right)^* \left(\psi_1(x) + \psi_2(x)\right) dx = 1$$

$$A^2 \int |\psi_1(x)|^2 + |\psi_2(x)|^2 + \psi_1^*(x)\psi_2(x) + \psi_2^*(x)\psi_1(x) dx = 1$$

$$A^2 \left[1 + 1 + 0 + 0\right] = 1$$

$$A = \frac{1}{\sqrt{2}}$$

(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 $c_1 = c_2 = \frac{1}{\sqrt{2}}$

$$\Psi(x,t) = \frac{1}{\sqrt{2}}\left[\psi_1(x)e^{-iE_1\frac{t}{\hbar}} + \psi_2(x)e^{-iE_2\frac{t}{\hbar}}\right] \tag{39}$$
$$= \frac{1}{\sqrt{2}}\left[\psi_1(x)e^{-i\frac{\pi^2\hbar}{2ma^2}t} + \psi_2(x)e^{-i\frac{4\pi^2\hbar}{2ma^2}t}\right] \tag{40}$$
$$= \frac{1}{\sqrt{2}}\left(\sqrt{\frac{2}{a}}\sin\left(\frac{\pi}{a}x\right)e^{-i\omega t} + \sqrt{\frac{2}{a}}\sin\left(\frac{2\pi}{a}x\right)e^{-i4\omega t}\right) \tag{41}$$
$$= \frac{1}{\sqrt{a}}\left(\sin\left(\frac{\pi x}{a}\right)e^{-i\omega t} + \sin\left(\frac{2\pi x}{a}\right)e^{-i4\omega t}\right) \tag{42}$$
$$\Psi^*(x,t)\cdot\Psi(x,t) = \frac{1}{a}\left(\sin\left(\frac{\pi x}{a}\right)e^{i\omega t} + \sin\left(\frac{2\pi x}{a}\right)e^{i4\omega t}\right)\cdot\left(\sin\left(\frac{\pi x}{a}\right)e^{-i\omega t} + \sin\left(\frac{2\pi x}{a}\right)e^{-i4\omega t}\right) \tag{43}$$
$$= \frac{1}{a}\left(\sin^2\left(\frac{\pi x}{a}\right) + \sin^2\left(\frac{2\pi x}{a}\right) + \sin\left(\frac{\pi x}{a}\right)\sin\left(\frac{2\pi x}{a}\right)\left(e^{i3\omega t} + e^{-i3\omega t}\right)\right) \tag{44}$$
$$= \frac{1}{a}\left(\sin^2\left(\frac{\pi x}{a}\right) + \sin^2\left(\frac{2\pi x}{a}\right) + 2\sin\left(\frac{\pi x}{a}\right)\sin\left(\frac{2\pi x}{a}\right)\cos(3\omega t)\right) \tag{45}$$

(c)

$$\langle x\rangle = \int_0^a x|\Psi(x,t)|^2 dx \tag{46}$$
$$= \int_0^a x\frac{1}{a}\left(\sin^2\left(\frac{\pi x}{a}\right) + \sin^2\left(\frac{2\pi x}{a}\right) + 2\sin\left(\frac{\pi x}{a}\right)\sin\left(\frac{2\pi x}{a}\right)\cos(3\omega t)\right)dx \tag{47}$$
$$= \frac{1}{a}\cos(3\omega t)\left(\int_0^a x\sin^2\left(\frac{\pi x}{a}\right)dx + \int_0^a x\sin^2\left(\frac{2\pi x}{a}\right)dx + 2\int_0^a x\sin\left(\frac{\pi x}{a}\right)\sin\left(\frac{2\pi x}{a}\right)dx\right) \tag{48}$$
$$= \frac{1}{a}\cos(3\omega t)\left(\frac{a^2}{4} + \frac{a^2}{4} + 2\left(\frac{-8a^2}{9\pi^2}\right)\right) \tag{49}$$

(d)

$$\langle p\rangle = m\frac{d\langle x\rangle}{dt} \tag{50}$$
$$= m\frac{16aw\sin(3tw)}{3\pi^2} \tag{51}$$

(e)

