Lecture 6

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1 Normalization and time evolution

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

$$i\hbar\frac{\partial\Psi(x,t)}{\partial t} = \Big(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x,t)\Big)\Psi(x,t)\,, \tag{1.1}$$

or more briefly

$$i\hbar\,\frac{\partial\Psi(x,t)}{\partial t} \;=\; \hat{H}\,\Psi(x,t)\,. \tag{1.2}$$

The interpretation of the wavefunction arises by declaring that dP, defined by

$$dP \;=\; |\Psi(x,t)|^2 dx\,, \tag{1.3}$$

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

$$\int_{-\infty}^{\infty}\Psi^*(x,t)\,\Psi(x,t)\,dx = 1\,. \tag{1.4}$$

We will try to understand how this equation is compatible with the time evolution prescribed by the Schrödinger equation. But before that let us examine what kind of conditions are required from wavefunctions in order to satisfy (1.4).

Suppose the wavefunction has well-defined limits as $x\to\pm\infty$. 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:

$$\boxed{\lim_{x\to\pm\infty}\Psi(x,t) = 0\,.} \tag{1.5}$$

It is in principle possible to have a wavefunction 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 (1.5) holds. It would also be natural to assume that the spatial derivative of Ψ vanishes as $x \to \pm\infty$ but, as we will see soon, it suffices to assume that the limit of the spatial derivative of Ψ is bounded

$$\boxed{\lim_{x\to\pm\infty} \frac{\partial\Psi(x,t)}{\partial x} < \infty\,.} \tag{1.6}$$

We have emphasized before that the overall numerical factor multiplying the wavefunction is not physical. But equation (1.4) seems to be in conflict with this: if a given Ψ satisfies it, the presumed equivalent 2Ψ will not! To make precise sense of probabilities it is *convenient* to work with normalized wavefunctions, but it is not necessary, as we show now. Since time plays no role in the argument, so assume in all that follows that the equations refer to some time t_0 arbitrary but fixed. Suppose you have a wavefunction such that

$$\int dx\, |\Psi|^2 \;=\; \mathcal{N} \;\neq\; 1\,. \tag{1.7}$$

Then I claim that the probability dP to find the particle in the interval dx about x is given by

$$dP \;=\; \frac{1}{\mathcal{N}}\,|\Psi|^2\,dx\,. \tag{1.8}$$

This is consistent because

$$\int dP \;=\; \frac{1}{\mathcal{N}}\int dx\,|\Psi|^2 \;=\; \frac{1}{\mathcal{N}}\cdot\mathcal{N} \;=\; 1\,. \tag{1.9}$$

Note that dP is not changed when Ψ is multiplied by any number. Thus, this picture makes it clear that the overall scale of Ψ contains no physics. As long as the integral $\int |\Psi|^2 dx < \infty$ the wavefunction is said to be **normalizable, or square-integrable**. By adjusting the overall coefficient of Ψ we can then make it **normalized**. Indeed, again assuming (1.7) the new wavefunction Ψ' defined by

$$\Psi' \;=\; \frac{1}{\sqrt{\mathcal{N}}}\,\Psi\,, \tag{1.10}$$

is properly normalized. Indeed

$$\int dx|\Psi'|^2 \;=\; \frac{1}{\mathcal{N}}\int |\Psi|^2 dx \;=\; 1\,. \tag{1.11}$$

We sometimes work with wavefunctions for which the integral (1.4) is infinite. Such wavefunctions can be very useful. In fact, the de Broglie plane wave $\Psi = \exp(ikx - i\omega t)$ for a free particle is a good example: since $|\Psi|^2 = 1$ the integral is in fact infinite. What this means is that $\exp(ikx - i\omega t)$ does not truly represent a single particle. To construct a square-integrable wavefunction 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 Wavefunction as a Probability Amplitude

