More on the Quantum Well.

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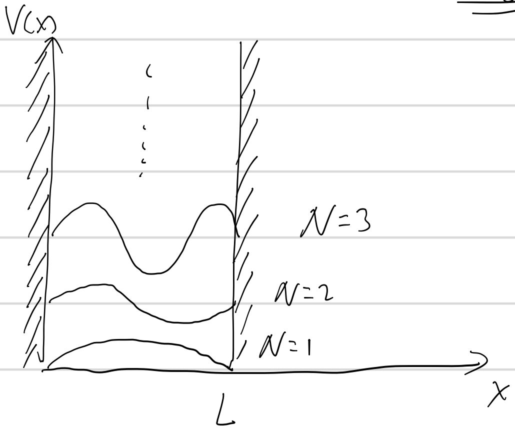
1. Measurements on Eigenstates



$$\psi_N(x,t) = \sqrt{\frac{2}{L}} \sin\frac{N\pi x}{L}\, e^{-iN^2\omega_0 t} \;;$$

$$E_N = \frac{\pi^2\hbar^2}{2mL^2} N^2 \;;\quad \omega_0 = \frac{E_{N=1}}{\hbar} = \frac{\pi^2\hbar}{2mL^2}.$$

1.1. Measurement on position x

a. probability density of measuring result x_0 $\quad |\psi_N(x_0,t)|^2$

$$= \frac{2}{L}\sin^2\frac{N\pi x_0}{L} \;;\quad \text{independent of time.}$$

b. expected value of position (must be $\frac{L}{2}$, symmetric)

$$\langle x\rangle = \int_0^L \psi_N^*(x,t)\cdot\hat{x}\,\psi_N(x,t)\,dx = \frac{2}{L}\int_0^L x\sin^2\frac{N\pi x}{L}\,dx$$

Use: $1-2\sin^2 x' = \cos 2x' \Rightarrow \sin^2 x' = \frac{1-\cos 2x'}{2}$

$$\therefore\quad \langle x\rangle = \frac{2}{L}\int_0^L \left(\frac{x}{2} - \frac{x}{2}\cos\frac{2N\pi x}{L}\right)dx$$

$$\int_0^L \frac{x}{2}dx = \int_0^L \frac{1}{4}dx^2 = \frac{1}{4}x^2\Big|_0^L = \frac{L^2}{4}$$

$$\therefore\quad \langle x\rangle = \frac{L}{2} - \int_0^L \frac{x}{L}\cos\frac{2N\pi x}{L}\,dx.$$

Two ways to calulate this integration:

1°. Integration by part. The difficulty is $x \cdot \cos$, but the derivative of x is 1, so you can use the integration trick to simplify it.

$$d(uv) = v\,du + u \cdot dv$$

$$\Downarrow$$

$$\int_{L_1}^{L_2} d(uv) = \int v\,du + \int u\,dv.$$

$$\| \qquad \downarrow$$

$$uv\Big|_{L_1}^{L_2}$$

Let this be

$$\int_0^L \frac{x}{L}\cos\left(\frac{2\pi N x}{L}\right)dx = \int_0^L \frac{x}{L}\, d\sin\left(\frac{2\pi N x}{L}\right) \times \frac{L}{2\pi N} = \int_0^L \frac{x}{2\pi N}\, d\sin\left(\frac{2\pi N x}{L}\right)$$

$\therefore$ $v = \dfrac{x}{2\pi N}$; $u = \sin\left(\dfrac{2\pi N x}{L}\right)$

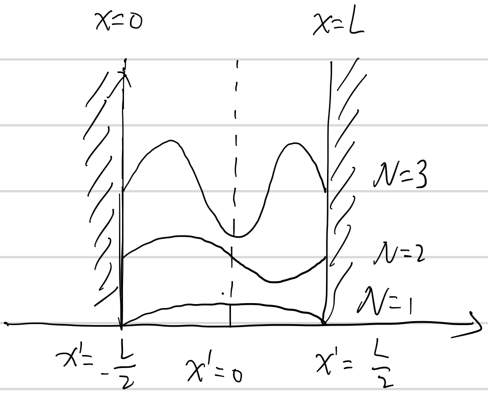
$$\therefore \int_0^L \frac{x}{L}\cos\left(\frac{2\pi N x}{L}\right)dx = \underbrace{\frac{x}{2\pi N}\sin\left(\frac{2\pi N x}{L}\right)\Big|_0^L}_{=0} - \underbrace{\int_0^L \sin\left(\frac{2\pi N x}{L}\right)d\,\frac{x}{2\pi N}}_{=0}$$

One period.

$$\therefore \langle x \rangle = \frac{L}{2} - 0 = \frac{L}{2}.$$

2°. The entire problem can be simplified a lot at the very beginning by noticing that the potential well is symmetric to $x = \frac{L}{2}$.