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

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

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

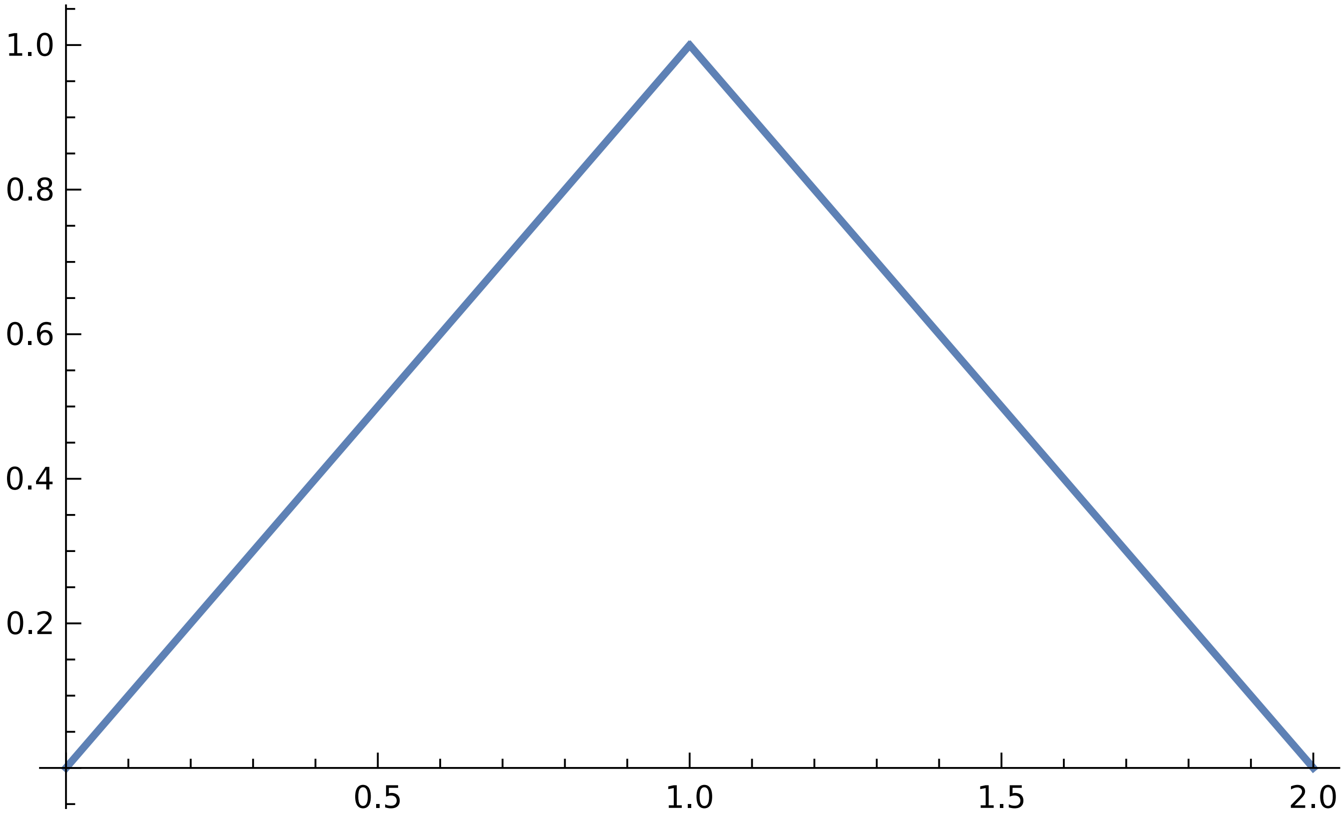

Figure 1: A = 1 and a = 2

Problem 2.7

(a)

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

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

$$\frac{a^3}{12} A^2 = 1 \tag{53}$$

$$A = \sqrt{\frac{12}{a^3}} \tag{54}$$

(b)

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

when $t = 0$

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

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

$$\tag{56}$$

$$\begin{aligned}
c_m &= \int_0^a \Psi(x,0)\psi_m(x)dx && (57)\\
&= \int_0^{\frac{a}{2}} Ax\psi_m(x)dx + \int_{\frac{a}{2}}^a A(a-x)\psi_m(x)dx && (58)\\
&= A\sqrt{\frac{2}{a}} \int_0^{\frac{a}{2}} xsin\left(\frac{m\pi x}{a}\right)dx + A\int_{\frac{a}{2}}^a (a-x)\sin\left(\frac{m\pi x}{a}\right)dx && (59)\\
&= A\sqrt{\frac{2}{a}} \left(\frac{a\left(-\frac{1}{2}am\pi\cos\left(\frac{m\pi}{2}\right) + a\sin\left(\frac{m\pi}{2}\right)\right)}{m^2\pi^2}\right) + A\left(\frac{a^2\left(m\pi\cos\left(\frac{m\pi}{2}\right) + 2\sin\left(\frac{m\pi}{2}\right) - 2\sin\left(m\pi\right)\right)}{2m^2\pi^2}\right) && (60)\\
&= \frac{4\sqrt{6}}{m^2\pi^2}(-1)^{\frac{m-1}{2}} && (61)
\end{aligned}$$

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

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

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

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

(d) The expectation value of the energy:

$$\begin{aligned}
\langle H \rangle &= \sum_{n=1}^{\infty} |c_n|^2 E_n && (62)\\
&= \sum_{n=1,3,5,\dots}^{\infty} \left(\frac{4\sqrt{6}}{n^2\pi^2}\right)^2 \frac{n^2\pi^2\hbar^2}{2ma^2} && (63)\\
&= \frac{48\hbar^2}{\pi^2 ma^2} \sum_{n=1,3,5,\dots}^{\infty} \frac{1}{n^2} && (64)
\end{aligned}$$

Problem 2.8

Normalizing $\Psi(x,0)$:

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

$$\int_0^{\frac{a}{2}} |A|^2 dx = 1 \tag{66}$$

$$\Rightarrow A = \sqrt{\frac{2}{a}} \tag{67}$$

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

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

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

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

$$= \frac{2}{a}\frac{a}{\pi} = \frac{2}{\pi} \tag{70}$$

$$\Rightarrow |c_1|^2 = \frac{4}{\pi^2} \tag{71}$$