THE FREE PARTICLE

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Reference: Griffiths, David J. (2005), Introduction to Quantum Mechanics, 2nd Edition; Pearson Education - Sec 2.4, Problem 2.21.

In a system in which there is no potential ($V(x) = 0$ everywhere), all particles are *free particles*. In principle, the solution of the Schrödinger equation is the easiest in this case:

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi \quad (1)$$

$$\frac{d^2\psi}{dx^2} = -\frac{2mE}{\hbar^2}\psi \quad (2)$$

$$\equiv -k^2\psi \quad (3)$$

$$k \equiv \frac{\sqrt{2mE}}{\hbar} \quad (4)$$

The stationary states, in terms of complex exponentials (the solutions can also be written in terms of sines and cosines by expanding the exponentials) are:

$$\psi(x) = Ae^{ikx} + Be^{-ikx} \quad (5)$$

$$\Psi(x,t) = (Ae^{ikx} + Be^{-ikx})e^{-iEt/\hbar} \quad (6)$$

Normally, at this point, we would impose some boundary conditions in an attempt to determine the constants A and B and also the allowed energies E. However, there are no boundary conditions in this problem since the potential is uniform everywhere, so we really can't go any further in specifying the stationary states. For a free particle, *any* positive energy E is allowable.

However, there is one big problem with the stationary states: they aren't normalizable. We can see this by calculating $|\Psi|^2$ directly:

$$|\Psi|^2 = \Psi^*\Psi \tag{7}$$
$$= (A^*e^{-ikx} + B^*e^{ikx})(Ae^{ikx} + Be^{-ikx}) \tag{8}$$
$$= |A|^2 + |B|^2 + A^*Be^{-2ikx} + B^*Ae^{2ikx} \tag{9}$$

Whatever the constants A and B are, this quantity must be real and positive (since it is the square modulus of a complex number) and, since the complex exponentials simply oscillate for all values of x, it is also clear that $|\Psi|^2$ does not decrease to zero at infinite distances, thus its integral over all x is infinite.

Thus we get the first important conclusion about a free particle: ***a free particle cannot exist in a stationary state***. So what does this mean? Does quantum mechanics predict that particles can't exist without some sort of potential to constrain them? If it did, this would be a fatal flaw in the theory, but before we panic, we need to remember another property of solutions to the Schrödinger equation: it is linear, so all linear combinations of solutions are also solutions. That is, even though a stationary state corresponding to one particular energy *cannot* on its own be a solution, maybe if we add up a bunch of stationary states, we *can* get a solution which is normalizable, and therefore physically acceptable.

Since any energy is allowable here, the linear combination of stationary states will be, in general, an integral rather than a sum. That is, the solution we want to try will look something like this:

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty}\phi(k)e^{ikx}e^{-iEt/\hbar}dk \tag{10}$$
$$= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty}\phi(k)e^{ikx}e^{-i\hbar k^2t/2m}dk \tag{11}$$

where in the second line we've substituted for $E = \hbar^2k^2/2m$ using the result above.

There are a few things we've done in this equation. First, we've replaced the sum $Ae^{ikx} + Be^{-ikx}$ by a single term $\phi(k)e^{ikx}/\sqrt{2\pi}$, but we're taking k over the entire set of real numbers, positive *and* negative. This has the same effect as integrating $Ae^{ikx} + Be^{-ikx}$ over k from 0 to ∞.

Second, we've introduced a function $\phi(k)/\sqrt{2\pi}$ (the $\sqrt{2\pi}$ is introduced to make this result more symmetric with another result that we'll get to in a minute; since $\phi(k)$ hasn't yet been specified, this is perfectly allowable). The function $\phi(k)$ plays the role of the c_n constants in the general solution of the particle in a box problem. It specifies how much of the stationary state with value k contributes to the overall solution $\Psi(x,t)$.

