More Infinite Square Well

QM Postulates as we know them

(1) The state of the system is fully determined by the wave function $\psi(x,t)$

(2) The probability density for the position of the particle is

$$\rho(x,t) = \psi^* \psi$$

$$\int \rho(x,t)\, dx = 1$$

(3) The momentum probability density is given by

$$\rho(p,t) = \Phi^*(p,t)\, \Phi(p,t)$$

$$\Phi(p,t) = \frac{1}{\sqrt{2\pi\hbar}} \int \psi(x,t)\, e^{-ipx/\hbar} dx$$

(4) The average of any classical mechanical quantity $Q(x,p)$ can be found by

$$\langle Q(x,p)\rangle(t) = \int \psi^*(x,t)\, Q(x,\hat{p})\, \psi(x,t)\, dx$$

$$\hat{p} = \frac{\hbar}{i}\frac{\partial}{\partial x}$$

(5) The observable energies of any experiment are energies found from the TISE

$$-\frac{\hbar^2}{2m}\frac{d^2\phi}{dx^2} + V\phi = E\phi$$

(6) The function associated with the observable energies $\{E_i\}$ are complete and can be made orthogonal $\Rightarrow$ for any $\psi(x,0)$

$$\psi(x,0) = \sum c_i \phi_i$$

for some c_i and

$$c_n = \int \phi_n^* \psi(x,0)\, dx$$

7 The time evolution of the wave function is given by

$$\psi(x,t) = \sum c_i \phi_i(x) e^{-i\omega_i t}$$

$$E_i = \hbar \omega_i$$

<u>Ex</u> An infinite square well $x \in [0, a]$ is prepared with initial wave function

$$\psi(x,0) = A\left(1 + \cos\frac{\pi x}{a}\right)\sin\frac{\pi x}{a}$$

<u>Calculate Everything</u>

(1) Normalized wave function

(2) $\psi(x,t)$

(3) Observable energies and probabilities

(4) Averages $\langle E \rangle$, $\langle x \rangle$, $\langle x^2 \rangle$, $\langle p \rangle$, $\langle p^2 \rangle$

(5) Uncertainty $\sigma_x \sigma_p$

(6) Momentum $\Phi(k)$ or $\Phi(p)$

Forgot a postulate - Although we could prove this

8 $$\psi(x,t) = \sum c_i(t)\phi_i(x)$$

$$c_i(t) = c_i(0)\, e^{-i\omega_i t} \equiv c_i e^{-i\omega_i t}$$

The probability of measuring E_i is given by $P_i = c_i^*(t)\, c_i(t) = c_i^* c_i$

so the average energy is constant and

$$\langle E\rangle = \sum E_i P_i = \sum c_i^* c_i E_i$$

Back to our example

<u>Normalize</u> $\psi(x,0) = A\left(1+\cos\frac{\pi x}{a}\right)\sin\frac{\pi x}{a}$

$$1 = AA^* \int_0^a \left(1+\cos\frac{\pi x}{a}\right)^2 \sin^2\frac{\pi x}{a}\, dx$$

$$= \int \psi^*\psi\, dx = \frac{5}{8} a A^2$$

$$A = \sqrt{\frac{8}{5a}}$$

$$\psi(x,0) = \sqrt{\frac{8}{5a}}\left(1+\cos\frac{\pi x}{a}\right)\sin\frac{\pi x}{a}$$

Expand in terms of solution of infinite square well.

$$\phi_i = \sqrt{\frac{2}{a}}\ \sin k_x x \qquad k_n = \frac{n\pi}{a}$$

$$\psi(x,0) = \sum c_i \phi_i$$

Fourier's Trick

$$\int_0^a \phi_n^* \sum c_i \phi_i \, dx = \int_0^a \phi_n^* \, \psi(x,0)\, dx$$

$$c_n = \int_0^a \phi_n^* \, \psi(x,0)\, dx$$

$$c_1 = \int_0^a \left(\sqrt{\frac{8}{5a}}\right)\left(1 + \cos\frac{\cancel{x}\pi}{a}\right) \sin\frac{\pi x}{a} \cdot \sqrt{\frac{2}{a}} \sin\left(\frac{\pi x}{a}\right) dx$$

$$= \frac{2}{\sqrt{5}}$$

$$c_2 = \int_0^a \sqrt{\frac{8}{5a}} \left(1 + \cos\frac{\pi x}{a}\right)\left(\sin\frac{\pi x}{a}\right) \sqrt{\frac{2}{a}} \sin\left(\frac{2\pi x}{a}\right) dx$$

$$= \frac{1}{\sqrt{5}}$$

etc. It turns out all other $c_i = 0$.

