1.2.1: Wave Quantization and Particle in a Box

Standing Waves

With the discovery of the wave-particle dualism of the electron, and the observation of the quantization of electronic states in atoms led physicists focus on a field in physics in which waves are quantized. The field of standing waves (Fig. 1.2.6).

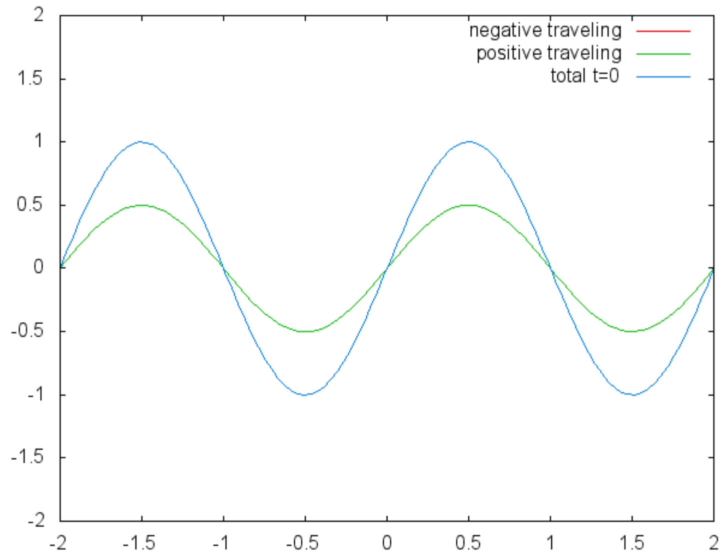

Figure 1.2.6 Two confined traveling waves (red and green) producing a standing wave (blue) due to their interference. (Attribution: Govindabalan [CC BY-SA (https://creativecommons.org/licenses/by-sa/3.0)], commons.wikimedia.org/wiki/F..._animation.gif)

Standing waves are a quite common phenomenon. You can for example trigger a standing waves by plucking a guitar string. This causes the guitar string to vibrate in standing waves with discreet, quantized wavelengths. The vibration with the longest wavelength is the so-called ground vibration. Its wavelength is two times the length of the guitar string. In addition, so-called higher harmonics are possible. The first harmonic has a wavelength equal to the length of the guitar string, the second one, has a wavelength equal to two-thirds of the length of the string, the third one has a wavelength equal to half of the length of the string, the fourth one has a wavelength equal to one third of the length of the guitar string, and so fourth (Fig. 1.2.7).

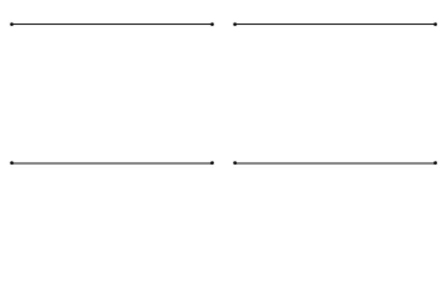

Figure 1.2.7 Standing waves (Attribution: Adjwilley [CC BY-SA (https://creativecommons.org/licenses/by-sa/3.0)], commons.wikimedia.org/wiki/F...n_a_string.gif)

It can be easily seen that the possible wavelengths at which the string can vibrate follow the equation $\lambda=2L/n$, whereby n is an integer, or a quantum number, and L is the length of the guitar string. Thus, we can say that the waves associated with the guitar string vibrations are quantized. Why are these waves called standing waves? This is because the positions of the crests and the troughs and the nodes do not move. They remain at the same position on the guitar string at any point in time. It should be said here that the standing nature of the waves is actually an illusion. There are actually two waves traveling in opposite direction on the guitar string, and these waves interfere with each other so that a standing wave is produced (this is illustrated in Fig. 1.2.6). When the guitar string is plucked two waves are sent into opposite direction on the guitar string toward the two opposite ends on the guitar string. Once they have reached these ends they get reflected and sent into the opposite direction until they again reach the ends of the guitar string where they get reflected again. During this process, which happens over and over again, the two waves interfere and produce the standing wave. In sum, the fact that the wave is confined within the guitar string, leads to the quantized standing waves.

Electron in a One-Dimensional Box

Let us know go from a vibrating guitar string to an electron in a one-dimensional box of length *a* having infinitely high walls. Inside the box the potential energy of the electron is zero, in the walls the potential energy is infinite (Figure 1.2.8).

