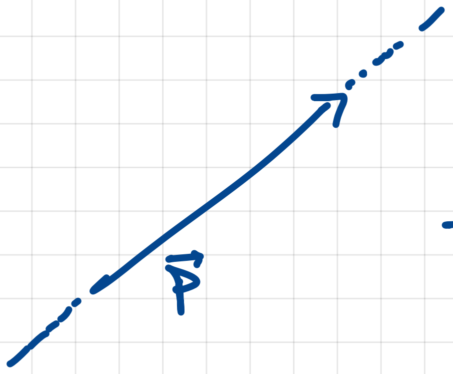
# Short Takes 331

## The quantum free particle

# The quantum free particle

- Classically, a free particle is one not affected by any external forces

$$\vec{F} = \frac{d\vec{p}}{dt} = 0 \quad , \quad \vec{p} = m\vec{v} = \text{constant}$$




travels in a straight line.

In the Hamiltonian formalism,

$$H = \frac{p^2}{2m} \qquad \frac{\partial}{\partial t}\frac{\partial H}{\partial p} = -\frac{\partial H}{\partial q} = 0 \Rightarrow \vec{p} = \text{constant}$$

- Quantum mechanically, the Hamiltonian is a linear operator:

$$\hat{H} = \frac{\hat{p}^2}{2m} = \frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2} \quad , \quad \hat{p} \equiv \frac{\hbar}{i}\frac{\partial}{\partial x} \quad , \quad \hbar = \frac{h}{2\pi} \quad , \quad h = \text{Planck's constant}$$

... and the stable states are given by the eigenvectors of $\hat{H}$, with corresponding energy given by the eigenvalues...

$$\hat{H}\psi(x) = E\,\psi(x) \quad \Rightarrow \quad \frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x) = E\,\psi(x)$$

What now...? We need boundary conditions to solve this eq.

- In the whole real line $\mathbb{R}$,

$$\psi_k(x) = C.\exp(ikx) \quad , \quad C = \frac{1}{(2\pi)^{1/2}} \quad \text{in 1d.}$$

$$E_k = \frac{\hbar^2 k^2}{2m}$$

Note: $\hat{p}\,\psi_k = \hbar k\,\psi_k$

The 3-dimensional generalization is

$$\hat{H} = -\frac{\hbar^2 \nabla^2}{2m} \quad , \quad \nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

and

$$\psi_{\vec{k}}(\vec{r}) = \frac{1}{(2\pi)^{3/2}} \exp(\pm i \vec{k}\cdot\vec{r}) \quad , \quad \vec{r} = (x, y, z)$$

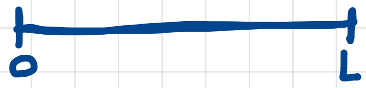
$$E_{\vec{k}} = \frac{\hbar^2 \vec{k}^2}{2m} \quad , \quad \vec{k} = (k_x, k_y, k_z)$$

Orthonormality: $\displaystyle\int_{-\infty}^{\infty} \psi^*_{\vec{k}}(\vec{r})\, \psi_{\vec{k}'}(\vec{r})\, d^3 r = \delta^{(3)}(\vec{k} - \vec{k}')$

Completeness: $\displaystyle\int_{-\infty}^{\infty} \psi^*_{\vec{k}}(\vec{r})\, \psi_{\vec{k}}(\vec{r}')\, d^3 k = \delta^{(3)}(\vec{r} - \vec{r}')$

- In a box, with $\psi(0) = \psi(L) = 0$ (1d)

  we have




$$\psi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right) \quad , \quad n = 1, 2, \ldots$$

$$E_n = \frac{\hbar^2}{2m}\left(\frac{n\pi}{L}\right)^2$$

These waves don't have well defined momentum, only momentum magnitude. It's a standing wave!

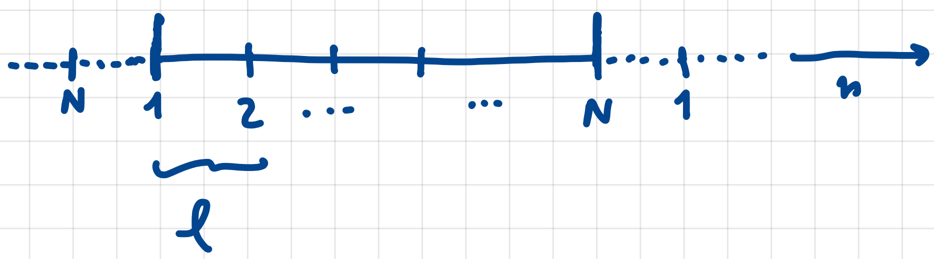
Orthonormality: $\displaystyle\int_0^L \psi^*_n(x)\, \psi_{n'}(x)\, dx = \delta_{nn'}$

Completeness: $\displaystyle\sum_{n=1}^{\infty} \psi^*_n(x)\, \psi_n(x') = \delta(x - x')$

- On the lattice, $n = 1, \ldots, N$, with periodic boundaries,

$$\psi_k(n) = \frac{1}{\sqrt{N}} \exp\left(i \frac{2\pi}{N} k n\right) \quad , \quad k = -\frac{N}{2}+1, \ldots, \frac{N}{2}$$

$$E_k = \frac{\hbar^2}{2m}\left(\frac{2\pi k}{N}\right)^2 \cdot \frac{1}{\ell^2}$$



$p$ : quasi-momentum

“ $-\frac{\pi}{\ell}+1, \dots, -\frac{2\pi}{L}, 0, \frac{2\pi}{L}, \dots, \frac{\pi}{\ell}$ , $L = N.\ell$

Orthogonality : $\sum_{n=1}^{N} \psi_k^*(n)\, \psi_{k'}(n) = \delta_{kk'}$

Completeness : $\sum_{k=-\frac{N}{2}+1}^{N/2} \psi_k^*(n)\, \psi_k(n') = \delta_{n,n'}$