Since we normalized, $\sum P(E_i) = 1 = \sum c_i^* c_i$

$$= c_1^* c_1 + c_2^* c_2 + c_3^* c_3 + \cdots$$

$$= \frac{4}{5} + \frac{1}{5} + 0 + 0 + 0$$

Time Evolution

$$\psi(x,t) = c_1 \phi_1 e^{-i\omega_1 t} + c_2 \phi_2 e^{-i\omega_2 t}$$

$$\omega_1 = E_1/\hbar = \frac{1}{\hbar} \cdot \frac{\hbar^2 k_1^2}{2m}$$

$$= \frac{\hbar}{2m} k_1^2 = \frac{\hbar}{2m}\left(\frac{\pi \cdot 1}{a}\right)^2$$

$$= \frac{\hbar \pi^2}{2ma^2} \equiv \frac{E_0}{\hbar} \quad \text{ground state energy}$$

$$\omega_2 = \frac{\hbar}{2m}\left(\frac{\pi \cdot 2}{d}\right)^2 = \frac{2\hbar\pi^2}{ma}$$

$$= 4E_0/\hbar$$

$$\psi(x,t) = \frac{2}{\sqrt{5}} \cdot \sqrt{\frac{2}{d}} \sin \frac{\pi x}{a} e^{-iE_0 t/\hbar}$$

$$+ \frac{1}{\sqrt{5}} \sqrt{\frac{2}{d}} \sin \frac{2\pi x}{d} e^{-4iE_0 t/\hbar}$$

Observation of Energy

Only energies $E_1 \equiv E_0$ and $E_2 = 4E_0$ can be observed with probability

$$P(E_1) = c_1^* c_1 = \frac{4}{5}$$

$$P(E_2) = c_2^* c_2 = \frac{1}{5}$$

Average Energy

$$\langle E \rangle = \sum P_i E_i = \sum c_i^* c_i E_i$$

$$= \frac{4}{5} \cdot E_1 + \frac{1}{5} \cdot E_2$$

$$= \frac{4}{5} \cdot E_0 + \frac{1}{5} \cdot 4E_0$$

$$= \frac{8}{5} \cdot E_0$$

Another way to get $\psi(x,0) = \sum c_i \phi_i(x)$

Work on given initial state

$$\psi(x,0) = A(1+\cos k_1 x)\sin k_1 x$$

$$= A\sin k_1 x + A\cos k_1 x \sin k_1 x$$

$$= A\sin k_1 x + \frac{A}{2}\sin 2k_1 x$$

$2k_1 = k_2$

$$= A'\left(\sqrt{\frac{2}{a}}\sin k_1 x + \frac{1}{2}\sqrt{\frac{2}{a}}\sin k_2 x\right)$$

$$= A'\left(\phi_1(x) + \frac{1}{2}\phi_2(x)\right)$$

$$= A''\left(2\phi_1(x) + \phi_2(x)\right)$$

Normalize like vectors

$\sqrt{2^2+1^2} = \sqrt{5}$ $\quad A'' = \frac{1}{\sqrt{5}}$

$$\psi(x,0) = \frac{2}{\sqrt{5}}\phi_1(x) + \frac{1}{\sqrt{5}}\phi_2(x)$$

Time evolution of averages

$$\langle x \rangle = \int \psi^*(x,t)\, x\, \psi^*(x,t)\, dx$$

We will need

$$\psi^*(x,t)\,\psi(x,t) = \left(\frac{2}{\sqrt{5}} \phi_1 e^{-i\omega t} + \frac{1}{\sqrt{5}} \phi_2 e^{-4i\omega t} \right)^*$$

$$\left(\frac{2}{\sqrt{5}} \phi_1 e^{-i\omega t} + \frac{1}{\sqrt{\cancel{8}}} \phi_2 e^{-4i\omega t} \right)$$

$$= \frac{1}{5} \Big[4\phi_1^2 + \phi_2^2 + 2\phi_1\phi_2 e^{-4i\omega t + i\omega t}$$

$$+ 2\phi_1\phi_2 e^{4i\omega t - i\omega t} \Big]$$

$$= \frac{1}{5} \left[4\phi_1^2 + \phi_2^2 + 2\phi_1\phi_2 \underbrace{\left(e^{3i\omega t} + e^{-3i\omega t} \right)}_{2\cos 3\omega t} \right]$$

$$= \frac{1}{5} \left[4\phi_1^2 + \phi_2^2 + 4\phi_1\phi_2 \cos 3\omega t \right]$$

where I used $\omega_1 = E_0/\hbar \equiv \omega$ $\quad \omega_2 = \dfrac{4E_0}{\hbar} \equiv 4\omega$

