POSITION AND MOMENTUM

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Reference: Griffiths, David J. (2005), Introduction to Quantum Mechanics, 2nd Edition; Pearson Education - Sec 1.5, Problem 1.6.

Once we have accepted the Schrödinger equation as the foundation of quantum mechanics and the interpretation of the square modulus of the wave function as the probability density that the particle is found at a certain location at a certain time, what, exactly, can we do with this information?

The key to quantum mechanics is the realization that many cherished notions in classical physics cannot be carried over in the same form to quantum mechanics. In particular, we can't ask a simple question like 'where is the particle' at a given time. What we *can* do, though, is ask for the particle's *average* or *mean* position as a function of time.

To see this, we need to recall (or learn, if you haven't met it before) how a probability function or probability density can be used. Consider first a simple case where there are a small number of discrete states in some system, say, the roll of a die. If the die is fair, then there is a probability of 1/6 that each of the numbers 1,2,3,4,5,6 comes up. In such a case, we cannot predict precisely which number will come up on the next roll of the die, but we can predict the average of the numbers that will be rolled, assuming that we roll the die a large number of times to smooth out any local blips in the run of numbers rolled.

If we know the probability function $P(n)$ which gives the probability that value$n$ will occur (as we do for a die) then to calculate the average of any quantity we multiply the value of that quantity by its probability of occurring and add up all these products. So in the case of a fair die, since each number between 1 and 6 has the same probability of 1/6, the average of the rolled values is

$$\begin{aligned}
\sum_{n=1}^{6} nP(n) &= \sum_{n=1}^{6} \frac{n}{6} && (1)\\
&= \frac{21}{6} && (2)\\
&= 3.5 && (3)
\end{aligned}$$

Obviously, the mean value is not an integer and therefore is not a value that will ever occur in any single roll of the die, but it is still a useful measure since if we rolled the die many times and the observed mean value was significantly different from 21/6 we would suspect that the die isn't fair. For example, suppose the die is weighted so that rolling a 6 is twice as likely as rolling any other number. Then the probability of rolling a number between 1 and 5 is 1/7 and the probability of rolling a 6 is 2/7 (note that the sum of probabilities for all possible outcomes must equal 1, so in this case, the total probability is $5\times(1/7)+(2/7)=1$). In this case, the average of the rolled numbers will be

$$\sum_{n=1}^{6} nP(n) = \frac{1}{7}\sum_{n=1}^{5} n+\frac{2}{7}6 \tag{4}$$

$$= \frac{27}{7} \tag{5}$$

$$= 3.86\ldots \tag{6}$$

Not surprisingly, the average value is higher than for a fair die.

Now, what about cases where the quantity being measured is continuous rather than discrete, such as the position of a particle in space (or in our case, along a straight line in one dimension)? In this case, the probability function is a continuous function of space (and possibly time), so instead of a discrete sum we need to use an integral to calculate means. If the probability density function $P(x)$ gives the probability that a particle is found in the interval $[x,x+dx]$, then the mean location of the particle, usually denoted $\langle x\rangle$ is

$$\langle x\rangle = \int xP(x,t)\,dx \tag{7}$$

where the limits on the integral cover all values of x where the probability density is non-zero.

This formula uses exactly the same idea as that for calculating the average number rolled on a die: we take the quantity of which we are trying to find the average (x in this case), multiply it by its probability of occurrence ($P(x,t)$) and sum (integrate) over all possible values of x. Thus the limits of the integral need to be chosen to cover all possible values of x. For a physical system, sometimes the limits will be infinite, while in other cases the particle will be restricted to some finite region; it all depends on the statement of the problem. Note, however, that I've included an explicit dependence on time, since the probability of being in a particular location can vary over time.