Let's begin with a normalized wavefunction at initial time t_0

$$\int_{-\infty}^{\infty} \Psi^*(x,t_0)\Psi(x,t_0)dx = 1\,. \tag{2.1}$$

Since $\Psi(x,t_0)$ and the Schrödinger equation determine Ψ for all times, do we then have

$$\int_{-\infty}^{\infty} \Psi^*(x,t)\Psi(x,t)dx \;=\; 1\;? \tag{2.2}$$

Define the **probability density** $\rho(x,t)$

$$\rho(x,t) \;\equiv\; \Psi^*(x,t)\Psi(x,t) \;=\; |\Psi(x,t)|^2\,. \tag{2.3}$$

Define also $\mathcal{N}(t)$ as the integral of the probability density throughout space:

$$\mathcal{N}(t) \;\equiv\; \int \rho(x,t)dx\,. \tag{2.4}$$

The statement in (2.1) that the wavefunction begins well normalized is

$$\mathcal{N}(t_0) = 1\,, \tag{2.5}$$

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

$$\frac{d\mathcal{N}(t)}{dt} = 0\,. \tag{2.6}$$

We call this *conservation* of probability. Let's check if the Schrödinger equation ensures this condition will hold:

$$\begin{aligned} \frac{d\mathcal{N}(t)}{dt} \;&=\; \int_{-\infty}^{\infty} \frac{\partial\rho(x,t)}{\partial t}dx \\ &=\; \int_{-\infty}^{\infty} \left(\frac{\partial\Psi^*}{\partial t}\Psi(x,t) + \Psi^*(x,t)\frac{\partial\Psi(x,t)}{\partial t}\right)dx\,. \end{aligned} \tag{2.7}$$

From the Schrödinger equation, and its complex conjugate

$$i\hbar\frac{\partial\Psi}{\partial t} = \hat{H}\Psi \quad\Longrightarrow\quad \frac{\partial\Psi}{\partial t} = -\frac{i}{\hbar}\hat{H}\Psi\,, \tag{2.8}$$

$$-i\hbar\frac{\partial\Psi^*}{\partial t} = (\hat{H}\Psi)^* \quad\Longrightarrow\quad \frac{\partial\Psi^*}{\partial t} = \frac{i}{\hbar}\,(\hat{H}\Psi)^*\,. \tag{2.9}$$

In complex conjugating the Schrödinger equation we used that the complex conjugate of the time derivative of Ψ is simply the time derivative of the complex conjugate of Ψ. To conjugate the right hand side we simply added the star to the whole of $\hat{H}\Psi$. We now use (2.8) and (2.9) in (2.7) to find

$$\begin{aligned} \frac{d\mathcal{N}(t)}{dt} &= \int_{-\infty}^{\infty} \Big(\frac{i}{\hbar}(\hat{H}\Psi)^* \, \Psi - \frac{i}{\hbar}\Psi^*(\hat{H}\Psi) \Big) dx \\ &= \frac{i}{\hbar}\Big(\int_{-\infty}^{\infty} (\hat{H}\Psi)^* \, \Psi dx - \int_{-\infty}^{\infty} \Psi^*(\hat{H}\Psi) dx \Big) \, . \end{aligned} \tag{2.10}$$

To show that the time derivative of $\mathcal{N}(t)$ vanishes, it suffices to show that

$$\boxed{\int_{-\infty}^{\infty} (\hat{H}\Psi)^* \, \Psi \; = \; \int_{-\infty}^{\infty} \Psi^*(\hat{H}\Psi) \, .} \tag{2.11}$$

Equation (2.11) is the condition on the Hamiltonian operator $\hat{H}$ for conservation of probability. In fact, if $\hat{H}$ is a Hermitian operator the condition will be satisfied. The operator $\hat{H}$ is a **Hermitian** operator if it satisfies

$$\boxed{\text{Hermitian operator:} \qquad \int_{-\infty}^{\infty} (\hat{H}\Psi_1)^* \, \Psi_2 \; = \; \int_{-\infty}^{\infty} \Psi_1^*(\hat{H}\Psi_2) \, .} \tag{2.12}$$

Here we have two wavefunctions that are arbitrary, but satisfy the conditions (1.5) and (1.6). As you can see, a Hermitian operator can be switched from acting on the first function to acting on the second function. When the two functions are the same, we recover condition (2.11).

It is worth closing this circle of ideas by defining the **Hermitian conjugate** $T^\dagger$ of the linear operator T. This is done as follows:

$$\int_{-\infty}^{\infty} \Psi_1^* \, (T\Psi_2) \; = \; \int_{-\infty}^{\infty} (T^\dagger \Psi_1)^* \, \Psi_2 \, . \tag{2.13}$$

The operator $T^\dagger$, which is also linear, is calculated by starting from the left-hand side and trying to recast the expression with no operator acting on the second function. An operator T is said to be Hermitian if it is equal to its Hermitian conjugate:

$$T \text{ is Hermitian if} \qquad T^\dagger = T \, . \tag{2.14}$$

Hermitian operators are very important in Quantum Mechanics. They have real eigenvalues and one can always find a basis of the state space in terms of orthonormal eigenstates. It turns out that observables in Quantum Mechanics are represented by Hermitian operators, and the possible measured values of those observables are given by their eigenvalues. Our quest to show that normalization is preserved under time evolution in Quantum Mechanics has come down to showing that the Hamiltonian operator is Hermitian.

