6.1: Fundamental Concepts

We have seen that in one dimension the instantaneous state of a single non-relativistic particle is fully specified by a complex wavefunction, $\psi(x,t)$. The probability of finding the particle at time t between x and $x+dx$ is $P(x,t)\,dx$, where

$$P(x,t) = |\psi(x,t)|^{\,2}. \tag{6.1.1}$$

Moreover, the wavefunction is normalized such that

$$\int_{-\infty}^{\infty}|\psi(x,t)|^{\,2}\,dx = 1 \tag{6.1.2}$$

at all times.

In three dimensions, the instantaneous state of a single particle is also fully specified by a complex wavefunction, $\psi(x,y,z,t)$. By analogy with the one-dimensional case, the probability of finding the particle at time t between x and $x+dx$, between y and $y+dx$, and between z and $z+dz$, is $P(x,y,z,t)\,dx\,dy\,dz$, where

$$P(x,y,z,t) = |\psi(x,y,z,t)|^{\,2}. \tag{6.1.3}$$

As usual, this interpretation of the wavefunction only makes sense if the wavefunction is normalized such that

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}|\psi(x,y,z,t)|^{\,2}\,dx\,dy\,dz = 1. \tag{6.1.4}$$

This normalization constraint ensures that the probability of finding the particle anywhere is space is always unity.

In one dimension, we can write the probability conservation equation (see Section [s4.5])

$$\frac{\partial|\psi|^{\,2}}{\partial t} + \frac{\partial j}{\partial x} = 0, \tag{6.1.5}$$

where

$$j = \frac{\mathrm{i}\,\hbar}{2\,m}\left(\psi\,\frac{\partial\psi^\ast}{\partial x} - \psi^\ast\,\frac{\partial\psi}{\partial x}\right) \tag{6.1.6}$$

is the flux of probability along the x-axis. Integrating Equation ([e6.5]) over all space, and making use of the fact that $\psi\rightarrow 0$ as $|x|\rightarrow\infty$ if ψ is to be square-integrable, we obtain

$$\frac{d}{dt}\int_{-\infty}^{\infty}|\psi(x,t)|^{\,2}\,dx = 0. \tag{6.1.7}$$

In other words, if the wavefunction is initially normalized then it stays normalized as time progresses. This is a necessary criterion for the viability of our basic interpretation of $|\psi|^{\,2}$ as a probability density.

In three dimensions, by analogy with the one dimensional case, the probability conservation equation becomes

$$\frac{\partial|\psi|^{\,2}}{\partial t} + \frac{\partial j_x}{\partial x} + \frac{\partial j_y}{\partial y} + \frac{\partial j_z}{\partial z} = 0. \tag{6.1.8}$$

Here,

$$j_x = \frac{\mathrm{i}\,\hbar}{2\,m}\left(\psi\,\frac{\partial\psi^\ast}{\partial x} - \psi^\ast\,\frac{\partial\psi}{\partial x}\right) \tag{6.1.9}$$

is the flux of probability along the x-axis, and

$$j_y = \frac{\mathrm{i}\,\hbar}{2\,m}\left(\psi\,\frac{\partial\psi^\ast}{\partial y} - \psi^\ast\,\frac{\partial\psi}{\partial y}\right) \tag{6.1.10}$$

the flux of probability along the y-axis, et cetera. Integrating Equation ([e6.8]) over all space, and making use of the fact that $\psi\rightarrow 0$ as $|\mathbf{r}|\rightarrow\infty$ if ψ is to be square-integrable, we obtain

$$\frac{d}{dt}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}|\psi(x,y,z,t)|^{\,2}\,dx\,dy\,dz=0. \tag{6.1.11}$$

Thus, the normalization of the wavefunction is again preserved as time progresses, as must be the case if $|\psi|^{\,2}$ is to be interpreted as a probability density.

