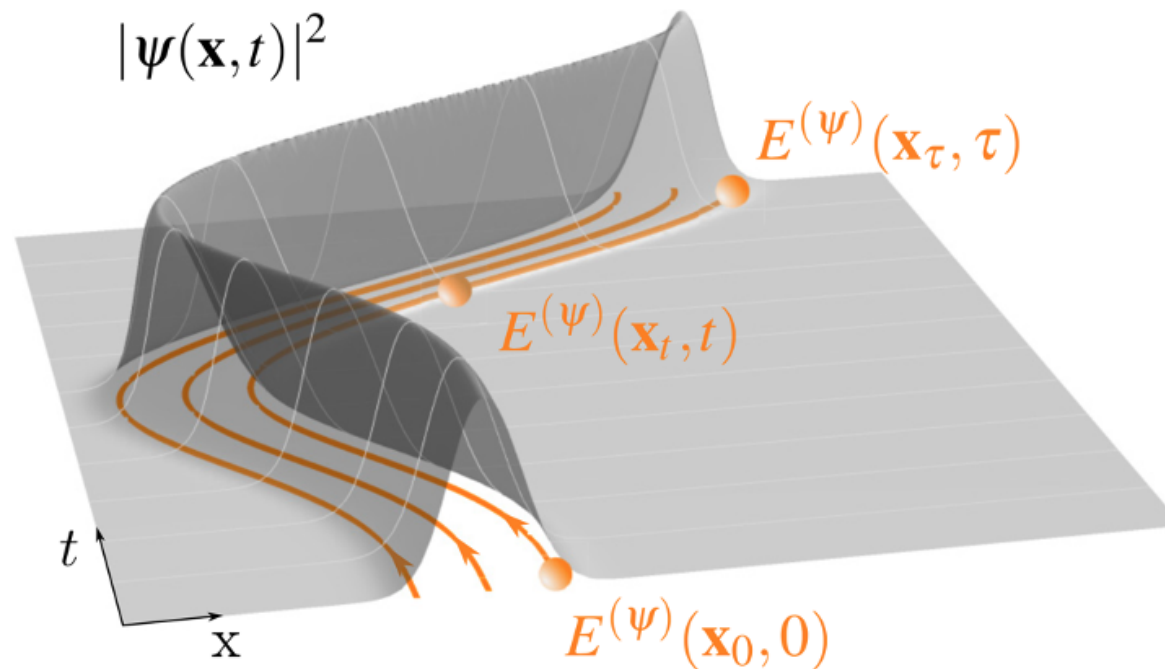


PHYS-C0252 - Quantum Mechanics Part 2

Sections 2-3

Tapio.Ala-Nissila@aalto.fi



2. Free Particles and Plane Waves

- Consider a free particle that does not experience any external potential in space. Going back to the symbolic notation, let us define the position and momentum (right) eigenvectors as

$$\hat{q}|x\rangle = x|x\rangle; \quad \hat{p}|p\rangle = p|p\rangle$$

and correspondingly the left eigenvectors

$$\langle x|\hat{q} = \langle x|x; \quad \langle p|\hat{p} = \langle p|p$$

The left and right eigenvectors are orthonormal:

$$\langle x'|x\rangle = \delta(x' - x); \quad \langle p'|p\rangle = \delta(p' - p)$$

and they form complete orthonormal sets that can be inserted between any states when necessary:

$$\int dx |x\rangle \langle x| = 1; \quad \int dp |p\rangle \langle p| = 1$$

Now we can define the *momentum operator in the position basis* as (can be derived by inserting p basis and partial integration)

$$\langle x' | \hat{p} | x \rangle = \delta(x' - x) \frac{\hbar}{i} \frac{d}{dx}$$

and the *position operator in the momentum basis* as

$$\langle p' | \hat{q} | p \rangle = -\delta(p' - p) \frac{\hbar}{i} \frac{d}{dp}$$

