# Particle in a Box

At the expense of any pretensions of historical accuracy, I am going to see how many interesting conclusions we can draw from one simple hypothesis posed by Louis Victor Pierre Raymond duc de Broglie in his 26-page doctoral thesis in 1924. It had been shown two decades earlier that *light*, which is certainly a *wave*, comes *quantized* in clumps like *particles* (called *photons*) with the energy of each photon equal to Planck's constant times its frequency: $E = h\nu$, where $h = 6.626 \times 10^{-34}$ J-s is Planck's constant. (It was the explanation of this phenomenon in 1905 that won Albert Einstein the Nobel prize. Relativity was just gravy.) It had already been shown earlier still (in the late Nineteenth Century) that an electromagnetic wave carries both energy $E$ and momentum $p$, in the ratio $E = pc$ where $c$ is the speed of light. This ratio holds also for quantized photons, which therefore have momentum $p = h\nu/c$. But for any wave, $c = \lambda\nu$, so

$$\lambda = \frac{h}{p}. \qquad (1)$$

Louis' hypothesis was amazingly simple: he reasoned that if *waves* are like *particles*, then maybe *particles* are like *waves*. In particular, an *electron* is in some mysterious sense a *wave* with its *wavelength* $\lambda$ given in terms of its *momentum* $p$ by Eq. (1). This simple suggestion was the basis for the WAVE/PARTICLE DUALITY that has perplexed generations of Physics students ever since (and formed the basis for all QUANTUM MECHANICS). But suppose we just take it at face value and examine a few "obvious" consequences.

## 24.1 A 1-Dimensional Box

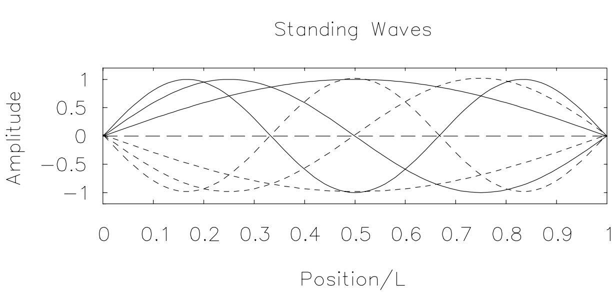


Figure 24.1 — First three allowed *modes* of a standing wave confined to a 1-dimensional box.

Suppose an electron is confined somehow to a "1-dimensional box" (like a bead on a wire). Actually there are many examples of such systems; a DNA molecule is an interesting example. The "box" (or string, or however you want to think of it) has a *length* $\ell$. If the electron is truly *confined* to the box, then its "wave" must have *nodes* (zeroes) at the *ends* of the box — and be zero everywhere outside the box. This is the familiar condition defining the allowed "modes" of vibrations in a string or in a closed organ pipe:

$$\lambda_n = \frac{2\ell}{n} \qquad (2)$$

where $n$ is any nonzero integer.

If we put this together with de Broglie's formula (1), we get an equation for the *momentum* of the electron in it's $n^{\text{th}}$ mode:

$$p_n = \frac{nh}{2\ell} \qquad (3)$$

and if we recall that the *kinetic energy* associated with a particle of mass $m$ having momentum $p$ is given by

$$E = \frac{p^2}{2m} \qquad (4)$$

then we have the *energy* of the electron in its $n^{\text{th}}$ mode:

$$E_n = \frac{n^2 h^2}{8m\ell^2}. \qquad (5)$$

The electron not only has *discrete* "energy levels" but it has an *irreducible minimum energy* for the lowest possible state (the "GROUND STATE"):

$$E_1 = \frac{h^2}{8m\ell^2}. \qquad (6)$$

The smaller the box, the bigger the ground state energy. **Particles don't "like" to be confined!** This has a number of profound consequences which we will revisit shortly. But first let's do a little trick and turn our string into a *circle*....

## 24.2 Fudging The Bohr Atom

If the electron travels in a *circular path* (as postulated by Niels Bohr in 1913) then we must apply de Broglie's hypothesis in a slightly different way: namely, the electron's "wave" must be *single valued* — it has to get back to the same value as it travels around the closed loop back to where it started. This means that the circumference of the loop is an integer number of wavelengths, or

$$2\pi r_n = n\lambda_n \qquad (7)$$

where $r_n$ is the radius of the orbit for the $n^{\text{th}}$ allowed mode. This in turn predicts a relationship between the radius and the momentum,

$$r_n p_n = n\hbar \qquad (8)$$

where $\hbar \equiv h/2\pi = 1.05458 \times 10^{-34}$ J-s. [Actually in any sensible system of units $\hbar = 1$, just like $c = 1$, but we are forced by tyrannical bureaucrats and twisted social conventions to use SI units.]

