particle between $x$ and $x + dx$ *in our space*. One may thus visualize $\psi(x)$ as a function in our space, whose modulus squared gives the probability density for finding a particle near $x$. Such a picture is useful in thinking about the double-slit experiment or the electronic states in a hydrogen atom.

But like all pictures, it has its limits. First of all it must be borne in mind that even though $\psi(x)$ can be visualized as a wave in our space, it is not a real wave, like the electromagnetic wave, which carries energy, momentum, etc. To understand this point, consider a particle in three dimensions. The function $\psi(x, y, z)$ can be visualized as a wave in our space. But, if we consider next a two-particle system, $\psi(x_1, y_1, z_1, x_2, y_2, z_2)$ is a function in a six-dimensional *configuration space* and cannot in general be visualized in our space.

Thus the case of the single particle is really an exception: there is only one position operator and the space of its eigenvalues *happens to coincide* with the space in which we live and in which the drama of physics takes place.

This brings us to the end of our general discussion of the postulates. We now turn to the application of quantum theory to various physical problems. For pedagogical reasons, we will restrict ourselves to problems of a single particle in one dimension in the next few chapters.

# 5

# Simple Problems in One Dimension

Now that the postulates have been stated and explained, it is all over but for the applications. We begin with the simplest class of problems—concerning a single particle in one dimension. Although these one-dimensional problems are somewhat artificial, they contain most of the features of three-dimensional quantum mechanics but little of its complexity. One problem we will not discuss in this chapter is that of the harmonic oscillator. This problem is so important that a separate chapter has been devoted to its study.

## 5.1. The Free Particle

The simplest problem in this family is of course that of the free particle. The Schrödinger equation is

$$i\hbar\,|\dot{\psi}\rangle = H\,|\psi\rangle = \frac{P^2}{2m}\,|\psi\rangle \tag{5.1.1}$$

The normal modes or stationary states are solutions of the form

$$|\psi\rangle = |E\rangle e^{-iEt/\hbar} \tag{5.1.2}$$

Feeding this into Eq. (5.1.1), we get the time-independent Schrödinger equation for $|E\rangle$:

$$H\,|E\rangle = \frac{P^2}{2m}\,|E\rangle = E\,|E\rangle \tag{5.1.3}$$

This problem can be solved without going to any basis. First note that any eigenstate of $P$ is also an eigenstate of $P^2$. So we feed the trial solution $|p\rangle$ into Eq. (5.1.3) and find

$$\frac{P^2}{2m}\,|p\rangle = E\,|p\rangle$$

or

$$\left(\frac{p^2}{2m} - E\right)|p\rangle = 0 \qquad (= |0\rangle) \tag{5.1.4}$$

Since $|p\rangle$ is not a null vector, we find that the allowed values of $p$ are

$$p = \pm(2mE)^{1/2} \tag{5.1.5}$$

In other words, there are two orthogonal eigenstates for each eigenvalue $E$:

$$|E, +\rangle = |p = (2mE)^{1/2}\rangle \tag{5.1.6}$$

$$|E, -\rangle = |p = -(2mE)^{1/2}\rangle \tag{5.1.7}$$

Thus, we find that to the eigenvalue $E$ there corresponds a degenerate two-dimensional eigenspace, spanned by the above vectors. Physically this means that a particle of energy $E$ can be moving to the right or to the left with momentum $|p| = (2mE)^{1/2}$. Now, you might say, "This is exactly what happens in classical mechanics. So what's new?" What is new is the fact that the state

$$|E\rangle = \beta\,|p = (2mE)^{1/2}\rangle + \gamma\,|p = -(2mE)^{1/2}\rangle \tag{5.1.8}$$

is also an eigenstate of energy $E$ and represents a *single* particle of energy $E$ that can be caught moving either to the right or to the left with momentum $(2mE)^{1/2}$!

To construct the complete orthonormal eigenbasis of $H$, we must pick from each degenerate eigenspace any two orthonormal vectors. The obvious choice is given by the kets $|E, +\rangle$ and $|E, -\rangle$ themselves. In terms of the ideas discussed in the past, we are using the eigenvalue of a compatible variable $P$ as an extra label within the space degenerate with respect to energy. Since $P$ is a nondegenerate operator, the label $p$ by itself is adequate. In other words, there is no need to call the state $|p, E = p^2/2m\rangle$, since the value of $E = E(p)$ follows, given $p$. We shall therefore drop this redundant label.