Now we can solve for the *momentum eigenstate in the position basis* $\psi_p(x) = \langle x|p\rangle$ from the DE

$$\langle x|\hat{p}|p\rangle = \frac{\hbar}{i} \frac{d}{dx} \langle x|p\rangle = p \langle x|p\rangle$$

This equation comes about from the fact that

$$\begin{aligned} \langle x|\hat{p}|p\rangle &= \int dx' \langle x|p|x'\rangle \langle x'|p\rangle = \int dx' \delta(x - x') \frac{\hbar}{i} \frac{d}{dx'} \langle x'|p\rangle \\ &= \frac{\hbar}{i} \frac{d}{dx} \langle x|p\rangle \end{aligned}$$

Thus we have the differential equation

$$\frac{\hbar}{i} \frac{d}{dx} \langle x|p\rangle = p \langle x|p\rangle$$

The solution to this DE is a simple plane wave

$$\langle x|p\rangle = \sqrt{\frac{1}{2\pi\hbar}} e^{ipx/\hbar}$$

where $p = \hbar k$. The corresponding *momentum eigenstate in the momentum basis* is

$$\psi_p(p') = \langle p'|p\rangle = \delta(p - p')$$

The normalized *position eigenstate in the momentum basis* can be obtained from

$$\langle p|x\rangle = \langle x|p\rangle^\dagger = \sqrt{\frac{1}{2\pi\hbar}} e^{-ipx/\hbar}$$

and the normalized *position eigenstate in the position basis* is (of course)

$$\psi_x(x) = \langle x'|x\rangle = \delta(x - x')$$

Note that these results can be immediately obtained from the Schrödinger equation (in the position basis)

$$-\frac{\hbar^2}{2m} \frac{d^2\psi(x)}{dx^2} = 0$$

- Let us next look at the time dependence of the plane waves in the **position basis**. The time-dependent Schrödinger equation is

$$i\hbar \frac{\partial\Psi(x, t)}{\partial t} = -\frac{\hbar^2}{2m} \frac{d^2\Psi(x, t)}{dx^2}$$

We look for separable solutions of the form

$$\Psi(x, t) = f(t)\psi(x)$$

This gives

$$\frac{i\hbar}{f(t)} \frac{\partial f(t)}{\partial t} = -\frac{1}{\psi(x)} \frac{\hbar^2}{2m} \frac{d^2\psi(x)}{dx^2}$$

Both sides must be constant (why?) and thus

$$f(t) = e^{-iEt/\hbar}$$

The solutions

$$\Psi(x, t) = e^{-iEt/\hbar} \psi_E(x)$$

are called *stationary states* because

$$\partial_t |\Psi(x, t)|^2 = 0$$

The general solution of the time-dependent wave equation can be obtained from the superposition principle

$$\Psi(x, t) = \sum_E c_E e^{-iEt/\hbar} e^{ipx/\hbar}$$

for the case of free particles (plane waves)

- An important generalization of this result is that if we use the completeness of the energy eigenfunctions to expand in terms of them $\psi_E(x)$, then in general

$$\Psi(x, t) = \sum_E c_E e^{-iEt/\hbar} \psi_E(x)$$

3. Particle in a Periodic Box

- Consider a free particle that traverses a box of finite (linear) size L , but no external $V(x)$ (periodic boundary conditions) s.t. $\psi_k(x) = \psi_k(x + L)$

The solution is that of the free particle, but now

$$k = \frac{2\pi n}{L}, \quad n \in \mathbb{Z}$$

The completeness relations now read as

$$\int_0^L dx |x\rangle \langle x| = 1; \quad \sum_{n=-\infty}^{\infty} |k\rangle \langle k| = 1$$

The wavevector eigenstate in the **position basis** is then simply

$$\psi_k(x) = \langle x|k\rangle = \langle k|x\rangle^\dagger = \frac{1}{L^{1/2}} e^{ikx}$$