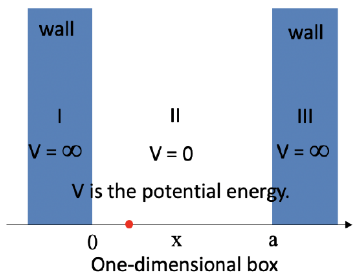

Figure 1.2.8 Electron (red dot) in a one-dimensional box with a potential energy V=0 within the box and infinite potential energy within the walls (the walls may be thought infinitely high).

Due to its kinetic energy the electron can travel on a line within the box until it hits the wall (Fig. 1.2.9, A). At the wall it is getting reflected and forced to travel into the opposite direction until it again hits the wall where it reverses direction again, and so forth. Consider now that the electron does not only have particle, but also wave properties. Because of that also a wave travels along the line, gets reflected at the wall, travels into opposite direction, gets reflected again and so on. These waves can interfere with it other just like the waves traveling on the guitar string to produce a standing wave. Thus, the electron in the one-dimensional box should behave like a standing wave, and this wave should be quantized (Fig. 1.2.9, B-F).

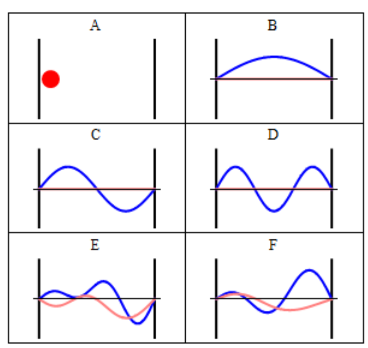

Figure 1.2.9 Electron traveling in a one-dimensional box acting as a standing wave (Attribution: Sbyrnes321 [CC0], commons.wikimedia.org/wiki/F...lAnimation.gif)

How can we mathematically describe the electron in the box as a standing wave? Generally, you can describe a standing wave by a wave function. A wave function tells the amplitude of the standing wave at a particular position in the one-dimensional box. How can we find the wave function? We can start out from a differential equation that is generally valid for standing waves (Eq. 1.2.1).

$$\frac{d^2\Psi(x)}{dx^2} = -\left(\frac{2\pi}{\lambda}\right)^2 \Psi(x)$$

Equation 1.2.1 Standing wave differential equation.

It says that the second derivative of the amplitude of the wave function at the position x is equal to $-(2\pi/\lambda)^2$ multiplied with the amplitude of the wave function at the position x. Let us now consider that the kinetic energy of the electron is $E = 1/2mv^2$ and expand the equation by m.

$$E = \tfrac{1}{2} mv^2$$

$$E = (mv)^2/2m \rightarrow (mv)^2 = 2mE \rightarrow mv=[2mE]^{1/2} \longrightarrow \lambda = h/[2mE]^{1/2}$$

$$\lambda = h/mv \longrightarrow mv=h/\lambda$$

Equation 1.2.2 Solving for λ from kinetic energy equation and De Broglie equation.

Let us then solve the equation for (mv) . Now let us solve the De Broglie equation for mv and insert mv by h/λ in the previous equation. Finally, let us solve the equation by λ and we will get $\lambda = h/[2mE]^{1/2}$, Eq. 1.2.2. We can now substitute λ by $h/[2mE]^{1/2}$ in the differential equation. Slightly rearranged this equation becomes the Schrödinger equation for the electron in the one-dimensional box (Equation 1.2.3).

$$\left[\frac{d^2}{dx^2} \frac{-h^2}{8\pi^2 m} \right] \Psi(x) = E_{kin}\Psi(x)$$

Equation 1.2.3 Schrödinger Equation for the electron in a 1-D box.

The Schrödinger equation is a differential equation. To get the wave function that describes the electron in the box we need to solve the differential equation. One possibility solve a differential equation is to guess its solution, and after that show that the solution is right. This is the approach we want to pursue here. A very general wave function is one that is a sum of a sinus term and a cosinus term of the coordinate x whereby we shall assume two general coefficients r and s in front of x, and two other general coefficients A and B in front of the sinus and the cosinus term, respectively.

$$\Psi = A \sin rx + B \cos sx$$

Equation 1.2.4 Generic solution to the differential equation.