In one dimension, position is represented by the algebraic operator x, whereas momentum is represented by the differential operator $-\mathrm{i}\,\hbar\,\partial/\partial x$. (See Section [s4.6].) By analogy, in three dimensions, the Cartesian coordinates x, y, and z are represented by the algebraic operators x, y, and z, respectively, whereas the three Cartesian components of momentum, p_x, p_y, and p_z, have the following representations:

$$\begin{aligned} p_x &\equiv -\mathrm{i}\,\hbar\,\frac{\partial}{\partial x},\\ p_y &\equiv -\mathrm{i}\,\hbar\,\frac{\partial}{\partial y},\\ p_z &\equiv -\mathrm{i}\,\hbar\,\frac{\partial}{\partial z}.\end{aligned}$$

Let $x_1=x$, $x_2=y$, $x_3=z$, and $p_1=p_x$, et cetera. Because the x_i are independent variables (i.e., $\partial x_i/\partial x_j=\delta_{ij}$), we conclude that the various position and momentum operators satisfy the following commutation relations:

$$\begin{aligned} [x_i,x_j] &= 0,\\ [p_i,p_j] &= 0,\\ [x_i,p_j] &= \mathrm{i}\,\hbar\,\delta_{ij}.\end{aligned}$$

Now, we know, from Section [smeas], that two dynamical variables can only be (exactly) measured simultaneously if the operators that represent them in quantum mechanics commute with one another. Thus, it is clear, from the previous commutation relations, that the only restriction on measurement in a system consisting of a single particle moving in three dimensions is that it is impossible to simultaneously measure a given position coordinate and the corresponding component of momentum. Note, however, that it is perfectly possible to simultaneously measure two different positions coordinates, or two different components of the momentum. The commutation relations ([commxx])–([commxp]) again illustrate the point that quantum mechanical operators corresponding to different degrees of freedom of a dynamical system (in this case, motion in different directions) tend to commute with one another. (See Section [sfuncon].)

In one dimension, the time evolution of the wavefunction is given by [see Equation ([etimed])]

$$\mathrm{i}\,\hbar\,\frac{\partial\psi}{\partial t}=H\,\psi, \tag{6.1.12}$$

where H is the Hamiltonian. The same equation governs the time evolution of the wavefunction in three dimensions.

Now, in one dimension, the Hamiltonian of a non-relativistic particle of mass m takes the form

$$H=\frac{p_x^{\,2}}{2\,m}+V(x,t), \tag{6.1.13}$$

where $V(x)$ is the potential energy. In three dimensions, this expression generalizes to

$$H=\frac{p_x^{\,2}+p_y^{\,2}+p_z^{\,2}}{2\,m}+V(x,y,z,t). \tag{6.1.14}$$

Hence, making use of Equations ([e6.12])–([e6.14]) and ([e6.15]), the three-dimensional version of the time-dependent Schröndiger equation becomes [see Equation ([e3.1])]

$$\mathrm{i}\,\hbar\,\frac{\partial\psi}{\partial t}=-\frac{\hbar^{\,2}}{2\,m}\,\nabla^{\,2}\psi+V\,\psi. \tag{6.1.15}$$

Here, the differential operator

$$\nabla^{\,2}\equiv\frac{\partial^{\,2}}{\partial x^{\,2}}+\frac{\partial^{\,2}}{\partial y^{\,2}}+\frac{\partial^{\,2}}{\partial z^{\,2}} \tag{6.1.16}$$

is known as the *Laplacian*. Incidentally, the probability conservation equation ([e6.8]) is easily derivable from Equation ([esh3d]). An eigenstate of the Hamiltonian corresponding to the eigenvalue E satisfies

$$H\,\psi = E\,\psi. \tag{6.1.17}$$

It follows from Equation ([e6.15]) that (see Section [sstat])

$$\psi(x,y,z,t) = \psi(x,y,z)\,{\rm e}^{-{\rm i}\,E\,t/\hbar}, \tag{6.1.18}$$

where the stationary wavefunction $\psi(x,y,z)$ satisfies the three-dimensional version of the time-independent Schröndiger equation [see Equation ([etimeii])]:

$$\nabla^{\,2}\psi = \frac{2\,m}{\hbar^{\,2}}\,(V-E)\,\psi, \tag{6.1.19}$$

where V is assumed not to depend explicitly on t.

Contributors and Attributions

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