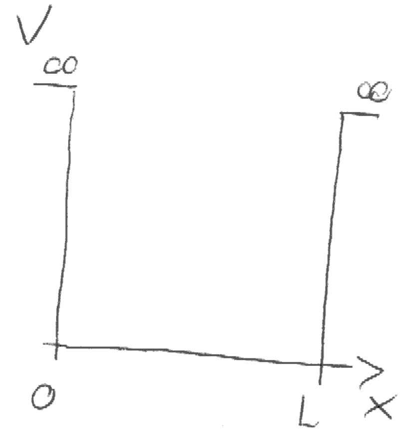
Summary

① Particle in box (1D)

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



$$\frac{d^2\psi}{dx^2} = -\underbrace{\frac{2mE}{\hbar^2}}_{k^2}\psi$$

V is infinite for $x<0$ or $x>L$

$\Rightarrow$ particle localized in the $(0,L)$ interval

$\psi(0)=\psi(L)=0$

$$\psi(x) = D\sin kx$$

$$k = \frac{n\pi}{L} = \sqrt{\frac{2mE}{\hbar^2}},$$

$n = 1, 2, \dots$

$$E_n = \frac{n^2h^2}{8mL^2}, \quad \psi_n = D\sin\left(\frac{n\pi}{L}x\right)$$

② postulate I. $\psi_n^*(x)\,\psi_n(x)$ is the probability density of the particle ($\rho(x)$)

$\Rightarrow \rho(x)\,dx$ is the probability that we find the particle in the given dx interval

$$\int_0^L \psi_n^*(x)\,\psi_n(x) = 1 = D^2\int_0^L \sin^2\left(\frac{n\pi}{L}x\right)dx$$

$$\Rightarrow D = \sqrt{\frac{2}{L}}$$

③ postulate II.:

$$\hat{H}_{\text{part. in box}} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \hat{V}(x)$$

It is the linear Hermitian op. assigned to the energy.

(it is zero in the $0<x<L$ interval)

$\hat{V}(x)\,\psi(x) = V(x)\,\psi(x)$ (it is a multiplication)

$$E_{kin} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} = \frac{1}{2m}\underbrace{\left(\frac{\hbar}{i}\frac{d}{dx}\right)}_{\hat{P}_x = -i\hbar\frac{d}{dx}}\left(\frac{\hbar}{i}\frac{d}{dx}\right) = \frac{1}{2m}\hat{P}_x^2$$

$\hat{P}_x$ is the op. of the linear momentum

④ Postulate IV.:

Measurable values of a phys. quantity are the eigenvalues of the op. of the given phys. property:

$\hat{H}\psi_n = E_n\psi_n$ eigenvector

eigenvalue

input: $\hat{H}$

outputs: E_n, ψ_n, $n=1,2,\ldots$

What are the measurable values for the momentum?

$$\hat{P}_x\psi_n = \frac{\hbar}{i}\frac{d}{dx}\psi_n = \frac{\hbar}{i}\frac{n\pi}{L}\cos\frac{n\pi}{L}\cdot x$$

it is not an eigenvalue equation!

What are the eigenfunctions of $\hat{P}_x$?

$$\frac{\hbar}{i}\frac{\partial}{\partial x}\psi_n^{(p)} = \hat{P}_x\psi_n^{(p)} = p_n\psi_n^{(p)} \Rightarrow \frac{d}{dx}\psi_n^{(p)} = \frac{i p_n}{\hbar}\psi_n^{(p)}$$

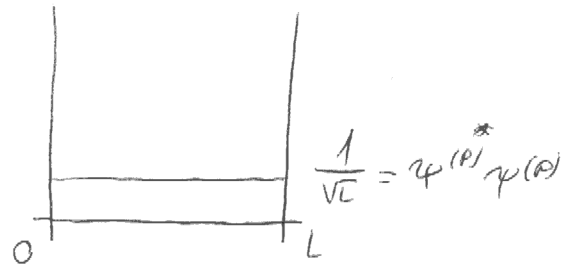
$$\Rightarrow \psi_n^{(p)} = D\,e^{\frac{i}{\hbar}p_x \cdot x}$$

Normalization factor N:

$$\psi_n^{(p)*}\psi_n^{(p)} = e^{-\frac{i}{\hbar}p_n} e^{\frac{i}{\hbar}p_n} = 1$$ $\Rightarrow$ the probability density is constant.

$$\int_0^L \psi_n^{(p)*}(x)\,\psi_n^{(p)}(x) = 1 \Rightarrow N = \frac{1}{\sqrt{L}}$$

problem: $\psi(0)=\psi(L)$ conditions are not satisfied.



⑤ Postulate V

The average of an observable quantity can be calculated as $\langle\omega\rangle = \int \psi^* \hat{\Omega}\psi\, d\tau$

If ψ_i is an eigenfunction of $\hat{\Omega}$:
$\hat{\Omega}\psi_i = \omega_i\psi_i$
$\langle\omega\rangle = \int \psi_i^*\hat{\Omega}\psi_i$
$= \omega_i \int \psi_i^*\psi_i$
$= \omega_i$

Example: Where is the particle?