We can now think of so-called boundary conditions for the wave function which will make the wave function more specific. A boundary condition is a property the wave function must have to be a sensible solution to the differential equation. We can assume a first boundary condition which assumes that at the position x=0 the amplitude of the wave function must be 0. This can be assumed because at these positions the "electron wave" gets reflected at the wall. That means that the wave function cannot have a cosinus term and thus B must be 0. If the wave function had a cosinus term it would not be 0 at x = 0 because the cosinus of 0 is not 0.

$$B = 0 \qquad \Psi = A \sin rx$$

Equation 1.2.5 Boundary condition 1 for the wave function

The second boundary condition is that the amplitude of the wave function is zero at x = a. Again, this is because the electron hits the wall at x = a and reverses its direction. The sinus function is only zero at x = a when ra is an integer number n times π: ra=nπ. This means that r must be nπ/a.

$$ra = n\pi \quad \text{or} \quad r = n\pi/a$$

Equation 1.2.6 Boundary condition 2 for the wave function

Thus, the wave function must be A=sin(nπx/a). We can see that the wave function that describes the electron as a standing wave in the one-dimensional box is quantized because the quantum number n appears.

$$\Psi = A \sin(n\pi x/a)$$

Equation 1.2.7 The wave function considering boundary conditions 1 and 2.

Inserting the quantum numbers n into the wave functions produces all the standing waves the electron can adopt (Fig. 1.2.10). You can see that the number of nodes and the wavelengths of the waves depend on the quantum number n. For n = 0 there is no node and the wavelength is twice the length of the box, for n = 2 there is one node and the wavelength is equal to the length of the box, for n =3 there are three nodes and the wavelength of the wave is 2/3 of the lengths of the box and so forth. We can illustrate that the wave function describes the waves depicted in Figure 1.2.10 by an example. The amplitude for the wave for n=2 is zero in the middle of the box where x = a/2. If we insert a/2 into the equation for Ψ then Ψ = A sin(nπ2a/a)= A sin(nπ) = 0 because it is the property of a sinus function to be 0 at an integer number multiple of π. We could also insert other values for x and n into the wave function, and would get the expected amplitude. This shows that the wave function correctly represents the standing waves the electron can adopt.

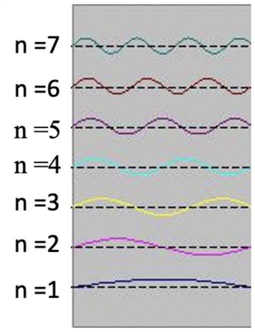

Figure 1.2.10 Standing waves corresponding to the wave function for different quantum numbers n.

We are still not quite finished with the wave function because we have not determined the parameter A in front of the sinus term. To obtain it we need to consider a third boundary condition (Eq. 1.2.8).

$$\int_0^a \Psi^2 dx = 1$$

Equation 1.2.8 Boundary condition 3.

It says that the integral of the square of the wave function over the length of the box must be equal to one. We can understand this boundary condition when we consider that the square of the wave function represents the probability to find the electron at a particular position in the box. The value the square of Ψ adopts at a position x within the box represents the probability to find the electron at this position when we consider the electron as a particle. This is called the Born interpretation of the wave function, named after the German physicist Max Born.

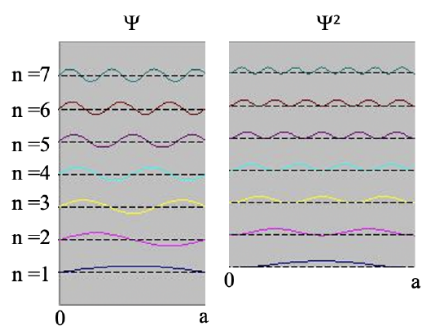

Figure 1.2.11 Standing waves corresponding to the wave function and its square.

Because the probability to find the electron anywhere in the box must be 100%, the integral of the square of the wave function over the entire box must be 100% or 1. One can show, and we omit the necessary mathematical steps for clarity here, that the boundary condition is only fulfilled when A is equal to the square root of 2/a. The final wave function is then psi is equal to 2/a sin(nπx/a). The factor square root of 2/a is called the normalization constant of the wave function because it adjusts the amplitude of the wave function so that the probability to find the electron anywhere in the box is 100%.

Dr. Kai Landskron (Lehigh University). If you like this textbook, please consider to make a donation to support the author's research at Lehigh University: Click Here to Donate.