The propagator is then

$$U(t) = \int_{-\infty}^{\infty} |p\rangle\langle p|\, e^{-iE(p)t/\hbar}\, dp$$
$$= \int_{-\infty}^{\infty} |p\rangle\langle p|\, e^{-ip^2t/2m\hbar}\, dp \tag{5.1.9}$$



*Exercise 5.1.1.* Show that Eq. (5.1.9) may be rewritten as an integral over $E$ and a sum over the $\pm$ index as

$$U(t) = \sum_{\alpha=\pm} \int_0^{\infty} \left[\frac{m}{(2mE)^{1/2}}\right] |E, \alpha\rangle\langle E, \alpha|\, e^{-iEt/\hbar}\, dE$$

*Exercise 5.1.2.** By solving the eigenvalue equation (5.1.3) in the $X$ basis, regain Eq. (5.1.8), i.e., show that the general solution of energy $E$ is

$$\psi_E(x) = \beta\,\frac{\exp[i(2mE)^{1/2}x/\hbar]}{(2\pi\hbar)^{1/2}} + \gamma\,\frac{\exp[-i(2mE)^{1/2}x/\hbar]}{(2\pi\hbar)^{1/2}}$$

[The factor $(2\pi\hbar)^{-1/2}$ is arbitrary and may be absorbed into $\beta$ and $\gamma$.] Though $\psi_E(x)$ will satisfy the equation even if $E < 0$, are these functions in the Hilbert space?

The propagator $U(t)$ can be evaluated explicitly in the $X$ basis. We start with the matrix element

$$U(x, t; x') \equiv \langle x|U(t)|x'\rangle = \int_{-\infty}^{\infty} \langle x|p\rangle\langle p|x'\rangle e^{-ip^2t/2m\hbar}\, dp$$
$$= \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} e^{ip(x-x')/\hbar} \cdot e^{-ip^2t/2m\hbar}\, dp$$
$$= \left(\frac{m}{2\pi\hbar i t}\right)^{1/2} e^{im(x-x')^2/2\hbar t} \tag{5.1.10}$$

using the result from Appendix A.2 on Gaussian integrals. In terms of this propagator, any initial-value problem can be solved, since

$$\psi(x, t) = \int U(x, t; x')\psi(x', 0)\, dx' \tag{5.1.11}$$

Had we chosen the initial time to be $t'$ rather than zero, we would have gotten

$$\psi(x, t) = \int U(x, t; x', t')\psi(x', t')\, dx' \tag{5.1.12}$$

where $U(x, t; x', t') = \langle x|U(t - t')|x'\rangle$, since $U$ depends only on the time interval $t - t'$ and not the absolute values of $t$ and $t'$. [Had there been a time-dependent potential such as $V(t) = V_0 e^{-\alpha t^2}$ in $H$, we could have told what absolute time it was by looking at $V(t)$. In the absence of anything defining an absolute time in the problem, only time differences have physical significance.] Whenever we set $t' = 0$, we will resort to our old convention and write $U(x, t; x', 0)$ as simply $U(x, t; x')$.

A nice physical interpretation may be given to $U(x, t; x', t')$ by considering a special case of Eq. (5.1.12). Suppose we started off with a particle localized at $x' = x_0'$, that is, with $\psi(x', t') = \delta(x' - x_0')$. Then

$$\psi(x, t) = U(x, t; x_0', t') \tag{5.1.13}$$

*In other words, the propagator (in the X basis) is the amplitude that a particle starting out at the space–time point* $(x_0', t')$ *ends with at the space–time point* $(x, t)$. [It can obviously be given such an interpretation in any basis: $\langle \omega | U(t, t') | \omega' \rangle$ is the amplitude that a particle in the state $|\omega'\rangle$ at $t'$ ends up with in the state $|\omega\rangle$ at $t$.] Equation (5.1.12) then tells us that the total amplitude for the particle's arrival at $(x, t)$ is the sum of the contributions from all points $x'$ with a weight proportional to the initial amplitude $\psi(x', t')$ that the particle was at $x'$ at time $t'$. One also refers to $U(x, t; x_0' t')$ as the "fate" of the delta function $\psi(x', t') = \delta(x' - x_0')$.