The position op: $\hat{x}\psi_n = x\cdot\sqrt{\frac{2}{L}}\sin\left(\frac{n\pi}{L}\cdot x\right)$

$\Rightarrow \psi_n$ is not a position eigenfunction...

$$\langle x\rangle = \int_0^L \psi_n^* \hat{x}\psi_n\, dx = \frac{2}{L}\int_0^L \sin\left(\frac{n\pi}{L}x\right)\cdot x \sin\left(\frac{n\pi}{L}x\right) dx$$

$$= \frac{2}{L}\int_0^L \sin^2\left(\frac{n\pi}{L}x\right)\cdot x\cdot dx = \frac{2}{L}\cdot\left(\frac{L}{n\pi}\right)^2\int_0^{n\pi} y\sin^2(y)\,dy$$

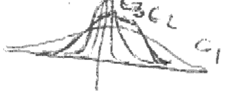
$$= \frac{L}{2}$$

Eigenfunctions of position $\int \delta_c(x)\,dx = 1$

$\hat{x}\,\delta(x-a) = a\,\delta(x-a)$ Dirac-delta

$$\delta_c(x) = \frac{1}{c\sqrt{\pi}}e^{-\frac{x^2}{c^2}}$$

$\delta_c(x) \xrightarrow[c \to 0]{} \delta(x)$



$c_4 < c_3 < c_2 < c_1$

⑥ Hermitian operators

Def.: $\int \phi^*(\tau)\,\hat{\Omega}\,\eta(\tau)\,d\tau = \int (\hat{\Omega}\phi)^*\,\eta\,d\tau$

$= \left[\int \eta^*\hat{\Omega}\phi\,d\tau\right]^*$

$[(\eta^*)^* = \eta]$

Eigenvalues of Ω are real numbers:

$\hat{\Omega}\psi_n = \lambda_n\psi_n \implies (\hat{\Omega}\psi_n)^* = \lambda_n^*\psi_n^*$

$\psi_n^*/$ $\quad \psi_n^*\hat{\Omega}\psi_n = \lambda_n\psi_n^*\psi_n \qquad \psi_n(\hat{\Omega}\psi_n)^* = \lambda_n^*\psi_n\psi_n^*$

$\int d\tau/$ $\quad \int \psi_n^*\hat{\Omega}\psi_n\,d\tau = \lambda_n\int\psi_n^*\psi_n\,d\tau$

$\int \psi_n(\hat{\Omega}\psi_n)^*\,d\tau = \lambda_n^*\int\psi_n\psi_n^*\,d\tau$

As Ω is Hermitian: $\lambda_n\int\psi_n^*\psi_n\,d\tau = \lambda_n^*\int\psi_n^*\psi_n\,d\tau$

$\implies \lambda_n = \lambda_n^*$ $\quad$ (λ_n is real)

If $\lambda_n \neq \lambda_m$ than ψ_n and ψ_m are orthogonal!

$\hat{\Omega}\psi_n = \lambda_n\psi_n \qquad \hat{\Omega}\psi_m = \lambda_m\psi_m$

$\int\psi_m^*/$ $\qquad$ $\hat{\Omega}$ is Hermitian $\quad \hat{\Omega}^*\psi_m^* = \lambda_m^*\psi_m^* \qquad \int\psi_n/$

$\int\psi_m^*\hat{\Omega}\psi_n\,d\tau = \int\psi_n\hat{\Omega}^*\psi_m^*\,d\tau = \lambda_n\int\psi_m^*\psi_n\,d\tau =$

$\implies$ as $\lambda_n \neq \lambda_m$ $\qquad \lambda_m\int\psi_m^*\psi_n\,d\tau$

$\int\psi_m^*\psi_n\,d\tau$ must be zero.

E.g., particle in box (1D)

$$\int_0^L \psi_n^*(x)\,\psi_m(x)\,d\tau = \frac{2}{L}\int_0^L \sin\left(\frac{\pi n}{L}x\right)\sin\left(\frac{\pi m}{L}x\right)dx$$

$$\left.\begin{aligned} \frac{n\pi}{L} &= \frac{\theta+\varphi}{2} \\ \frac{m\pi}{L} &= \frac{\theta-\varphi}{2} \end{aligned}\right\} \quad \begin{aligned} \theta &= \frac{(n+m)\pi}{L} \\ \varphi &= \frac{(n-m)\pi}{L} \end{aligned}$$

$$= \frac{1}{L}\left(\int_0^L \cos\varphi x\,dx - \int_0^L \cos\theta x\,dx\right) =$$

$$\frac{1}{L\varphi}\int_0^{(n-m)\pi} \cos z\,dz - \frac{1}{L\theta}\int_0^{(n+m)\pi} \cos z\,dz =$$

$$\frac{1}{L\varphi}\left[\sin z\right]_0^{(n-m)\pi} - \frac{1}{L\theta}\left[\sin z\right]_0^{(n+m)\pi} = 0 + 0$$