3 The Probability Current

Let's take a closer look at the integrand of equation (2.10). Using the explicit expression for the Hamiltonian we have

$$
\begin{aligned}
\frac{\partial \rho}{\partial t} &= \frac{i}{\hbar}\big((\hat{H}\Psi)^*\,\Psi - \Psi^*(\hat{H}\Psi)\big) \\
&= \frac{i}{\hbar}\left[-\frac{\hbar^2}{2m}\left(\frac{\partial^2\Psi^*}{\partial x^2}\Psi - \Psi^*\frac{\partial^2\Psi}{\partial x^2}\right) + V(x,t)\Psi^*\Psi - \Psi^* V(x,t)\Psi\right].
\end{aligned}
\tag{3.1}
$$

The contributions from the potential cancel and we then get

$$
\frac{i}{\hbar}\big((\hat{H}\Psi)^*\,\Psi - \Psi^*(\hat{H}\Psi)\big) \;=\; \frac{\hbar}{2im}\left(\frac{\partial^2\Psi^*}{\partial x^2}\Psi - \Psi^*\frac{\partial^2\Psi}{\partial x^2}\right). \tag{3.2}
$$

The only chance to get to show that the integral of the right-hand side is zero is to show that it is a total derivative. Indeed, it is!

$$
\begin{aligned}
\frac{i}{\hbar}\big((\hat{H}\Psi)^*\,\Psi - \Psi^*(\hat{H}\Psi)\big) \;&=\; \frac{\partial}{\partial x}\left[\frac{\hbar}{2im}\left(\frac{\partial\Psi^*}{\partial x}\Psi - \Psi^*\frac{\partial\Psi}{\partial x}\right)\right] \\
&=\; -\frac{\partial}{\partial x}\left[\frac{\hbar}{2im}\left(\Psi^*\frac{\partial\Psi}{\partial x} - \frac{\partial\Psi^*}{\partial x}\Psi\right)\right] \\
&=\; -\frac{\partial}{\partial x}\left[\frac{\hbar}{2im}\,2i\,\mathrm{Im}\left(\Psi^*\frac{\partial\Psi}{\partial x}\right)\right] \\
&=\; -\frac{\partial}{\partial x}\left[\frac{\hbar}{m}\,\mathrm{Im}\left(\Psi^*\frac{\partial\Psi}{\partial x}\right)\right],
\end{aligned}
\tag{3.3}
$$

where we used that $z - z^* = 2i\,\mathrm{Im}(z)$. Recall that the left-hand side we have evaluated is actually $\frac{\partial\rho}{\partial t}$ and therefore the result obtained so far is

$$
\frac{\partial\rho}{\partial t} + \frac{\partial}{\partial x}\left[\frac{\hbar}{m}\,\mathrm{Im}\left(\Psi^*\frac{\partial\Psi}{\partial x}\right)\right] \;=\; 0\,. \tag{3.4}
$$

This equation encodes charge conservation and is of the type

$$
\frac{\partial\rho}{\partial t} + \frac{\partial J}{\partial x} \;=\; 0\,, \tag{3.5}
$$

where $J(x,t)$ is the current associated with the charge density ρ. We have therefore identified a probability current

$$
\boxed{J(x,t) \equiv \frac{\hbar}{m}\mathrm{Im}\left(\Psi^*\frac{\partial\Psi}{\partial x}\right).} \tag{3.6}
$$

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, as we now verify.

For one spatial dimension, $[\Psi] = L^{-1/2}$, which is easily seen from the requirement that $\int dx |\Psi|^2$ is unit free. (When working with d spatial dimensions the wavefunction will have units of $L^{-d/2}$). We then have

$$\left[\Psi^* \frac{\partial \Psi}{\partial x}\right] = \frac{1}{L^2}, \quad [\hbar] = \frac{ML^2}{T}, \quad \left[\frac{\hbar}{m}\right] = \frac{L^2}{T}, \tag{3.7}$$

$$\implies [J] = \frac{1}{T} = \text{probability per unit time} \tag{3.8}$$

We can now show that the time derivative of $\mathcal{N}$ is zero. Indeed, using (3.5) we have

$$\frac{d\mathcal{N}}{dt} = \int_{-\infty}^{\infty} dx \frac{\partial \rho}{\partial t} = -\int_{\infty}^{\infty} \frac{\partial J}{\partial x} dx = -(J(\infty, t) - J(-\infty, t)). \tag{3.9}$$