### Time Evolution of the Gaussian Packet

There is an unwritten law which says that the derivation of the free-particle propagator be followed by its application to the Gaussian packet. Let us follow this tradition.

Consider as the initial wave function the wave packet

$$\psi(x', 0) = e^{ip_0x'/\hbar} \frac{e^{-x'^2/2\Delta^2}}{(\pi\Delta^2)^{1/4}} \tag{5.1.14}$$

This packet has mean position $\langle X \rangle = 0$, with an uncertainty $\Delta X = \Delta/2^{1/2}$, and mean momentum $p_0$ with uncertainty $\hbar/2^{1/2}\Delta$. By combining Eqs. (5.1.10) and (5.1.12) we get

$$\psi(x, t) = \left[\pi^{1/2}\left(\Delta + \frac{i\hbar t}{m\Delta}\right)\right]^{-1/2} \cdot \exp\left[\frac{-(x - p_0t/m)^2}{2\Delta^2(1 + i\hbar t/m\Delta^2)}\right] \times \exp\left[\frac{ip_0}{\hbar}\left(x - \frac{p_0t}{2m}\right)\right] \tag{5.1.15}$$

The corresponding probability density is

$$P(x, t) = \frac{1}{\pi^{1/2}(\Delta^2 + \hbar^2t^2/m^2\Delta^2)^{1/2}} \cdot \exp\left\{\frac{-[x - (p_0/m)t]^2}{\Delta^2 + \hbar^2t^2/m^2\Delta^2}\right\} \tag{5.1.16}$$

The main features of this result are as follows:



(1) The mean position of the particles is

$$\langle X \rangle = \frac{p_0t}{m} = \frac{\langle P \rangle t}{m}$$

In other words, the classical relation $x = (p/m)t$ now holds between average quantities. This is just one of the consequences of the *Ehrenfest theorem* which states that the classical equations obeyed by dynamical variables will have counterparts in quantum mechanics as relations among expectation values. The theorem will be proved in the next chapter.

(2) The width of the packet grows as follows:

$$\Delta X(t) = \frac{\Delta(t)}{2^{1/2}} = \frac{\Delta}{2^{1/2}}\left(1 + \frac{\hbar^2t^2}{m^2\Delta^4}\right)^{1/2} \tag{5.1.17}$$

The increasing uncertainty in position is a reflection of the fact that any uncertainty in the initial velocity (that is to say, the momentum) will be reflected with passing time as a growing uncertainty in position. In the present case, since $\Delta V(0) = \Delta P(0)/m = \hbar/2^{1/2}m\Delta$, the uncertainty in $X$ grows approximately as $\Delta X \simeq \hbar t/2^{1/2}m\Delta$ which agrees with Eq. (5.1.17) for large times. Although we are able to understand the spreading of the wave packet in classical terms, the fact that the initial spread $\Delta V(0)$ is *unavoidable* (given that we wish to specify the position to an accuracy $\Delta$) is a purely quantum mechanical feature.

If the particle in question were macroscopic, say of mass 1 g, and we wished to fix its initial position to within a proton width, which is approximately $10^{-13}$ cm, the uncertainty in velocity would be

$$\Delta V(0) \simeq \frac{\hbar}{2^{1/2}m\Delta} \simeq 10^{-14} \text{ cm/sec}$$

It would be over 300,000 years before the uncertainty $\Delta(t)$ grew to one millimeter! We may therefore treat a macroscopic particle classically for any reasonable length of time. This and similar questions will be taken up in greater detail in the next chapter.

*Exercise 5.1.3. (Another Way to Do the Gaussian Problem).* We have seen that there exists another formula for $U(t)$, namely, $U(t) = e^{-iHt/\hbar}$. For a free particle this becomes

$$U(t) = \exp\left[\frac{i}{\hbar}\left(\frac{\hbar^2t}{2m}\frac{d^2}{dx^2}\right)\right] = \sum_{n=0}^{\infty}\frac{1}{n!}\left(\frac{i\hbar t}{2m}\right)^n \frac{d^{2n}}{dx^{2n}} \tag{5.1.18}$$

Consider the initial state in Eq. (5.1.14) with $p_0 = 0$, and set $\Delta = 1$, $t' = 0$:

$$\psi(x, 0) = \frac{e^{-x^2/2}}{(\pi)^{1/4}}$$

Find $\psi(x, t)$ using Eq. (5.1.18) above and compare with Eq. (5.1.15).

