ZCT 205 Quantum Mechanics

Tutorial 2.1 (40%)

Q1 Separation of Variables

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

LHS is a function of t alone while the RHS is a function of x alone. Equation above is true only if both sides equal to a constant. We will call this constant E, so that

$$\frac{d\varphi}{dt} = -\frac{iE}{\hbar}\varphi \qquad\qquad -\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V(x) = E\psi$$

Show the solution to the time-independent part is

$$\varphi(t) = e^{-iEt/\hbar}$$

(2%)

<u>Solution</u>

Time-independent part of the equation : $\frac{d\varphi}{dt} = -\frac{iE}{\hbar}\varphi$

By using separation of variables,

$\int \frac{1}{\varphi} d\varphi = -\frac{iE}{\hbar}\int dt$

$\ln \varphi = -\frac{iE}{\hbar}t + C$ ✓

$\varphi = Ae^{-iEt/\hbar}$ where $A = e^C$

As the arbitrary constant is being absorbed, the solution to the time-independent part is

$\varphi(t) = e^{-iEt/\hbar}$ (Shown) ✓

Q2

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

Show that the total solution (above) is a solution to the time-dependent Schroedinger equation (TDSE), which is given by

$$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 \Psi}{\partial x^2} + V\Psi$$

(6%)

<u>*Solution*</u>

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

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

$$\frac{\partial^2 \Psi(x,t)}{\partial x^2} = \sum_{n=1}^{\infty} c_n \frac{\partial^2 \psi_n(x)}{\partial x^2} e^{-iE_n t/\hbar}$$ ✓

LHS of TDSE : $i\hbar \frac{\partial \Psi}{\partial t} = i\hbar \left[-\frac{i}{\hbar}\sum_{n=1}^{\infty} c_n \psi_n(x) E_n e^{-iE_n t/\hbar}\right]$

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

$$= \sum_{n=1}^{\infty} E_n \Psi_n(x,t)$$ ✓

RHS of TDSE : $-\frac{\hbar^2}{2m}\frac{\partial^2 \Psi}{\partial x^2} + V\Psi = -\frac{\hbar^2}{2m}\left[\sum_{n=1}^{\infty} c_n \frac{\partial^2 \psi_n(x)}{\partial x^2} e^{-\frac{iE_n t}{\hbar}}\right] + V\sum_{n=1}^{\infty} \Psi_n(x,t)$

$$= -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\sum_{n=1}^{\infty} c_n \psi_n(x) e^{-iE_n t/\hbar} + V\sum_{n=1}^{\infty} \Psi_n(x,t)$$ ✓

$$= \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V\right)\sum_{n=1}^{\infty} \Psi_n(x,t)$$

$$= \hat{H}\sum_{n=1}^{\infty} \Psi_n(x,t)$$ ✓

$\therefore \sum_{n=1}^{\infty} E_n \Psi_n(x,t) = \hat{H}\sum_{n=1}^{\infty} \Psi_n(x,t)$ (Shown) ✓

Q3

(i) For an infinite square well,

$$\frac{d^2\psi}{dx^2} = -k^2\psi \text{, where } k \equiv \frac{\sqrt{2mE}}{\hbar} \text{ ; } k^2 \geq 0$$

E must be positive. Why?

(ii) Using Euler relation, show that

$$\psi(x) = C_1 e^{ikx} + C_2 e^{-ikx}$$
$$= A \sin kx + B \cos kx$$

(2%)

<u>*Solution*</u>

(i) For an infinite square well, $V_{min} = 0$. E must be larger than V_{min} so that the wave function is valid and normalizable. ✓

(ii) Euler relation is given by $e^{ikx} = \cos kx + i \sin kx$

$$\psi(x) = C_1 e^{ikx} + C_2 e^{-ikx}$$
$$= C_1(\cos kx + i \sin kx) + C_2(\cos kx - i \sin kx)$$
$$= i(C_1 - C_2) \sin kx + (C_1 + C_2) \cos kx$$

Let $A = i(C_1 - C_2)$ and $B = (C_1 + C_2)$

$\psi(x) = A \sin kx + B \cos kx$ (Shown) ✓

Q4 The TISE solutions are mutually orthogonal

Given ψ_n solution to a time-independent Schroedinger equation (TISE)

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V(x) = E\psi$$

Prove

$$\int \psi_m{}^*(x)\psi_n(x)dx = \delta_{mn}$$

(8%)

