Lecture notes: QM 02

Time evolution of normalized wave function

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Contents

1 Wave function normalization

The wave function $\Psi(x,t)$ that describes the quantum mechanics of a particle of mass m moving in a potential $V(x,t)$ satisfies the Schrödinger equation

$$i\hbar\frac{\partial\Psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi(x,t)}{\partial x^2} + V(x,t)\Psi(x,t) \tag{1}$$

or briefly

$$i\hbar\frac{\partial\Psi(x,t)}{\partial t} = \hat{H}\Psi(x,t). \tag{2}$$

Here $\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x,t)$ is the Hamiltonian operator. The interpretation of the wave function arises by declaring that $\mathrm{d}P$, defined by

$$\mathrm{d}P = |\Psi(x,t)|^2\mathrm{d}x = \Psi^*(x,t)\Psi(x,t)\mathrm{d}x, \tag{3}$$

is the probability to find the particle in the interval $\mathrm{d}x$ centered on x at time t. It follows that the probabilities of finding the particle at all possible points must add up to one:

$$\boxed{\int_{-\infty}^{\infty}\Psi^*(x,t)\Psi(x,t)\mathrm{d}x = 1} \tag{4}$$

Suppose we have a wave function such that

$$\int_{-\infty}^{\infty} |\Psi(x,t)|^2 \mathrm{d}x = \mathcal{N} \neq 1. \tag{5}$$

If $\mathcal{N} < \infty$ the wave function $\Psi(x,t)$ is said to be **normalizable** or **square-integrable** and we define the **normalized** wave function as

$$\Psi'(x,t) = \frac{1}{\sqrt{\mathcal{N}}}\Psi(x,t). \tag{6}$$

This process is called **normalizing** the wave function. Indeed

$$\int_{-\infty}^{\infty} |\Psi'(x,t)|^2 \mathrm{d}x = \frac{1}{\mathcal{N}}\int_{-\infty}^{\infty} |\Psi(x,t)|^2 \mathrm{d}x = \frac{1}{\mathcal{N}} \times \mathcal{N} = 1. \tag{7}$$

We also claim that the probability $\mathrm{d}P$ to find the particle in the interval $\mathrm{d}x$ about x is given by

$$\mathrm{d}P = \frac{1}{\mathcal{N}}|\Psi(x,t)|^2 \mathrm{d}x. \tag{8}$$

This is consistent because

$$\int_{-\infty}^{\infty} \mathrm{d}P = \frac{1}{\mathcal{N}}\int_{-\infty}^{\infty} |\Psi(x,t)|^2 \mathrm{d}x = \frac{1}{\mathcal{N}} \times \mathcal{N} = 1. \tag{9}$$

Note that $\mathrm{d}P$ is not changed when $\Psi(x,t)$ is multiplied by any number. Thus, the overall scale of $\Psi(x,t)$ contains no physics.

If a wave function has well-defined limits as $x \to \pm\infty$ and if those limits are different from zero, the integral around infinity would produce an infinite result, which is inconsistent with the claim that the total integral is one. Therefore the limits should be zero:

$$\boxed{\lim_{x\to\pm\infty} \Psi(x,t) = 0.} \tag{10}$$

It is in principle possible to have a wave function that has no well-defined limit at infinity but is still is square integrable. But such cases do not seem to appear in practice so we will assume that (10) holds. It would also be natural to assume that the spatial derivative of $\Psi(x,t)$ vanishes as $x \to \pm\infty$ but, it suffices to assume that the limit of the spatial derivative of $\Psi(x,t)$ is bounded:

$$\boxed{\left|\lim_{x\to\pm\infty} \frac{\partial\Psi(x,t)}{\partial x}\right| < \infty.} \tag{11}$$

We sometimes work with wave functions for which the integral (4) is infinite. Such wave functions can be very useful. In fact, the de Broglie plane wave $\Psi(x,t) = \exp(ikx - \omega t)$ for a free particle is a good example: since $|\Psi(x,t)|^2 = 1$ the integral is in fact infinite. What this means is that $\Psi(x,t) = \exp(ikx - \omega t)$ does not truly represent a single particle. To construct a square-integrable wave function we can use a superposition of plane waves. It is indeed a pleasant surprise that the superposition of infinitely many non-square integrable waves is square integrable!

