1/24/01

Lecture 7 Properties of Wave Functions

Last time: Infinite square well

$$V = \begin{cases} 0 & 0 \le x \le a \\ \infty & \text{else} \end{cases}$$

Time indep. Schrodinger eq. $\hat{H}\psi = E\psi$

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

Full wave function $\Psi(x,t) = \psi(x)\, e^{-iEt/\hbar}$

Solution for square well

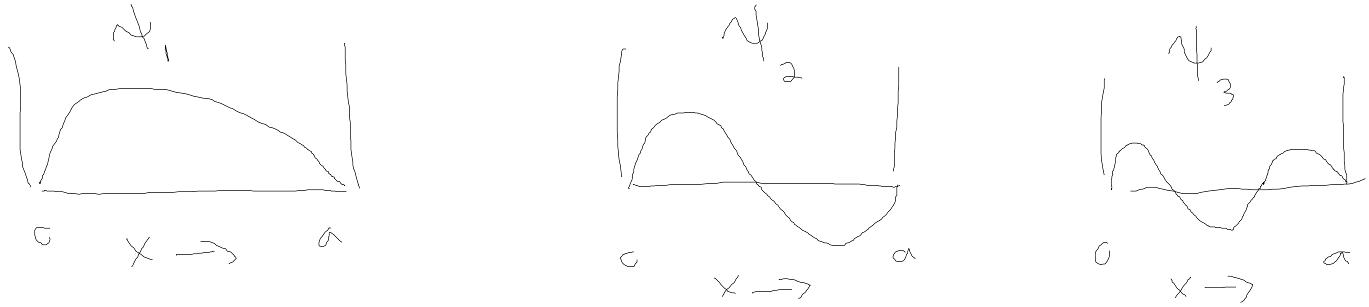
$$\psi_n(x) = A \sin k_n x \qquad \psi(0) = \psi(a) = 0$$

$$\text{B.C.} \Rightarrow \quad k_n = \frac{n\pi}{a} \qquad \boxed{E_n = \frac{\hbar^2 k_n^2}{2m} = \frac{n^2\pi^2\hbar^2}{2ma^2}}$$

Boundary conditions give quantized energies

Normalize $\int_0^a dx\, \psi_n^*(x)\,\psi_n(x) = 1 \Rightarrow A = \sqrt{\frac{2}{a}}$

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



Properties of $\psi_n(x)$

Note: these properties are general and don't just apply to the inf. square well.

① As one goes up in energy each wave function has one more node

② The wave functions are orthogonal

$$\int_{-\infty}^{\infty} dx \; \psi_m^*(x)\, \psi_n(x) = \begin{cases} 0 & m \neq n \\ 1 & m = n \end{cases}$$

Overlap of two different wave functions is zero. This is very important and useful

For square well

$$\int_0^a dx \; \frac{2}{a} \sin\frac{m\pi x}{a} \sin\frac{n\pi x}{a}$$

$$= \frac{1}{\pi}\left\{ \frac{\sin(m-n)\pi}{m-n} - \frac{\sin(m+n)\pi}{m+n} \right\} = \begin{cases} 0 & m \neq n \\ 1 & m = n \end{cases}$$

③ The wave functions are complete

Can expand any function F in eigenfunctions ψ_n

$$F(x) \approx \sum_{n=1}^{\infty} c_n \psi_n(x)$$

For some choice of expansion coef. c_n

If we truncate sum at some finite but large N

$$f_N(x) \equiv \sum_{n=1}^{N} c_n \psi_n(x)$$

Consider error

$$\lim_{N\to\infty} \int dx \left| F(x) - f_N(x) \right|^2 = 0$$

Completeness says error goes to zero for any function $F(x)$ that satisfies boundary conditions. Note, we have not proved completeness.