Now in quantum mechanics, the probability function is *assumed* to be the square modulus of the wave function, that is

$$P(x) \equiv |\Psi(x,t)|^2 = \Psi^*(x,t)\Psi(x,t) \tag{8}$$

so

$$\begin{aligned}
\langle x \rangle &= \int xP(x,t)\,dx && (9)\\
&= \int x|\Psi(x,t)|^2\,dx && (10)
\end{aligned}$$

To go any further, of course, we would need to know the actual form of $\Psi(x,t)$, but we'll leave that until we consider some specific examples.

What we can do at this point is ask another naughty question: what is the *velocity* of the particle? As with the position, quantum mechanics doesn't allow us to ask for the precise velocity of a particle at a given time, since everything has to arise from the wave function, and all the wave function can tell us is the *probability* that something has a certain value. So instead, we'll ask what the *average* velocity is. Since the velocity is the derivative of the position, we should be able to get this by working out $d\langle x \rangle/dt$.

Since we have an expression for the average position as a function of time, we should be able to do this. At this point we will, without justification, do something that usually makes mathematicians cringe. From above, we know that

$$\langle x \rangle = \int x|\Psi(x,t)|^2\,dx \tag{11}$$

Now the time dependence is tucked away inside the integral. Ordinarily we need to justify taking a derivative inside an integral, but we can console ourselves with the knowledge that for any wave function for which this is *not* a valid operation, that function is also not a possible description of a physical state (for one reason or another). Physicists are notoriously sloppy about things like this, but remember that all their results have to pass the test of experimental verification, so if we do something wrong, then the experiments will catch us out, and so far they agree with the calculations so we seem to be safe.

Anyway, if we proceed with taking the derivative, we get

$$\frac{d\langle x\rangle}{dt} = \frac{d}{dt}\int x|\Psi(x,t)|^2\,dx \tag{12}$$
$$= \int x\frac{\partial}{\partial t}|\Psi(x,t)|^2\,dx \tag{13}$$
$$= \int x\frac{\partial}{\partial t}(\Psi^*\Psi)\,dx \tag{14}$$
$$= \int x\left[\frac{\partial\Psi^*}{\partial t}\Psi+\Psi^*\frac{\partial\Psi}{\partial t}\right]\,dx \tag{15}$$

where we've used the product rule for derivatives in the last step. Notice also that when we took the derivative inside the integral, we changed it to a partial derivative, since inside the integral, the wave function $\Psi(x,t)$ is a function of two variables and we want only the derivative with respect to time.

Note that we can't apply integration by parts directly to 13, since the derivative inside the integrand is with respect to *time* and the integration is with respect to *distance*. To go any further, we need to somehow convert the time derivatives into space derivatives, and we can do this by using the Schrödinger equation

$$-\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2}+V(x,t)\Psi = i\hbar\frac{\partial\Psi}{\partial t} \tag{16}$$
$$\frac{\partial\Psi}{\partial t} = -\frac{\hbar}{2mi}\frac{\partial^2\Psi}{\partial x^2}+\frac{1}{i\hbar}V(x,t)\Psi \tag{17}$$
$$\frac{\partial\Psi^*}{\partial t} = \frac{\hbar}{2mi}\frac{\partial^2\Psi^*}{\partial x^2}-\frac{1}{i\hbar}V(x,t)\Psi^* \tag{18}$$

where the last line is just the complex conjugate of the second line. Putting these last two lines into the expression above we find the terms containing the potential $V(x,t)$ cancel and we are left with

$$\frac{\partial\Psi^*}{\partial t}\Psi+\Psi^*\frac{\partial\Psi}{\partial t}=\frac{\hbar}{2mi}\left[\Psi\frac{\partial^2\Psi^*}{\partial x^2}-\Psi^*\frac{\partial^2\Psi}{\partial x^2}\right] \tag{19}$$

