1 Probability Conservation

The conventional interpretation of the wavefunction, ψ, associated with a particle is that $|\psi(x)|^2 = \psi^*(x)\psi(x)$ expresses the relative probability of finding the particle at point x. (The superscripted asterisk indicates complex conjugation.) If particles aren't created or destroyed, then the probability integrated over the x-domain must satisfy

$$P = \int_{-\infty}^{\infty} \psi^* \psi dx = 1, \tag{1}$$

and should not change with time. In order to test whether the theory satisfies this condition, we first need to derive the time-dependent form of the Schrödinger equation. We can then take the time derivative of P and see if it is indeed zero.

1.1 Time-Dependent Schrödinger Equation

The time independent Schrödinger equation in one space dimension for a particle with total (non-relativistic) energy E is

$$\frac{\partial^2 \psi_E}{\partial x^2} + \frac{2m(E-U)}{\hbar^2}\psi_E = 0. \tag{2}$$

(Note that we have dropped the prime on E for convenience.) Using $E = \hbar\omega$, the time-dependent wavefunction is simply $\psi(x,t) = \psi_E(x)\exp(-iEt/\hbar)$.

Since the principle of superposition applies to quantum mechanical waves, the wavefunction for an arbitrary mix of possible energy states is obtained as a weighted sum of such expressions:

$$\psi(x,t) = \sum_E W_E \psi_E(x) \exp(-iEt/\hbar), \tag{3}$$

where W_E is the (possibly complex) weight for the wavefunction associated with energy E. Normally, the time-independent wavefunctions are normalized such that

$$\int_{-\infty}^{\infty} |\psi_E(x)|^2 dx = 1. \tag{4}$$

With this normalization, $|W_E|^2$ just becomes the probability of the particle having energy E. Note that the sum is over just the *possible* energies, i. e., those energies for which equation (2) and its associated boundary conditions are satisfied.

We now rearrange equation (2) and multiply by $\exp(-iEt/\hbar)$ to incorporate the time dependence of the wavefunction,

$$E\psi_E \exp(-iEt/\hbar) = -\frac{\hbar^2}{2m}\frac{\partial\psi_E \exp(-iEt/\hbar)}{\partial x^2} + U\psi_E \exp(-iEt/\hbar), \qquad (5)$$

and then note that the right side can be written $i\hbar\partial\psi_E \exp(-iEt/\hbar)/\partial t$. Multiplying by W_E and summing over E finally results in the time-dependent Schrödinger equation:

$$i\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + U\psi. \qquad (6)$$

This partial differential equation governs the fully time-dependent behavior of non-relativistic particles in one dimension. (The three-dimensional version is obtained by replacing $\partial^2\psi/\partial x^2$ with $\nabla^2\psi$.)

1.2 Probability Flux

Let us now ask a somewhat more complex question than the one posed in the introduction. Suppose we want to know how the probability of a particle being within some interval $[a, b]$ on the x-axis changes with time. This probability is obtained by replacing the infinite limits in equation (1) with a and b:

$$P_{ab} = \int_a^b \psi^*\psi dx. \qquad (7)$$

Taking the time derivative of this yields

$$\frac{dP_{ab}}{dt} = \int_a^b \left(\frac{\partial\psi^*}{\partial t}\psi + \psi^*\frac{\partial\psi}{\partial t}\right) dx. \qquad (8)$$

The Schrödinger equation can now be substituted into the above formula, yielding

$$\frac{dP_{ab}}{dt} = \frac{\hbar}{2im}\int_a^b \left(\frac{\partial^2\psi^*}{\partial x^2}\psi - \psi^*\frac{\partial^2\psi}{\partial x^2}\right) dx. \qquad (9)$$

Note that the equation for ψ^* is obtained by taking the complex conjugate of equation (6), which changes the sign of i on the left side, resulting in the minus sign in the above equation.