2 The probability current

Suppose we have a normalized wave function at an initial time $t = t_0$

$$\int_{-\infty}^{\infty} \Psi^*(x, t_0)\Psi(x, t_0)\mathrm{d}x = 1. \tag{12}$$

Will it remain normalized as time goes on and Ψ evolves? Since $\Psi(x, t_0)$ and the Schrödinger equation determine Ψ for all times, do we then have, for a later time t,

$$\int_{-\infty}^{\infty} \Psi^*(x, t)\Psi(x, t)\mathrm{d}x = 1? \tag{13}$$

Fortunately, the Schrödinger equation has the remarkable property that is automatically preserves the normalization of the wave function. Without this crucial feature the Schrödinger equation would be incompatible and the whole theory would crumble.

Let us define the **probability density** $\rho(x, t)$ as

$$\rho(x, t) \equiv \Psi^*(x, t)\Psi(x, t) = |\Psi(x, t)|^2 \tag{14}$$

and $\mathcal{N}(t)$ a the integral of the probability density throughout the space

$$\mathcal{N}(t) \equiv \int_{-\infty}^{\infty} \rho(x, t)\mathrm{d}x. \tag{15}$$

The statement in (12) that the wave function begins well normalized is

$$\mathcal{N}(t_0) = 1, \tag{16}$$

and the condition that it remain normalized for all later times is $\mathcal{N}(t) = 1$. This would be guaranteed if we showed that for all times

$$\frac{\mathrm{d}\mathcal{N}(t)}{\mathrm{d}t} = 0. \tag{17}$$

We call this *conservation of probability*. To check that the Schrödinger equation ensures this condition we begin with

$$\begin{aligned} \frac{\mathrm{d}\mathcal{N}(t)}{\mathrm{d}t} &= \int_{-\infty}^{\infty} \frac{\partial \rho(x, t)}{\partial t}\mathrm{d}x \\ &= \int_{-\infty}^{\infty} \left(\frac{\partial \Psi^*(x, t)}{\partial t}\Psi(x, t) + \Psi^*(x, t)\frac{\partial \Psi(x, t)}{\partial t} \right) \mathrm{d}x. \end{aligned} \tag{18}$$

(Note that $\mathcal{N}(t)$ is a function only of t, so we used a total derivative but $\rho(x, t)$ is a function of x as well as t, so a partial derivative is used.) Now the Schrödinger equation says that

$$\frac{\partial \Psi(x, t)}{\partial t} = \frac{i\hbar}{2m}\frac{\partial^2 \Psi(x, t)}{\partial x^2} - \frac{i}{\hbar}V(x, t)\Psi(x, t) \tag{19}$$

and hence also (taking complex conjugate)

$$\frac{\partial \Psi^*(x,t)}{\partial t} = -\frac{i\hbar}{2m}\frac{\partial^2 \Psi^*(x,t)}{\partial x^2} + \frac{i}{\hbar}V(x,t)\Psi^*(x,t), \tag{20}$$

since the complex conjugate of the derivative of Ψ is simply the derivative of the complex conjugate of Ψ. We therefore have