The what you can do is to move the axis of x to the symmetric point.



$$\therefore \quad x' = x - \frac{L}{2} \Rightarrow \langle x' \rangle = \langle x \rangle - \frac{L}{2}.$$

$$\langle x \rangle = \langle x' \rangle + \frac{L}{2}$$

$$\psi(x,t) = \psi\left(x' + \frac{L}{2}\right) = \sqrt{\frac{2}{L}} \sin\left(\frac{N\pi}{L}\left(x' + \frac{L}{2}\right)\right) e^{-iN\omega_0 t}$$

$$= \sqrt{\frac{2}{L}} \sin\left(\frac{N\pi}{L}x' + \frac{N\pi}{2}\right) e^{-iN\omega_0 t}.$$

It's important to notice that $\psi(x',t)$ is odd/even symmetry along $x'=0$.

$N=1$, $\sin(\ldots) = \sin\left(\frac{N\pi x'}{L} + \frac{\pi}{2}\right) = \cos\left(\frac{N\pi x'}{L}\right)$ even

$N=2$, $\sin(\ldots) = \sin\left(\frac{N\pi x'}{L} + \pi\right) = -\sin\left(\frac{N\pi x'}{L}\right)$ odd

$N=3$, $\sin(\ldots) = \sin\left(\frac{N\pi x'}{L} + \frac{\pi}{2} + \pi\right) = -\cos\left(\frac{N\pi x'}{L}\right)$, even

$N=4$, $\sin(\ldots) = \sin\left(\frac{N\pi x'}{L} + 2\pi\right) = \sin\left(\frac{N\pi x'}{L}\right)$, odd

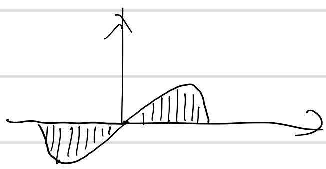
$\vdots$

Rest is just repeat these four.

$f_e(x) = f_e(-x)$: even function

$f_o(x) = -f_o(-x)$, odd function.

$f_o^2(x) = \left(-f_o(-x)\right)^2 = f_o^2(-x) \rightarrow$ even function.



$$\langle x' \rangle = \int_{-\frac{L}{2}}^{\frac{L}{2}} \underbrace{x'}_{\text{odd}} \cdot \frac{2}{L} \underbrace{\sin^2\left(\frac{N\pi x'}{L} + \frac{N\pi}{2}\right)}_{\text{even}} dx' = \int_{-\frac{L}{2}}^{\frac{L}{2}} f_o(x)\, dx$$

$$= 0$$

$\therefore \quad \langle x' \rangle = 0 \quad ; \quad \langle x \rangle = \langle x' \rangle + \frac{L}{2} = \frac{L}{2}.$

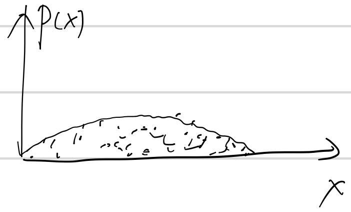
This conclusion is true for potential well with even symmetry.

If $V(x) = V(-x)$; And symmetric B.C. $\psi(x)\big|_{x=L} = \psi(x)\big|_{x=-L}$

Then $\langle x \rangle$ for the eigenstates of the system is zero.

Not true for arbitary states!

C. What about the measurement deviation of x?



Definition of deviation:

$$\sigma_x^2 = \langle (x - \langle x \rangle)^2 \rangle$$

Average of how much you deviate from average value.

$$\sigma_x^2 = \langle (x - \langle x \rangle)^2 \rangle = \langle (x^2 - 2x\langle x \rangle + \langle x \rangle^2) \rangle = \langle x^2 \rangle - 2\langle x \rangle \langle x \rangle + \langle x \rangle^2$$
$$= \langle x^2 \rangle - \langle x \rangle^2$$