This solution is acceptable, provided $\Psi(x,t)$ can be normalized. To see that it can, we can use the standard procedure for specifying and solving the Schrödinger equation: specify some initial conditions and use them to determine the initial distribution of stationary states. That is, we specify $\Psi(x,0)$ (which, to be physically realistic, must be normalizable) and use it to find the function $\phi(k)$. That is, the problem is, given:

$$\Psi(x,0) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty}\phi(k)e^{ikx}dk$$

find $\phi(k)$.

Remember that in the particle in a box problem, we solved the analogous problem using the orthonormal properties of the stationary states. In the continuous case, the solution isn't quite as easy to prove, but the results are similar in spirit. The result is known as Plancherel's theorem, and it states that if we know the function $\Psi(x,0)$ and want to find $\phi(k)$ then we can invert the relation between $\Psi(x,0)$ and $\phi(k)$ to get:

$$\phi(k) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty}\Psi(x,0)e^{-ikx}dx \tag{12}$$

(This was the reason for introducing the weird factor of $\sqrt{2\pi}$ in the original equation - it makes Plancherel's theorem work out symmetrically.) For readers familiar with Fourier transforms, the two functions $\Psi(x,0)$ and $\phi(k)$ are Fourier transforms of each other.

Once we have $\phi(k)$, we can get the general time-dependent solution by plugging it back into the equation above:

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty}\phi(k)e^{ikx}e^{-i\hbar k^2t/2m}dk \tag{13}$$

although this integral is often not easy to work out(!)

Example: Suppose we have $\Psi(x,0) = Ae^{-a|x|}$. How far can we get in working out this system's behaviour as a free particle?

First, we need to normalize the initial condition, so we do the usual integral

$$1 = \int_{-\infty}^{\infty} |\Psi(x,0)|^2 dx \tag{14}$$

$$= A^2 \int_{-\infty}^{\infty} e^{-2a|x|} dx \tag{15}$$

$$= A^2/a \tag{16}$$

$$A = \sqrt{a} \tag{17}$$

Next, we can use Plancherel's theorem to work out $\phi(x)$:

$$\phi(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \Psi(x,0) e^{-ikx} dx \tag{18}$$

$$= \sqrt{\frac{a}{2\pi}} \int_{-\infty}^{+\infty} e^{-a|x|} e^{-ikx} dx \tag{19}$$

$$= \sqrt{\frac{2}{\pi}} \frac{a^{3/2}}{a^2+k^2} \tag{20}$$

The full solution, including time-dependence, is therefore

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \phi(k) e^{ikx} e^{-i\hbar k^2 t/2m} dk \tag{21}$$

$$= \frac{1}{\pi} a^{3/2} \int_{-\infty}^{\infty} \frac{e^{ikx - i\hbar k^2 t/2m}}{a^2+k^2} dk \tag{22}$$

This integral is clearly not easy and probably doesn't have a closed form, but the idea of how a problem is solved should be clear from this example.

Despite the intractability of the integral, there are a few things we can say about this result. First, the initial condition $\Psi(x,0)$ defines a wave function that is peaked at $x=0$ and falls off symmetrically as x gets further from 0. The rate of fall-off is determined by the constant a; for small a the function falls off very slowly and for large a the function is a very sharp spike at $x=0$.

When translated into $\phi(k)$, we see that for small a,

$$\phi(k) = \sqrt{\frac{2}{\pi}} \frac{1}{\sqrt{a} + k^2/a^{3/2}} \tag{23}$$

which has a peak around $k=0$ and falls off fairly rapidly once k gets larger. Thus when the wave function is spread out over x the values of k (and hence of energy E) that contribute to this function are quite restricted.

Conversely, if a is large, the k^2 term in the denominator of $\phi(k)$ becomes negligible and $\phi(k)$ becomes more or less constant. Thus when the particle is restricted to a narrow spatial area (x is peaked), pretty well all energies contribute to the wave function.

This is an illustration of the uncertainty principle: when the location is well known, the energy (and hence the momentum, since $E = p^2/2m$) is uncertain; conversely when the location is uncertain, the energy and momentum are known. You can't measure both position and momentum accurately at the same time.

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