Solution

For an infinite square well, $\psi_n(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi}{a}x\right)$

$\int_0^a \psi_m(x)^*\psi_n(x)dx = \frac{2}{a}\int_0^a \sin\left(\frac{m\pi}{a}x\right)\sin\left(\frac{n\pi}{a}x\right)dx$ ✓

When $m = n$, $\int_0^a \psi_n(x)^*\psi_n(x)dx = \frac{2}{a}\int_0^a \sin^2\left(\frac{n\pi}{a}x\right)dx = \frac{2}{a}\int_0^a \frac{1}{2}\left[1 - \cos^2\left(\frac{n\pi}{a}x\right)\right]dx$ ✓

$$= \frac{1}{a}\left[x - \frac{a}{2n\pi}\sin\left(\frac{n\pi}{a}x\right)\right]_0^a$$ ✓

$$= 1$$ ✓

When $m \neq n$, employing trigonometry identity : $\sin\alpha\sin\beta = \frac{\cos(\alpha-\beta)-\cos(\alpha+\beta)}{2}$

$\int_0^a \psi_m(x)^*\psi_n(x)dx = \frac{1}{a}\int_0^a \left[\cos\left(\frac{m-n}{a}\pi x\right) - \cos\left(\frac{m+n}{a}\pi x\right)\right]dx$ ✓

$$= \frac{1}{a}\left[\frac{a}{(m-n)\pi}\sin\left(\frac{m-n}{a}\pi x\right) - \frac{a}{(m+n)\pi}\sin\left(\frac{m+n}{a}\pi x\right)\right]_0^a$$ ✓

$$= 0$$ ✓

$\therefore \int \psi_m(x)^*\psi_n(x)dx = \begin{Bmatrix} 0 \ ; \ m \neq n \\ 1 \ ; \ m = n \end{Bmatrix} = \delta_{mn}$ (Shown) ✓

Q5

Prove that

$$c_n = \int \psi_n(x)^* f(x)\, dx$$

This can be simply proven by making use of the orthogonally of the TISE solutions :

$$\int \psi_m(x)^* \psi_n(x) dx = \delta_{mn}$$

(3%)

Solution

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

Let $\quad f(x) = \Psi(x,0) = \sum_{m=1}^{\infty} c_m \psi_m(x)$

$\int \psi_n(x)^* f(x)\, dx = \int \psi_n(x)^* [\sum_{m=1}^{\infty} c_m \psi_m(x)]\, dx$ ✓

$= \sum_{m=1}^{\infty} c_m \int \psi_n(x)^* \psi_m(x)\, dx \quad ; \quad \int \psi_m(x)^* \psi_n(x) dx = \delta_{mn}$

$= \sum_{m=1}^{\infty} c_m \delta_{mn}$ ✓

Since $\delta_{mn} = \begin{cases} 0 \ ; \ m \neq n \\ 1 \ ; \ m = n \end{cases}$, all terms vanish except for c_n.

$\therefore \int \psi_n(x)^* f(x)\, dx = c_n$ (Shown) ✓

Q6

Use

$$\int |\Psi(x,t)|^2 \, dx = 1 \qquad \text{and} \qquad \int \psi_m(x)^* \psi_n(x) dx = \delta_{mn}$$

to prove

$$\sum_{n=1}^{\infty} |c_n|^2 = 1$$

(3%)

Solution

At $t = 0$,

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

$\int [\sum_{m=1}^{\infty} c_m \psi_m(x)]^* [\sum_{n=1}^{\infty} c_n \psi_n(x)] \, dx = 1$ ✓

$\sum_{m=1}^{\infty} \sum_{n=1}^{\infty} c_m{}^* c_n \int \psi_m(x)^* \psi_n(x) dx = 1 \qquad ; \qquad \int \psi_m(x)^* \psi_n(x) dx = \delta_{mn}$

$\sum_{m=1}^{\infty} \sum_{n=1}^{\infty} c_m{}^* c_n \delta_{mn} = 1$ ✓

Since $\delta_{mn} = \begin{cases} 0 \ ; \ m \neq n \\ 1 \ ; \ m = n \end{cases}$, all terms vanish except for $m = n$.

$\sum_{n=1}^{\infty} c_n{}^* c_n = 1 \qquad ; \qquad c_n{}^* c_n = |c_n|^2$

$\therefore \ \sum_{n=1}^{\infty} |c_n|^2 = 1$ (Shown) ✓

Q8

Consider the solutions to a quantum harmonic potential.