For N-th eigenstate:

$$\langle x^2 \rangle_N = \int_0^L \psi_N^*(x,t)\, x^2\, \psi_N(x,t)\, dx = \int_0^L \frac{2}{L} \cdot x^2 \sin^2\left(\frac{N\pi x}{L}\right) dx$$

use: $\sin^2 y = \frac{1 - \cos 2y}{2}$ $\Rightarrow \langle x^2 \rangle_N = \int_0^L \frac{2}{L} x^2 \times \frac{1}{2}\left(1 - \cos \frac{2N\pi x}{L}\right) dx$

$$= \underbrace{\int_0^L \frac{x^2}{L} dx}_{\int_0^L \frac{1}{3L} d x^3 = \frac{L^3}{3L} = \frac{L^2}{3}} - \int_0^L \frac{x^2}{L} \cos \frac{2N\pi x}{L}\, dx = \frac{L^2}{3} - \int_0^L \frac{x^2}{L} \cos \frac{2N\pi x}{L}\, dx$$

$$\int_0^L \frac{x^2}{L} \cos\frac{2N\pi x}{L}\, dx$$

Use: $\displaystyle \int d(uv) = \int u\,dv + \int v\,du$

$$\therefore \int \dots = \frac{L}{2N\pi}\int_0^L \frac{x^2}{L}\cdot d\sin\left(\frac{2N\pi x}{L}\right) = \int_0^L \underbrace{\frac{x^2}{2N\pi}}_{u}\cdot d\,\underbrace{\sin\left(\frac{2N\pi x}{L}\right)}_{v}$$

$$= \underbrace{\frac{x^2}{2N\pi}\sin\left(\frac{2N\pi x}{L}\right)\Bigg|_0^L}_{=0} - \int_0^L \frac{1}{2N\pi}\sin\left(\frac{2N\pi x}{L}\right)\cdot dx^2$$

$$= -\int_0^L \frac{1}{N\pi}\, x \sin\left(\frac{2N\pi x}{L}\right) dx = \int_0^L \frac{x}{N\pi}\,\frac{L}{2N\pi}\, d\cos\left(\frac{2N\pi x}{L}\right)$$

$$= \frac{L}{2N^2\pi^2}\int_0^L \underbrace{x}_{u}\, d\,\underbrace{\cos\left(\frac{2N\pi x}{L}\right)}_{v} = \frac{L}{2N^2\pi^2}\left\{ x\cos\left(\frac{2N\pi x}{L}\right)\Bigg|_0^L - \underbrace{\int_0^L \cos\left(\frac{2N\pi x}{L}\right) dx}_{=0} \right\}$$

$$= \frac{L^2}{2N^2\pi^2}\cos(2N\pi) = \frac{L^2}{2N^2\pi^2}$$

$$\therefore\ \sigma_x^2 = \frac{L^2}{3} - \frac{L^2}{2N^2\pi^2}$$

Continue:

1.2. Measurement of momentum for eigenstates

For eigenstate ψ_N, it has energy $E_N = N^2 \hbar \omega_0$, does it mean it also has a well defined momentum? $E_N = \frac{P_N^2}{2m}$?

If yes, then ψ_N must be eigenstates of $\hat{p}$ as well, because

$$\hat{p}\,\psi_N \rightarrow p_N \cdot \psi_N .$$

Give it a try: $\hat{p} = \frac{\hbar}{i}\frac{\partial}{\partial x}$; $\psi_N = \sqrt{\frac{2}{L}} \sin\left(\frac{N\pi}{L}x\right) e^{-iN^2\omega_0 t}$

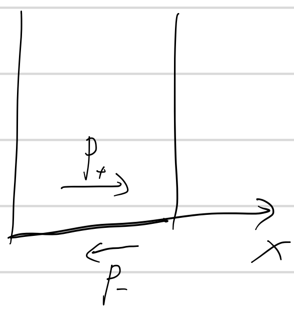
$$\hat{p}\,\psi_N = \frac{N\pi}{L}\sqrt{\frac{2}{L}} \cos\left(\frac{N\pi}{L}x\right) e^{-iN^2\omega_0 t} \neq p\,\psi_N$$

So what happened?

$E_N = \frac{P_N^2}{2m} \longrightarrow P_N = \pm\sqrt{2mE_N}$, so there are two momentum,

one forward, one backward.

It makes a lot of physics sense.



If the state only has forward momentum, it will go outside of the potential well and move to infinity eventually.

But the infinite potential well reflect it, so in combine, your electron is confined in the potential well.

In general, the eigenstates of $\hat{H}$, are not eigenstates of $\hat{p}$, unless it's free particle.

1°. What are the possible measurement result of p?