The term in square brackets can be expressed as a single derivative:

$$\Psi\frac{\partial^2\Psi^*}{\partial x^2}-\Psi^*\frac{\partial^2\Psi}{\partial x^2}=\frac{\partial}{\partial x}\left[\Psi\frac{\partial\Psi^*}{\partial x}-\Psi^*\frac{\partial\Psi}{\partial x}\right] \tag{20}$$

so going back to our original integral, we get

$$\frac{d\langle x\rangle}{dt} = \int x\left[\frac{\partial\Psi^*}{\partial t}\Psi + \Psi^*\frac{\partial\Psi}{\partial t}\right]dx \tag{21}$$

$$= \frac{\hbar}{2mi}\int x\frac{\partial}{\partial x}\left[\Psi\frac{\partial\Psi^*}{\partial x} - \Psi^*\frac{\partial\Psi}{\partial x}\right]dx \tag{22}$$

$$= \frac{\hbar}{2mi}x\left[\Psi\frac{\partial\Psi^*}{\partial x} - \Psi^*\frac{\partial\Psi}{\partial x}\right] - \frac{\hbar}{2mi}\int\left[\Psi\frac{\partial\Psi^*}{\partial x} - \Psi^*\frac{\partial\Psi}{\partial x}\right]dx$$

where we used integration by parts to get the last line.

To proceed further, we need to make another assumption in the physics. We assume that all wave functions of physical relevance will be zero at the boundaries within which the system is contained, or failing that, at infinite distances, and further, that they will go to zero fast enough that multiplying them by powers of x or any other function isn't enough to stop them from becoming zero. This is a reasonable assumption, since we are simply stating that a particle cannot exist (the wave function being zero at a location implies the probability of finding it at that location is zero) outside the region in which we have confined it.

Under that assumption, the first term in the last line above will be zero, since in any application of this formula to a real physical case, that term needs to be evaluated at limits at the extent of the region of physical interest. We can therefore write

$$\frac{d\langle x\rangle}{dt} = -\frac{\hbar}{2mi}\int\left[\Psi\frac{\partial\Psi^*}{\partial x} - \Psi^*\frac{\partial\Psi}{\partial x}\right]dx \tag{23}$$

$$= \frac{\hbar}{mi}\int\Psi^*\frac{\partial\Psi}{\partial x}\,dx \tag{24}$$

where we used another integration by parts on the first term and threw away the boundary term for the same reason as before. We now have an expression for the mean velocity of the particle in terms of the wave function:

$$\langle v\rangle = \frac{\hbar}{mi}\int\Psi^*\frac{\partial\Psi}{\partial x}\,dx \tag{25}$$

or, since it is more common to work with the momentum which is defined in classical physics as $p = mv$, we can write an expression for the mean momentum (assuming the mass is constant, as it is for elementary particles like electrons)

$$\begin{aligned} \langle p\rangle &= m\langle v\rangle && (26)\\ &= \frac{\hbar}{i}\int\Psi^{*}\frac{\partial\Psi}{\partial x}\,dx && (27)\end{aligned}$$

Now for yet another postulate (yes, quantum mechanics has a lot of postulates, but they tend to be justified by the fact that the theory gives stunningly accurate predictions, although it does leave the reader with a sense that something is missing at the foundation of the theory). We note that this expression for the mean momentum can be put into the standard form for the mean of a quantity if we identify the *differential operator* $(\hbar/i)\partial/\partial x$ with the actual momentum. In other words:

$$p=\frac{\hbar}{i}\frac{\partial}{\partial x} \tag{28}$$

since we can then write

$$\langle p\rangle=\int\Psi^{*}p\Psi\,dx \tag{29}$$

which has the form of a quantity (momentum) multiplied by the probability density and summed (integrated) over the region of interest.

In fact, this is the recipe for finding the average values of *any* quantity in quantum mechanics: first, express the quantity you're interested in in terms of position and momentum (and all *classical* quantities such as angular momentum and so forth can be so expressed; there are other quantities such as spin that can't, but they have their own special treatment), and then sandwich this expression between Ψ^* and Ψ as we've done with the momentum, and then integrate.

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