We can use orthogonality to calculate expansion coef. c_n

$$F(x) = \sum_{n=1}^{\infty} c_n \psi_n(x)$$

Multiply by $\psi_m^*(x)$ and integrate

$$\int \psi_m^*(x)\, F(x)\, dx = \sum_n c_n \underbrace{\int dx\, \psi_m^* \psi_n}_{\delta_{mn}}$$

$$\delta_{mn} = \begin{cases} 1 & m = n \\ 0 & \text{else} \end{cases}$$

$$\sum_n c_n \delta_{nm} = c_m$$

$$\boxed{c_m = \int \psi_m^*(x)\, F(x)\, dx}$$

Full time dep. of wave function $\Psi(x,t)$

If at $t=0$ full wave function is $\Psi(x,0)$ what is wave function at all later times?

① Expand $\Psi(x,0)$ in eigenstates $\psi_n(x)$

② Time dep. of eigenstates is $e^{-iE_nt/\hbar}$

$$\Psi(x,0) = \sum_n c_n \psi_n(x)$$

$$c_n = \int \psi_n^*(x)\, \Psi(x,0)\, dx$$

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

Note different terms in sum have different energies.

<u>Example Problem 2.8</u>

Given $\Psi(x,0) = A\,x(a-x)$

(a) Normalize to find A

(b) What ψ_n is $\Psi(x,0)$ close to

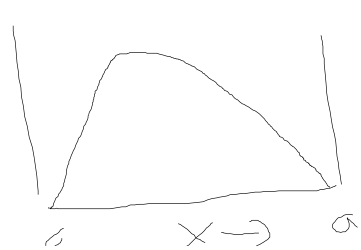
(c) Find $\langle \hat{H} \rangle$ for $\Psi(x,0)$ and compare with $\psi_n(x)$

Note, want wave function that satisfies b.c.

$$\Psi(0) = \Psi(a) = 0 \qquad (\text{for all } t) \quad ✓$$

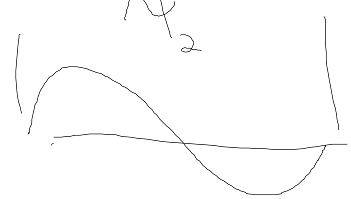
Normalize $A^2 \int_0^a x^2 (a-x)^2\, dx = 1$

(a) $\boxed{A = \sqrt{\dfrac{30}{a^5}}}$

(b) $\Psi(x,0) =$  (Parabola)

Compare this to

(sin func)



. . .

$\Psi(x,0)$ is close to ψ_1. Expect c_1 to be large ~ 1 and $c_2, c_3 \ldots$ to be small. Note higher c_i are nonzero because a parabola is not quite a sin function so small correction terms must be added.

Note could calculate

$$c_1 = \int_0^a \sqrt{\frac{2}{a}} \sin\frac{\pi x}{a} \sqrt{\frac{30}{a^5}}\, x(a-x)\, dx$$

$$c_1 = \sqrt{\frac{60}{a^6}}\ \frac{4}{\pi^3} a^3 = \frac{4}{\pi^3}\sqrt{60} = 0.9993$$

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

(c) Calculate $\langle E \rangle = \langle \hat{H} \rangle$

$$\langle \hat{H} \rangle = \int dx\ \Psi^*(x,0)\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V\right]\Psi(x,0)$$

$$= \int_0^a dx \left(\frac{-\hbar^2}{2m}\right) |A|^2\, x(a-x)\ \frac{d^2}{dx^2}\, x(a-x)$$

Note $V=0$, $0<x<a$

$$\frac{d^2}{dx^2}(a-x)\,x = -2$$

$$\langle \hat{H} \rangle = \frac{\hbar^2}{m}\left(\frac{30}{a^5}\right)\int_0^a x(a-x)\, dx$$

$$\langle \hat{H} \rangle = \frac{\hbar^2}{m}\left(\frac{30}{a^5}\right)\left(\frac{a^3}{2} - \frac{a^3}{3}\right) = \boxed{\frac{5\hbar^2}{ma^2}}$$

Compare this to $E_1 = \frac{\hbar^2 \pi^2}{2ma^2} = 4.935 \frac{\hbar^2}{ma^2}$

Expectation value is just a little bit above E_1 because there are some small bits of higher excited states in wave function

Later we will show

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