# PH354 HW3

classmate
Date
Page

Q16) $$\hat{H} = \frac{-\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)$$

$$\psi(x) = \sum_{n=1}^{\infty} \psi_n \sin\left(\frac{n\pi x}{L}\right)$$

gn $$\int_0^L \sin\frac{m\pi x}{L}\cdot\sin\frac{n\pi x}{L}\,dx = \begin{cases} \frac{L}{2}, & m=n \\ 0, & \text{otherwise} \end{cases}$$

Now: $\hat{H}\psi(x) = E\psi(x)$ ~~consider LHS~~

$$\hat{H}\psi(x) = \hat{H}\left(\sum_{n=1}^{\infty}\psi_n \sin\left(\frac{n\pi x}{L}\right)\right)$$

$\hat{H}\psi(x) = E\psi(x)$

in matrix form

$H\psi = E\psi$ where $H, \psi$ in the same basis of functions $\left\{ \sin\frac{n\pi x}{L} \; n \in \mathbb{N} \right\}$

$$\Rightarrow \begin{pmatrix} H_{11} & H_{12} & H_{13} & \cdots \\ H_{21} & H_{22} & H_{23} & \cdots \\ \vdots & \vdots & \vdots & \end{pmatrix} \begin{pmatrix} \psi_1 \\ \psi_2 \\ \vdots \end{pmatrix} = E \begin{pmatrix} \psi_1 \\ \psi_2 \\ \vdots \end{pmatrix}$$

$\Rightarrow$ for some row index $m$:

$LHS = \sum_{n=1}^{\infty} H_{mn}\psi_n$ $\qquad$ $RHS = E\psi_m$

$$\Rightarrow \sum_{n=1}^{\infty} H_{mn}\psi_n = E\psi_m$$

We know $H_{mn} = \frac{2}{L}\int_0^L \sin\frac{\pi m x}{L}\, \hat{H}\, \sin\frac{\pi n x}{L}\, dx$

Substituting:

$$\sum_{n=1}^{\infty} \left(\frac{2}{L}\right)\left(\int_0^L \sin\left(\frac{m\pi x}{L}\right) \hat{H} \sin\left(\frac{n\pi x}{L}\right) dx\right)\psi_n$$

$$= E\psi_m$$

$\Rightarrow$

$$\sum_{n=1}^{\infty}\left(\int_0^L \sin\left(\frac{m\pi x}{L}\right) \hat{H} \sin\left(\frac{n\pi x}{L}\right) dx\right)\psi_n$$

$$= \cancel{2}\ \frac{1}{2} L\, E\psi_m$$

(ii) $H_{mn} = \frac{2}{L}\int_0^L \sin\left(\frac{m\pi x}{L}\right)\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)\right]\sin\left(\frac{n\pi x}{L}\right) dx$

$\left(V(x) = \frac{ax}{L}\right)$

$$= \frac{2}{L}\left\{\int_0^L \sin\left(\frac{m\pi x}{L}\right)\left(\frac{\hbar^2}{2m}\right)\left(\frac{n\pi}{L}\right)^2 \times \sin\left(\frac{n\pi x}{L}\right) dx + \int_0^L \sin\left(\frac{m\pi x}{L}\right)\cdot\left(\frac{ax}{L}\right)\sin\left(\frac{n\pi x}{L}\right) dx\right\}$$

$$= \frac{2}{L}\left[\left(\frac{\hbar^2}{2m_e}\right)\left(\frac{n\pi}{L}\right)^2 \int_0^L \sin\left(\frac{m\pi x}{L}\right)\cdot\sin\left(\frac{n\pi x}{L}\right) dx + \left(\frac{a}{L}\right)\int_0^L x\sin\left(\frac{m\pi x}{L}\right)\sin\left(\frac{n\pi x}{L}\right) dx\right]$$

$\int_0^L \sin\left(\frac{m\pi x}{L}\right)\sin\left(\frac{n\pi x}{L}\right) dx \rightarrow \begin{cases} \frac{L}{2}, & m=n \\ =0 & \text{otherwise} \end{cases}$

$\int_0^L x\sin\left(\frac{m\pi x}{L}\right)\sin\left(\frac{n\pi x}{L}\right) dx \rightarrow \begin{cases} 0, & m\neq n, \text{ both even or both odd} \\ -\left(\frac{2L}{\pi}\right)^2 \frac{mn}{(m^2-n^2)^2} & m\neq n, \text{ one even, other is odd} \\ \frac{L^2}{4} & \text{if } m=n \end{cases}$

$H_{mn} =$

$$\begin{cases} = \frac{2}{L}\left[\frac{\hbar^2}{2m_e}\left(\frac{n^2\pi^2}{L^2}\right)\cdot\left(\frac{L}{2}\right) + \left(\frac{a}{L}\right)\left(\frac{L^2}{4}\right)\right] & m=n \\ = \frac{2}{L}\left[-\left(\frac{a}{L}\right)\left(\frac{2L}{\pi}\right)^2 \frac{mn}{(m^2-n^2)^2}\right] & m\neq n \text{ one is odd, other is even} \\ = 0 & m\neq n \text{ both are odd or both are even} \end{cases}$$

$\therefore H_{mn}$

$$= \begin{cases} \dfrac{\hbar^2}{2m_e}\left(\dfrac{n^2\pi^2}{L^2}\right) + \left(\dfrac{a}{2}\right) & m = n \\[2ex] -\dfrac{8}{\pi^2}\,\dfrac{mn}{(m^2-n^2)^2}\cdot(a) & m \neq n \text{ one is even, other is odd } (m+n \text{ is odd}) \\[2ex] 0 & (m \neq n,\ m+n \text{ is even}) \end{cases}$$