*Hints*: (i) Write $\psi(x, 0)$ as a power series:

$$\psi(x, 0) = (\pi)^{-1/4} \sum_{n=0}^{\infty} \frac{(-1)^n x^{2n}}{n!(2)^n}$$

(ii) Find the action of a few terms

$$1, \quad \left(\frac{i\hbar t}{2m}\right)\frac{d^2}{dx^2}, \quad \frac{1}{2!}\left(\frac{i\hbar t}{2m}\frac{d^2}{dx^2}\right)^2$$

etc., on this power series.

(iii) Collect terms with the same power of $x$.

(iv) Look for the following series expansion in the coefficient of $x^{2n}$:

$$\left(1 + \frac{it\hbar}{m}\right)^{-n-1/2} = 1 - (n + 1/2)\left(\frac{i\hbar t}{m}\right) + \frac{(n + 1/2)(n + 3/2)}{2!}\left(\frac{it\hbar}{m}\right)^2 + \cdots$$

(v) Juggle around till you get the answer.

*Exercise 5.1.4*: *A Famous Counterexample*. Consider the wave function

$$\begin{aligned}\psi(x, 0) &= \sin\left(\frac{\pi x}{L}\right), \quad &|x| \leq L/2\\ &= 0, &|x| > L/2\end{aligned}$$

It is clear that when this function is differentiated any number of times we get another function confined to the interval $|x| \leq L/2$. Consequently the action of

$$U(t) = \exp\left[\frac{i}{\hbar}\left(\frac{\hbar^2 t}{2m}\right)\frac{d^2}{dx^2}\right]$$

on this function is to give a function confined to $|x| \leq L/2$. What about the spreading of the wave packet?

[*Answer*: Consider the derivatives at the boundary. We have here an example where the (exponential) operator power series doesn't converge. *Notice that the convergence of an operator power series depends not just on the operator but also on the operand.* So there is no paradox: if the function dies abruptly as above, so that there seems to be a paradox, the derivatives are singular at the boundary, while if it falls off continuously, the function will definitely leak out given enough time, no matter how rapid the falloff.]



### Some General Features of Energy Eigenfunctions

Consider now the energy eigenfunctions in some potential $V(x)$. These obey

$$\psi'' = -\frac{2m(E - V)}{\hbar^2}\psi$$

where each prime denotes a spatial derivative. Let us ask what the continuity of $V(x)$ implies. Let us start at some point $x_0$ where $\psi$ and $\psi'$ have the values $\psi(x_0)$ and $\psi'(x_0)$. If we pretend that $x$ is a time variable and that $\psi$ is a particle coordinate, the problem of finding $\psi$ everywhere else is like finding the trajectory of a particle (for all times past and future) given its position and velocity at some time and its acceleration as a function of its position and time. It is clear that if we integrate these equations we will get continuous $\psi'(x)$ and $\psi(x)$. This is the typical situation. There are, however, some problems where, for mathematical simplicity, we consider potentials that change abruptly at some point. This means that $\psi''$ jumps abruptly there. However, $\psi'$ will still be continuous, for the area under a function is continuous even if the function jumps a bit. What if the change in $V$ is infinitely large? It means that $\psi''$ is also infinitely large. This in turn means that $\psi'$ *can* change abruptly as we cross this point, for the area under $\psi''$ can be finite over an infinitesimal region that surrounds this point. But whether or not $\psi'$ is continuous, $\psi$, which is the area under it, will be continuous.‡

Let us turn our attention to some specific cases.

## 5.2. The Particle in a Box

We now consider our first problem with a potential, albeit a rather artificial one:

$$\begin{aligned}V(x) &= 0, \quad &|x| < L/2\\ &= \infty, &|x| \geq L/2\end{aligned} \tag{5.2.1}$$

This potential (Fig. 5.1a) is called the box since there is an infinite potential barrier in the way of a particle that tries to leave the region $|x| < L/2$.

‡ We are assuming that the jump in $\psi'$ is finite. This will be true even in the artificial potentials we will encounter. But can you think of a potential for which this is not true? (Think delta.)