

THE WAVE FUNCTION AS A PROBABILITY

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Reference: Griffiths, David J. (2005), Introduction to Quantum Mechanics, 2nd Edition; Pearson Education - Chapter 1.

In quantum mechanics, the wave function is the mathematical description of the state of the system under study, and contains all the available information about that system as a function of position and time. It is obtained by solving the Schrödinger equation, in which we need to specify the *potential* in which the particle or particles are moving. Although it is always dangerous to use analogies in attempting to understand quantum mechanics, we can view this process of solving the Schrödinger equation to obtain the wave function as roughly similar to solving Newton's equation $F = ma$ to obtain the positions of all particles in the system as functions of time. In Newton's equation, we must specify the force as a function of position and time (for example, for two masses moving in a gravitational field, F is given by Newton's formula $F = Gm_1m_2/r^2$ where m_1 and m_2 are the two masses, r is the distance between them and G is the gravitational constant). Newton's equation requires solving because it is actually a differential equation in disguise. The acceleration a of a particle is in reality the second derivative of the position: $a = d^2x/dt^2$ (in one dimension). If the force F is also given as a function of position (and, in general, the velocity $v = dx/dt$ and of time itself) then we are faced with a second-order differential equation that needs to be solved to obtain the particle's position as a function of time. In practice, a neat, closed-form solution of Newton's deceptively simple equation is possible only for very simple systems. For more complex systems, only approximate solutions are possible.

The Schrödinger equation, at least, doesn't hide the fact that it is a differential equation, since that's how it is presented:

$$-\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} + V\Psi = i\hbar \frac{\partial \Psi}{\partial t} \quad (1)$$

In fact, it's potentially worse than Newton's equation since it is a partial differential equation (PDE), with derivatives with respect to both position and time. Newton's equation usually has only ordinary derivatives with respect to time, so it is an ordinary differential equation (ODE). PDEs are usually more difficult to solve than ODEs, although of course it all depends on what the force or potential functions are.

In any case, the wave function Ψ that is the solution of the Schrödinger equation is, in general, a function of position and time, and to make things worse (or more fun, depending on your viewpoint) it is also a complex function, whose values are complex numbers. As pointed out on the page where it was introduced, this means that Ψ itself cannot represent a physically measurable quantity, but it was proposed by Max Born that its square modulus $|\Psi|^2$ can be interpreted as a probability density for finding the particle at a particular location at a particular time.

A probability density is similar to an ordinary probability, except it applies to a continuous variable rather than a discrete one. When we roll a die, the probability of getting any of the six numbers is $1/6$. Since there are six possible outcomes, the total probability of getting any one of these six values is $6 \times (1/6) = 1$. This is a requirement on any set of probabilities: if we add up the probabilities for all possible outcomes, we must always get 1, which is just another way of saying that if we allow an event to happen, we have to get one of the possible outcomes.

For a continuous variable, however, this simple approach doesn't seem to work. Suppose we are told that a computer will generate a random number between 0 and 1, and that all numbers within this range are equally probable (we are assuming that the computer is capable of generating *any* value between 0 and 1, so the number of decimal places it can print out is unlimited). What is the probability that the computer will generate 0.72731723934? If we try to assign a non-zero probability to each real number between 0 and 1, then since there are an infinite number of real numbers within that range, when we try to add up the probabilities for all these numbers, we will get infinity. Clearly something is wrong.

The concept of a probability density solves this problem. A function such as $|\Psi(x)|^2$ specifies the probability per unit length at the location x that the value x will be generated. If this confuses you, think of it like an ordinary density. If you have a block of a solid in which the density varies from place to place, we can define a function $\rho(r)$ that gives the density at each point r within the solid. Clearly it doesn't make sense to ask someone to measure the density at a geometric point, since a point has zero volume, so the amount of material within a geometric point is zero. But what you can do is measure the mass of a little volume around the point r and calculate an approximation to $\rho(r)$ by dividing this mass by the little volume. If you keep doing this by reducing the volume, then in the (mathematical) limit, you will get a value for $\rho(r)$ that is exact.

It's the same idea with a probability density. We start out by measuring (or calculating) the probability that a number within a small interval around x will be generated and divide this value by the length of the interval. By choosing successively smaller intervals, we will get a better approximation

for the probability density until ultimately, in the limit, we will get an exact value for $|\Psi(x)|^2$.

If we define the probability density in this way, there is now a way we can add up all the probabilities and get a finite value. Since the density is the probability per unit length that a number will be generated, then the actual probability that a number in the interval $[x, x + \Delta x]$ will be generated is $|\Psi(x)|^2 \Delta x$ (since the length of the interval is Δx). An approximation to the total probability can then be found by adding up terms like this for all the little intervals between 0 and 1. In the limit, we let $\Delta x \rightarrow 0$ and replace the sum with an integral, so we get the condition

$$\int_0^1 |\Psi(x)|^2 dx = 1 \quad (2)$$

This is the *normalization* condition on a probability density: the integral of the density over the range for which it is defined must sum to 1, since whatever number is generated must come from that interval. If the density is defined over a different set of events (such as a different interval from which the numbers are chosen), then the limits on the integral are adjusted, but the overall normalization condition remains the same.

In quantum mechanics, we are interpreting $|\Psi(x, t)|^2$ as the probability density for finding the particle at position x at time t . Since at every instant in time, the particle has to be *somewhere*, if we integrate this function over all possible values of x , the result must be 1, and it must *remain* 1 for all time, since the particle always has to be somewhere.

This has an immediate consequence for solving the Schrödinger equation, since any solution that is not normalizable can immediately be rejected. Notice that this is a case where a requirement of the physics (the statement that the particle must be found somewhere) leads to a restriction on the mathematics (the wave function must be normalizable). The physics here is an assumption of the theory; the mathematics is a way of expressing this assumption in a precise form.

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