ENERGY STATES: BOUND AND SCATTERING STATES

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Reference: Griffiths, David J. (2005), Introduction to Quantum Mechanics, 2nd Edition; Pearson Education - Sec. 2.5.1.

In classical physics, a particle's energy consists of kinetic and potential energy, the sum of which is a constant, provided we have accounted for all the forces acting on the system. For example, in the simple harmonic oscillator system (mass on a spring), the kinetic energy is given, as usual, by the term $\frac{1}{2}mv^2$ and the potential energy by $\frac{1}{2}kx^2$ where k is a constant that measures the strength of the force and x is the particle's displacement from equilibrium. The particle's total energy is

$$E=\frac{1}{2}mv^2+\frac{1}{2}kx^2 \tag{1}$$

which is a constant, provided that the spring is the only force acting on the particle.

In classical physics, this energy can take any positive value (although in practice, of course, any real spring would break down if stretched too far, so there are limits, but we're considering the ideal case).

In quantum physics, the particle is represented by a wave function which is found as the solution to the Schrödinger equation. For the harmonic oscillator, the mathematics required to solve the equation is non-trivial, but one outcome of the analysis is that the allowed energies of the particle are discrete or quantized, and must be one of $E=(n+\frac{1}{2})\hbar\omega$ where $\omega=\sqrt{k/m}$ is the frequency of oscillation and $n=0,1,2,3,\ldots$.

We find a similar situation in other cases where the potential function creates a well in which the particle must move. The harmonic oscillator potential is $V(x)=\frac{1}{2}kx^2$, and is a parabola that goes to infinity in both directions. The particle in a box potential (or infinite square well) has infinitely high walls at the ends of a fixed interval. Any such potential in which there is an infinitely high barrier in both directions results in quantized, rather than continuous, energy levels in quantum mechanics.

It would be nice to get some sort of physical intuition as to why this happens. We can hide behind the mathematics and say "that's what the equations tell us", but a better explanation should be possible.

Ultimately it comes down to the fact that solutions of the Schrödinger equation in regions where the total energy is greater than the potential function are, in some sense, waves. In classical physics, a particle is just a particle: it is a point-sized bit of matter that can rattle around inside a potential well and it has no wave-like properties at all. The wave properties of a quantum particle, however, mean that it has an extent larger than a geometric point. Trying to confine a wave inside a well means that the wave will interact with the boundaries of the well, and it is these boundary conditions that impose restrictions on what types of wave can exist inside a potential well.

If we have a particle in a box, where the ends of the box are absolute barriers that are infinitely high, then there is no probability of the particle existing outside the boundaries of the box. Since the particle's wave function measures this probability, it *has* to be zero at the boundaries of the box, so that effectively pins down the particle at both ends. The fact that the wave function (in the case of the infinite square well) is a pure sine wave means that only those waves that go to zero at the ends of the box are permissible solutions, which in turn means that only multiples of half a full cycle of the sine wave are allowed as solutions, and since the energy of the particle is related to its wavelength, this requirement in turn puts restrictions on the allowable energies. That is, it is the act of confining the particle that results in the quantization of its energy, and the reason that confining the particle has this effect is that that particle is defined by a wave function. So ultimately it is the wave nature of the particle that causes the quantization.

For potentials which go to infinity gradually (such as the harmonic oscillator) rather than abruptly (like the infinite square well), the particle is still being confined, but in a box with soft end points rather than hard ones. The wave is allowed to penetrate slightly into the barriers rather than be reflected from a hard surface, so it's a bit like building a box with spongy walls rather than steel ones. There is a small chance that the particle can be found outside the end points of the box, but ultimately we are still confining the particle within a box. Going further with a qualitative description doesn't help much, but we need to recognize that because the particle is still a wave, confining it within any type of box, no matter what type of endpoints the box has, will result in only certain wave functions being allowed. So ultimately it's the boundary conditions that result in quantization of energy.

What happens if the potential does *not* go to infinity at some point? In that case, it is possible for the total energy of a particle to be greater than the maximum potential energy, which means that it is not restricted within a box. In that case, there is no restriction on energy levels of the particle, and in both the classical and quantum cases, the allowed energy levels are not quantized. In the quantum case, the particle still retains its wave-like qualities, but since the wave is not restricted by any barriers, there is no restriction on the allowable wavelengths, and thus, on the energies. The simplest example of such a case is that of the free particle, where a particle moves without any forces acting on it.

It should be added that potentials that don't go to infinity at both ends can still give rise to bound states, if the total energy is less than the maximum value of the potential. The point is that for a potential that is finite everywhere, any total energy that is greater than the maximum of the potential is possible, and these states are scattering states. For a potential that goes to infinity at both ends, only bound, quantized states are possible.

This is not to say that a particle whose total energy is greater than the maximum potential energy is unaffected by the presence of the potential, however. If a particle, represented as a wave, travels in from the left (say) and encounters a potential barrier (or in fact, any change in the potential) at some point, then if the energy of the particle is greater than the barrier, there will be both reflected and transmitted components of the wave function past that point. Note that this doesn't mean that the particle splits in two, with half of it being reflected and the other half transmitted. Rather, it is the *wave function* that effectively splits, and since the wave function is a measure of the probability of finding the particle at a given place and time, this means that there is now a certain probability that the particle (all of it!) will get reflected by the potential barrier, and another probability that it will get transmitted and proceed beyond the barrier.

A similar effect can be seen with classical wave physics. For example, if you watch the wave patterns on the surface of the sea at a point near the shore where the level of the seabed changes you will see changes in the surface waves as they move over the seabed. Even if there are no abrupt changes in the seabed (for example, if you are on a gradually sloping sandy beach), the waves will change form as the depth of the water varies. It is for this reason that waves will eventually tip over and 'break' as they near the shore.

These two types of quantum states are known as *bound* states (for states that are quantized, and in which the energy is constrained by a potential well that is infinite at both ends) and *scattering* states (for states where the potential fails to reach infinite height in either one or both directions).

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