Further progress comes from using the identity

$$\frac{\partial}{\partial x}\left(\frac{\partial \psi^*}{\partial x}\psi\right) = \frac{\partial^2 \psi^*}{\partial x^2}\psi + \frac{\partial \psi^*}{\partial x}\frac{\partial \psi}{\partial x} \tag{10}$$

and its complex conjugate to eliminate the second derivatives in equation (9),

$$\frac{dP_{ab}}{dt} = \frac{\hbar}{2im}\int_a^b \frac{\partial}{\partial x}\left(\frac{\partial \psi^*}{\partial x}\psi - \psi^*\frac{\partial \psi}{\partial x}\right) dx, \tag{11}$$

which can then be easily integrated to yield

$$\frac{dP_{ab}}{dt} = \frac{\hbar}{2im}\left(\frac{\partial \psi^*}{\partial x}\psi - \psi^*\frac{\partial \psi}{\partial x}\right)\Bigg|_a^b. \tag{12}$$

The quantity

$$F(x,t) = -\frac{\hbar}{2im}\left(\frac{\partial \psi^*}{\partial x}\psi - \psi^*\frac{\partial \psi}{\partial x}\right) \tag{13}$$

is called the *probability flux*. Notice that F is real even though ψ is in general complex. (Prove this by showing that $F^* = F$.) Equation (12) can be written

$$\frac{dP_{ab}}{dt} = F(a,t) - F(b,t), \tag{14}$$

which in words says that the rate of change of the probability of finding a particle within the interval $[a,b]$ equals the probability flux into the left side of the interval minus the flux out of the right side.

Notice that where $\psi = 0$, the flux is zero. It is often the case that $\psi = 0$ at $\pm\infty$, which means that $dP_{-\infty\infty}/dt = 0$. This constitutes a proof of the hypothesis posed in the introduction; the probability of finding a particle *somewhere* doesn't change with time in non-relativistic quantum mechanics. Also note that if ψ is real, so that $\psi^* = \psi$, then $F = 0$. This explains why the quantum mechanical wavefunction must in general be complex — if it weren't, nothing would ever go anywhere!

1.3 The Relativistic Case

Oddly enough, the above proof does not extend to the relativistic case. To see this, note that the relativistic form of the wavenumber squared is

$$k^2 = \frac{p^2}{\hbar^2} = \frac{E^2 - m^2 c^4}{\hbar^2 c^2} \tag{15}$$

when no potential energies are involved. The total energy, E, appears quadratically in this equation as opposed to linearly in the non-relativistic form, leading inevitably to a second time derivative of ψ in the relativistic wave equation:

$$\frac{1}{c^2}\frac{\partial^2 \psi}{\partial t^2} = \frac{\partial^2 \psi}{\partial x^2} - \frac{m^2 c^2}{\hbar^2}\psi. \tag{16}$$

This is called the *Klein-Gordon* equation, and it resembles the ordinary wave equation of electromagnetism with an additional term proportional to ψ added on.

The interpretation of $|\psi|^2$ as the probability of finding a single particle doesn't work, because the spatially integrated value of $|\psi|^2$ can change with time. To see this, note that $\psi = \cos(kx)\cos(\omega t)$ is a solution to equation (16) if $\omega^2 = k^2c^2 + m^2c^4/\hbar^2$. The probability of finding a particle at point subject to this wave equation oscillates between zero and $\cos^2(kx)$ with a frequency 2ω. Thus, probability is not conserved for this solution to the Klein-Gordon equation.

What does this mean? It turns out that equations of this type have a different interpretation in relativistic quantum mechanics — the wavefunction represents an *ensemble* of zero or more particles of a given type. In the relativistic case, all particles can be created and destroyed by various processes, so it is not surprising that the probability of finding a particle is not generally conserved over time. *Quantum field theory* governs the rules for particle creation and destruction, and it arises as an inevitable consequence of the collision of quantum mechanics with special relativity.