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

$$J = \frac{\hbar}{2im}\left(\Psi^* \frac{\partial \Psi}{\partial x} - \Psi \frac{\partial \Psi^*}{\partial x}\right), \tag{3.10}$$

we see that the current indeed vanishes because we restrict ourselves to wavefunctions 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

$$\boxed{\frac{d\mathcal{N}}{dt} = 0,} \tag{3.11}$$

as we wanted to show.

To illustrate how probability conservation works more generally in one dimension, focus on a segment $x \in [a, b]$. Then the probability P_{ab} to find the particle in the segment $[a, b]$, is given by

$$P_{ab} = \int_a^b \rho(x, t)\, dx. \tag{3.12}$$

If we now take the time derivative of this and, as before, use current conservation we get

$$\frac{dP_{ab}}{dt} = -\int_a^b \frac{\partial J(x, t)}{\partial x} dt = -J(b, t) + J(a, t). \tag{3.13}$$

This is the expected result. If the amount of probability in the region $[a, b]$ changes in time, it must be due to probability current flowing in or out at the edges of the interval. Assuming the currents at $x = b$ and at $x = a$ are positive, we note that probability is flowing out at $x = b$ and is coming in at $x = a$. The signs in the above right-hand side correctly reflect the effect of these flows on the rate of change of the total probability inside the segment.

4 Probability current in 3D and current conservation

The determination of the probability current $\mathbf{J}$ for a particle moving in three dimensions follows the route taken before, but we use the 3D version of the Schrödinger equation. After some work (homework) the probability density and the current are determined to be

$$\boxed{\rho(\mathbf{x},t) \;=\; |\Psi(\mathbf{x},t)|^2\,, \qquad \mathbf{J}(x,t) \;=\; \frac{\hbar}{m}\,\mathrm{Im}\,(\Psi^*\nabla\Psi)\,,} \tag{4.1}$$

and satisfy the conservation equation

$$\frac{\partial\rho}{\partial t} + \nabla\cdot\mathbf{J} \;=\; 0\,. \tag{4.2}$$

In three spatial dimensions, $[\Psi] = L^{-\frac{3}{2}}$ and the units of $\mathbf{J}$ are quickly determined

$$[\Psi^*\nabla\Psi] = \frac{1}{L^4}\,, \qquad \left[\frac{\hbar}{m}\right] = \frac{L^2}{T} \tag{4.3}$$

$$\implies [\mathbf{J}] = \frac{1}{TL^2} = \text{probability per unit time per unit area} \tag{4.4}$$

The conservation equation (4.2) is particularly clear in integral language. Consider a fixed region V of space and the probability $Q_V(t)$ to find the particle inside the region:

$$Q_V(t) \;=\; \int_V \rho(\mathbf{x},t)d^3\mathbf{x}\,. \tag{4.5}$$

The time derivative of the probability is then calculated using the conservation equation

$$\frac{dQ_V}{dt} \;=\; \int_V \frac{\partial\rho}{\partial t}\,d^3\mathbf{x} \;=\; -\int_V \nabla\cdot\mathbf{J}\,d^3\mathbf{x}\,. \tag{4.6}$$

Finally, using Gauss' law we find

$$\frac{dQ_V}{dt} \;=\; -\int_S \mathbf{J}\cdot\mathbf{da}\,, \tag{4.7}$$

where S is the boundary of the volume V. The interpretation here is clear. The probability that the particle is inside V may change in time if there is flux of the probability current across the boundary of the region. When the volume extends throughout space, the boundary is at infinity, and the conditions on the wavefunction (which we have not discussed in the 3D case) imply that the flux across the boundary at infinity vanishes.

Our probability density, probability current, and current conservation are in perfect analogy to electromagnetic charge density, current density, and current conservation. In electromagnetism charges flow, in quantum mechanics probability flows. The terms of the correspondence are summarized by the table.

	Electromagnetism	Quantum Mechanics
ρ	charge density	probability density
Q_V	charge in a volume V	probability to find particle in V
$\mathbf{J}$	current density	probability current density

Sarah Geller transcribed Zwiebach's handwritten notes to create the first LaTeX version of this document.