Expectation Value $\langle x \rangle$

$$\langle x \rangle = \int x \, \psi^* \psi \, dx$$

$$= \frac{1}{5} \left[4 \int x \, \phi_1^2 dx + \int x \, \phi_2^2 \right.$$

$$\left. + 4 \cos 3\omega t \int_0^a x \, \phi_1 \phi_2 \, dx \right.$$

$$\langle x \rangle_1 \equiv \int x \, \phi_1^2 dx = a/2$$

$$\langle x \rangle_2 \equiv \int x \, \phi_2^2 dx = a/2$$

$$\int_0^a x \, \phi_1 \phi_2 \, dx = \int_0^a x \sqrt{\frac{2}{a}} \sin \frac{\pi x}{a} \cdot \sqrt{\frac{2}{a}} \sin \frac{2\pi x}{a} \, dx$$

$$= \frac{-16a}{9\pi^2}$$

$$\langle x \rangle = \frac{1}{5} \left[\frac{5a}{2} - \frac{64a}{9\pi^2} \cos 3\omega t \right]$$

$$\langle x \rangle = \frac{a}{2}\left(1 - \frac{128}{45\pi^2}\cos 3\omega t\right)$$

$$= \frac{a}{2}\left(1 - 0.29\cos 3\omega t\right)$$

Momentum Average

$$\langle p \rangle = m\frac{d\langle x \rangle}{dt} = \frac{ma}{2}\left(\frac{(128)(3\omega)}{45\pi^2}\sin 3\omega t\right)$$

Higher Moments

$$\langle x^2 \rangle = \int x^2 \psi^* \psi \, dx$$

$$\langle p^2 \rangle = \int \psi^* \left(\frac{\hbar}{i}\frac{d}{dx}\right)^2 \psi \, dx$$

$$\neq \int \left(\frac{\hbar}{i}\frac{d}{dx}\right)^2 \psi^* \psi \, dx$$

$$\langle p^2 \rangle = \int \psi^* \left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right)^2 \psi \, dx$$

$$\neq \int \left(\frac{\hbar}{i}\frac{\partial}{\partial x}\right)^2 |\psi|^2 \, dx$$

$$\psi(x,t) = \frac{2}{\sqrt{5}} \phi_1 e^{-i\omega_1 t} + \frac{1}{\sqrt{5}} \phi_2 e^{-i\omega_2 t}$$

$$\frac{\partial}{\partial x}\psi = \frac{2k_1}{\sqrt{5}} \sqrt{\frac{2}{a}} \cos k_1 x \, e^{-i\omega_1 t}$$

$$+ \frac{k_2}{\sqrt{5}} \sqrt{\frac{2}{a}} \cos k_2 x \, e^{-i\omega_2 t}$$

$$\frac{\partial^2 \psi}{\partial x^2} = -\frac{2}{\sqrt{5}} k_1^2 \sqrt{\frac{2}{a}} \sin k_1 x \, e^{-i\omega_1 t}$$

$$- \frac{1}{\sqrt{5}} k_2^2 \sqrt{\frac{2}{a}} \sin k_2 x \, e^{-i\omega_2 t}$$

$$= -\frac{2k_1^2}{\sqrt{5}} \phi_1 e^{-i\omega_1 t} - \frac{1}{\sqrt{5}} k_2^2 \phi_2 e^{-i\omega_2 t}$$

$$\langle p^2 \rangle = -\hbar^2 \int \psi^* \frac{\partial^2 \psi}{\partial x^2}\, dx$$

$$= \int_{-\infty}^{\infty} -\hbar^2 \left[\frac{2}{\sqrt{5}} \phi_1 e^{i\omega t} + \frac{1}{\sqrt{5}} \phi_2 e^{i4\omega t} \right] \cdot$$