(i) Assume n is 1, write down $h(\xi)$, hence the stationary wave function, $\psi_1(\xi)$.

(ii) Assume n is 2, write down $h(\xi)$, hence the stationary wave function, $\psi_2(\xi)$.

(5%)

Solution

$$h(\xi) = \sum_{j=0}^{n} a_j \xi^j = h(\xi)_{odd} + h(\xi)_{even}$$

$$a_{j+2} = \frac{j+2-K}{(j+1)(j+2)} a_j \qquad ; \qquad K = 2n+1$$

$$\psi(\xi) = h(\xi) e^{-\xi^2/2}$$

(i) $h_1(\xi) = a_1 \xi$ ✓

$\psi_1(\xi) = a_1 \xi e^{-\xi^2/2}$ ✓

(ii) $K = 5 \quad ; \quad a_2 = -2a_0$ ✓

$h_2(\xi) = a_0 + a_2 \xi^2 = (1 - 2\xi^2) a_0$ ✓

$\psi_2(\xi) = (1 - 2\xi^2) a_0 e^{-\xi^2/2}$ ✓

Q9

Consider the solutions to a quantum harmonic potential.

(i) Derive H_1, H_2, H_3 from the Rodrigues formula.

(ii) Derive H_3, H_4 from H_1, H_2 using the recursion relation.

(iii) As a check, the function H_3 derived using both methods must agree.

(9%)

Solution

(i) Rodrigues formula : $H_n(\xi) = (-1)^n e^{\xi^2} \left(\frac{d}{d\xi}\right)^n e^{-\xi^2}$

$$H_1(\xi) = (-1)e^{\xi^2} \frac{d}{d\xi}\left(e^{-\xi^2}\right) = 2\xi$$ ✓✓

$$H_2(\xi) = (1)e^{\xi^2} \left(\frac{d}{d\xi}\right)^2 e^{-\xi^2} = 4\xi^2 - 2$$ ✓✓

$$H_3(\xi) = (-1)^3 e^{\xi^2} \left(\frac{d}{d\xi}\right)^3 e^{-\xi^2} = 8\xi^3 - 12\xi$$ ✓✓

(ii) Recursion relation : $H_{n+1}(\xi) = 2\xi H_n(\xi) - 2nH_{n-1}(\xi)$

$$\begin{aligned} H_3(\xi) &= H_{n+1}(\xi) \qquad ; \quad n = 2 \\ &= 2\xi H_2(\xi) - 2(2)H_1(\xi) \\ &= 2\xi(4\xi^2 - 2) - 4(2\xi) \\ &= 8\xi^3 - 12\xi \end{aligned}$$ ✓

$$\begin{aligned} H_4(\xi) &= H_{3+1}(\xi) \qquad ; \quad n = 3 \\ &= 2\xi H_3(\xi) - 2(3)H_2(\xi) \\ &= 2\xi(8\xi^3 - 12\xi) - 4(4\xi^2 - 2) \\ &= 16\xi^4 - 48\xi^2 + 12 \end{aligned}$$ ✓

(iii) Function $H_3(\xi)$ derived from both Rodrigues formula and recursion formula are the same. ✓

Q10

The time-dependent "stationary" solution is a travelling plane wave :

$$\Psi_k(x,t) = Ae^{ik\left(x-\frac{\hbar k}{2m}t\right)}$$

Show

$$\int_{-\infty}^{\infty} \Psi_k{}^*\Psi_k \, dx \to \infty$$

(2%)

Solution

$$\Psi_k(x,t) = Ae^{ik\left(x-\frac{\hbar k}{2m}t\right)}$$

$$\Psi_k{}^*(x,t) = A^*e^{-ik\left(x-\frac{\hbar k}{2m}t\right)}$$

$$\int_{-\infty}^{\infty} \Psi_k{}^*\Psi_k \, dx = \int_{-\infty}^{\infty} \left[A^*e^{-ik\left(x-\frac{\hbar k}{2m}t\right)}\right]\left[Ae^{ik\left(x-\frac{\hbar k}{2m}t\right)}\right] dx$$

$$= |A|^2 \int_{-\infty}^{\infty} dx$$ ✓

$$= |A|^2 [x]_{-\infty}^{\infty}$$

$\therefore \int_{-\infty}^{\infty} \Psi_k{}^*\Psi_k \, dx \to \infty$ (Shown) ✓