Expand wavefunction $\psi_N(x)$ to eigenstates of $\hat{p}$

$$\psi_N(x,t) = \sum_k \alpha_k e^{-ikx} \quad ; \quad \text{Use: } \sin x' = \frac{e^{ix'} - e^{-ix'}}{2i}$$

$$\psi_N(x,t) = \sqrt{\frac{2}{L}} e^{-iN^2\omega_0 t} \sin\left(\frac{N\pi x}{L}\right)$$

$$= \sqrt{\frac{2}{L}} e^{-iN^2\omega_0 t} \left(\frac{e^{i\frac{N\pi}{L}x} - e^{-i\frac{N\pi}{L}x}}{2i}\right)$$

$$= i\sqrt{\frac{1}{2L}} e^{-iN^2\omega_0 t} \left(e^{-\frac{iN\pi}{L}x} - e^{+\frac{iN\pi}{L}x}\right)$$

$$k_+ = \frac{N\pi}{L} \qquad k_- = \frac{-N\pi}{L}$$

Two possible momentum result: $P_+ = \hbar k_+ = \frac{N\pi\hbar}{L}$; $P_- = \hbar k_- = -\frac{N\pi\hbar}{L}$

probability: $|\alpha_{k_+}| = |\alpha_{k_-}|$, equal probability : $\frac{1}{2}$.

2°. expected value of momentum:

$$\langle p \rangle = \sum_k \tilde{P}_k \cdot \hbar k \quad ; \quad \hat{P}_k \text{ is the probability of getting } p = \hbar k$$

$$= \frac{1}{2} P_+ + \frac{1}{2} P_- = 0.$$

Another way:

$$\langle p \rangle = \int_0^L \psi_N^*(x,t)\, \hat{p}\, \psi_N(x,t)\, dx = \frac{\hbar}{i} \int_0^L \frac{2}{L} \sin\left(\frac{N\pi x}{L}\right) \frac{\partial}{\partial x}\left(\sin\frac{N\pi x}{L}\right) \cdot dx$$

$$= \frac{2\hbar}{iL} \int_0^L \frac{N\pi}{L} \sin\left(\frac{N\pi x}{L}\right) \cos\left(\frac{N\pi x}{L}\right) dx$$

$$= \frac{\hbar}{iL} \int_0^L \frac{N\pi}{L} \sin\left(\frac{2N\pi x}{L}\right) dx \quad ; \quad \boxed{2\sin x' \cos x' = \sin 2x'.}$$

$$= 0$$

Is the expected momentum zero for all confined states?

In general, yes for eigenstates of $\hat{H}$, but no for arbitary confined states.

We will see examples in the next class.

3°. Deviation of momentum for eigenstates.

$$\sigma_{p,N}^2 = \langle (p - \langle p \rangle)^2 \rangle_N = \langle p^2 \rangle_N = \frac{p_+^2 + p_-^2}{2} = p_N^2$$

$$\therefore \quad \sigma_{p,N}^2 = \left(\frac{N\pi\hbar}{L}\right)^2 = \frac{N^2\pi^2\hbar^2}{L^2}$$

You can also calculate it as:

$$\langle p^2 \rangle_N = \int_0^L \psi_N^* \hat{p}^2 \psi_N \, dx = -\hbar^2 \int_0^L \psi_N^* \frac{\partial^2}{\partial x^2} \psi_N \, dx$$

$$= -\hbar^2 \cdot \frac{2}{L} \cdot \int_0^L \sin\left(\frac{N\pi x}{L}\right) \frac{\partial^2}{\partial x^2} \sin\left(\frac{N\pi x}{L}\right) dx$$

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

$$= \frac{2}{L} \left(\frac{N\pi\hbar}{L}\right)^2 \int_0^{N\pi} \sin^2\left(\frac{N\pi x}{L}\right) \cdot d\left(\frac{N\pi x}{L}\right) \cdot \frac{L}{N\pi}$$

$$= 2\left(\frac{N\pi\hbar^2}{L}\right) \cdot \underbrace{\frac{1}{N\pi} \int_0^{N\pi} \sin^2 x' \, dx'}_{\text{Average of } \sin^2 x' = \frac{1}{2}}$$

$$= \left(\frac{N\pi\hbar}{L}\right)^2$$

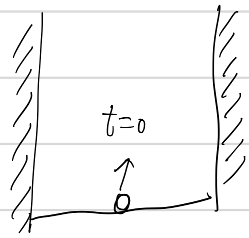
Can we extend the results of eigenstates directly to arbitary states?

Think about this state:

At time $t=0$, I put an electron at position $x=\frac{L}{2}$,

so:

$$\psi(x, t=0) = \delta\left(x-\frac{L}{2}\right)$$



Does it stay there?

How it moves?

We will discuss non-eigenstates next.