$$\begin{aligned}
\frac{\partial \rho(x,t)}{\partial t} &= -\frac{i\hbar}{2m}\frac{\partial^2\Psi^*}{\partial x^2}\Psi + \frac{i}{\hbar}V(x,t)\Psi^*\Psi + \frac{i\hbar}{2m}\Psi^*\frac{\partial^2\Psi}{\partial x^2} - \frac{i}{\hbar}\Psi^* V(x,t)\Psi \\
&= -\frac{i\hbar}{2m}\left(\frac{\partial^2\Psi^*}{\partial x^2}\Psi - \Psi^*\frac{\partial^2\Psi}{\partial x^2}\right) \\
&= \frac{\partial}{\partial x}\left[-\frac{i\hbar}{2m}\left(\frac{\partial\Psi^*}{\partial x}\Psi - \Psi^*\frac{\partial\Psi}{\partial x}\right)\right] \\
&= -\frac{\partial}{\partial x}\left[-\frac{i\hbar}{2m}\left(\Psi^*\frac{\partial\Psi}{\partial x} - \frac{\partial\Psi^*}{\partial x}\Psi\right)\right] \\
&= -\frac{\partial J(x,t)}{\partial x}.
\end{aligned} \tag{21}$$

This equation encodes charge conservation and is of the type

$$\frac{\partial \rho}{\partial t} + \frac{\partial J}{\partial x} = 0, \tag{22}$$

where J is the current associated with the charge density ρ. We have therefore identified a probability current

$$\begin{aligned}
J(x,t) &\equiv -\frac{i\hbar}{2m}\left(\Psi^*\frac{\partial\Psi}{\partial x} - \frac{\partial\Psi^*}{\partial x}\Psi\right) \\
&= \frac{\hbar}{2im}\left(\Psi^*\frac{\partial\Psi}{\partial x} - \frac{\partial\Psi^*}{\partial x}\Psi\right) \\
&= \frac{\hbar}{m}\,\mathrm{Im}\left(\Psi^*\frac{\partial\Psi}{\partial x}\right),
\end{aligned} \tag{23}$$

where we used that $z - z^* = 2i\,\mathrm{Im}(z)$. There is just one component for this current since the particle moves in one dimension. The units of J are one over time, or probability per unit time.

In case of a particle moving in three dimension one can easily show, using the three dimensional version of Schrödinger equation, that the probability density and the probability current are determined to be

$$\boxed{\rho(\mathbf{r},t) = |\Psi(\mathbf{r},t)|^2, \qquad \mathbf{J}(\mathbf{r},t) = \frac{\hbar}{m}\,\mathrm{Im}(\Psi^*\nabla\Psi),} \tag{24}$$

and satisfy the conservation equation

$$\frac{\partial \rho}{\partial t} + \nabla\cdot\mathbf{J} = 0. \tag{25}$$

In the three spatial dimensions the units of $\mathbf{J}$ are probability per unit time per unit area.

3 Conservation of probability

From (18) and (21) we have

$$\begin{aligned}\frac{\mathrm{d}\mathcal{N}(t)}{\mathrm{d}t} &= \int_{-\infty}^{\infty} \frac{\partial \rho(x,t)}{\partial t}\mathrm{d}x \\ &= -\int_{-\infty}^{\infty} \frac{\partial J(x,t)}{\partial x}\mathrm{d}x \\ &= -[J(\infty,t) - J(-\infty,t)]. \end{aligned} \tag{26}$$

The derivative vanishes if the probability current vanishes at infinity. Recalling that

$$J(x,t) = \frac{\hbar}{2im}\left(\Psi^* \frac{\partial \Psi}{\partial x} - \frac{\partial \Psi^*}{\partial x}\Psi\right)$$

we see that the current indeed vanishes because we restrict ourselves to wave functions for which $\lim_{x\to\pm\infty}\Psi = 0$ and $\lim_{x\to\pm\infty}\frac{\partial\Psi}{\partial x}$ remains bounded. We therefore have

$$\boxed{\frac{\mathrm{d}\mathcal{N}}{\mathrm{d}t} = 0,} \tag{27}$$

as we wanted to show. Hence $\mathcal{N}$ is constant (independent of time) and if Ψ is normalized at time $t = t_0$, it remains normalized for all future time.

Note: Most of the materials in this lecture note are taken from the lecture on Quantum Physics by Prof. Barton Zwiebach for the course 8.04 in the year of 2016 at MIT, USA.

References

1. Quantum Mechanics by Nouredine Zettili
2. Introduction to Quantum Mechanics by David J. Griffiths