$$\left[-\frac{2\pi^2}{a^2\sqrt{5}} \phi_1 e^{-i\omega t} - \frac{4\pi^2}{a^2\sqrt{5}} \phi_2 e^{-4i\omega t} \right] dx$$

$$k_1^2 = \frac{\pi^2}{a^2} \qquad k_2^2 = \frac{4\pi^2}{a^2}$$

$$\omega_2 = 4\omega$$

$$\omega_1 = \omega$$

$$\omega = \frac{\hbar k_1^2}{2m} = \frac{\hbar \pi^2}{2ma^2}$$

$$\langle p^2 \rangle = \int_{-\infty}^{\infty} + \frac{\hbar^2}{5} \frac{\pi^2}{a^2} \left[2\phi_1 e^{i\omega t} + \phi_2 e^{4i\omega t} \right]$$

$$\left[2\phi_1 e^{-i\omega t} + 4\phi_2 e^{-4i\omega t} \right] dx$$

$$[\,][\,] = 4\phi_1^2 + 4\phi_2^2 + 16\phi_1\phi_2 \cos 3\omega t$$

$$\int [\,][\,]\,dx = 4 + 4 + 0 = 8$$

$$\langle p^2 \rangle = \frac{8}{5}\frac{\hbar^2\pi^2}{a^2}$$

$$\sigma_p = \sqrt{\langle p^2 \rangle - \langle p \rangle^2}$$

$$= \left(\left(\frac{8}{5}\frac{\hbar^2\pi^2}{a^2} \right)^2 - \frac{1}{25}\left(\frac{5a}{2} - \frac{64a}{9\pi^2}\cos 3\omega t \right)^2 \right)^{1/2}$$

Uncertainty oscillates in time.

$\phi(k)$ – what will this tell us?

$$\phi^*(k)\,\phi(k) = \text{Probability density for } k$$

and therefore momentum $\hbar k$.

$\cancel{\phi}$

Also in this case, we could have used

$$\psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dk\, \phi(k)\, e^{ikx}\, e^{-i\frac{\hbar k^2}{2m}t}$$

but this doesn't always work. It works for the infinite square well because $E = p^2/2m \Rightarrow$ The energy has a simple relation to the momentum.

$$\phi(k) = \frac{1}{\sqrt{2\pi}} \int_0^a dx \; \psi(x,0) \, e^{-ikx}$$

$$= \frac{\cancel{A}}{\sqrt{2\pi}} \int dx \left(\frac{2}{\sqrt{5}} \phi_1 + \frac{1}{\sqrt{5}} \phi_2 \right) e^{-ikx}$$

$$= \left(\sqrt{\frac{2}{a}} \right) \left(\frac{1}{\sqrt{5}} \right) \frac{1}{\sqrt{2\pi}} \int_0^a dx \left(2 \sin k_1 x + \sin k_2 x \right) \cdot e^{-ikx}$$

$$\sin x = \frac{e^{x} - e^{-x}}{2i}$$

$$\phi(k) = \frac{1}{2i} \frac{1}{\sqrt{50\pi}} \int_0^a dx \left[2\left(e^{ik_1 x} - e^{-ik_1 x}\right) + \left(e^{ik_2 x} - e^{-ik_2 x}\right) \right] \cdot e^{-ikx}$$

$$[\;] e^{-ikx} = 2 e^{i(k_1 - k)x} - 2 e^{-i(k + k_1)x} + e^{i(k_2 - k)x} - e^{-i(k_2 + k)x}$$

$$\int_0^a e^{bx}\,dx = \frac{1}{b} e^{bx} \Big|_0^a$$

$$= \frac{1}{b}\left(e^{a} - 1\right)$$

$$\int_0^a [\,]\, e^{-ikx}\,dx$$

$$= \frac{2}{i(k_1 - k)}\left(e^{i(k_1-k)a} - 1\right) - \frac{2}{-i(k+k_1)}\left(e^{-i(k+k_1)a} - 1\right)$$

$$+ \frac{1}{i(k_2 - k)}\left(e^{i(k_2-k)a} - 1\right) - \frac{1}{-i(k_2+k)}\left(e^{-i(k_2+k)a} - 1\right)$$

I'm bored, but this is done

$$\phi(k) = \frac{1}{2i}\,\frac{1}{\sqrt{5a\pi}} \int_0^a dx\, [\,]\, e^{-ikx}$$