But what *is* the product of the radius and the momentum for a circular orbit? The ANGULAR MOMENTUM! Thus *Voila!* We have Bohr's hypothesis, namely that *angular momentum L is quantized* in units of $\hbar$:

$$L_n = n\hbar \tag{9}$$

### 24.2.1 The Bohr Radius

We can play more games with Bohr's hydrogen atom if we like, using just Eq. (8) to relate $r_n$ and $p_n$. Suppose we ask, "What is keeping the electron in its orbit?" The answer is, of course, "The Coulomb force of attraction between the positive nucleus and the negative electron!" This centripetal force has the value (in SI units)

$$F(r) = \frac{1}{4\pi\epsilon_\circ}\frac{e^2}{r^2} \tag{10}$$

where $e = 1.60217733 \times 10^{-19}$ C is the magnitude of the charge on either an electron ($-e$) or a proton ($+e$) and the ugly mess out front is the legacy of SI units — a constant stuck in to make it come out right. The corresponding *electrostatic potential energy* is

$$V(r) = -\frac{1}{4\pi\epsilon_\circ}\frac{e^2}{r} \tag{11}$$

(relative to $V \to 0$ at $r \to \infty$). We'll need that momentarily.

A simple application of NEWTON'S SECOND LAW gives

$$m\frac{v^2}{r} = \frac{p^2}{mr} = \frac{1}{4\pi\epsilon_\circ}\frac{e^2}{r^2}$$

where $m$ is the mass of the electron. Cancelling one $r$ and rearranging gives

$$p^2 = \frac{1}{4\pi\epsilon_\circ}\frac{me^2}{r}. \tag{12}$$

Substituting Eq. (8) into Eq. (12) gives

$$\left(\frac{n\hbar}{r_n}\right)^2 = \frac{1}{4\pi\epsilon_\circ}\frac{me^2}{r_n}$$

or (after some shuffling)

$$r_n = \frac{4\pi\epsilon_\circ n^2\hbar^2}{me^2} \tag{13}$$

for the radius of the $n^{\text{th}}$ Bohr orbit of the H atom. The lowest orbit ($n = 1$) has a special name and symbol: the BOHR RADIUS,

$$a_\circ = \frac{4\pi\epsilon_\circ\hbar^2}{me^2} = 0.529189379\text{Å} \tag{14}$$

where 1 Å $= 10^{-10}$ m.

### 24.2.2 Bohr's Energy Levels

Going on, we can calculate the net *energy* (kinetic plus potential) of an electron in the $n^{\text{th}}$ Bohr orbital of the H atom:

$$E_n = \frac{p_n^2}{2m} - \frac{1}{4\pi\epsilon_\circ}\frac{e^2}{r_n}$$

or [again using Eq. (8) to substitute $n\hbar/r_n$ for $p_n$]

$$E_n = \frac{n^2\hbar^2}{2mr_n^2} - \frac{1}{4\pi\epsilon_\circ}\frac{e^2}{r_n}.$$

Now we replace $r_n$ with our expression (13) to get

$$E_n = \frac{n^2\hbar^2}{2m}\left(\frac{me^2}{4\pi\epsilon_\circ n^2\hbar^2}\right)^2 - e^2\left[\frac{me^2}{(4\pi\epsilon_\circ)^2\, n^2\hbar^2}\right]$$

which simplifies to

$$E_n = -\left(\frac{1}{4\pi\epsilon_\circ}\right)^2\frac{me^4}{n^2\hbar^2} = -\frac{E_0}{n^2} \tag{15}$$

where $E_0 = 2.18 \times 10^{-18}$ J = 13.6055 eV (where 1 eV = $1.60219 \times 10^{-19}$ J). We have thus reproduced Bohr's explanation for the empirical formulae of Balmer and Rydberg! Note that whereas the energy of *confinement* of a particle in a box increases as $n^2$ (where $n - 1$ is the number of *nodes* inside the box), the Bohr energy levels of an *atom* increase as $-1/n^2$ (they get less negative and closer together as $n$ increases). Of course, so far all these calculations have been done in the classical (nonrelativistic) limit. If the momenta get big enough ($p$ comparable to or greater than $mc$) we have to do our calculations differently. . . .

## 24.3 Relativistic Energy

Let's generalize our formula for *kinetic energy* so that it is relativistically correct. For a *massless* particle (like a *photon*) the expression (4) doesn't make any sense and is in fact wrong. Without stopping now to explain where it comes from, I will just give you the relativistically correct and completely general formula for the total energy of a particle:

$$E^2 = p^2c^2 + m^2c^4. \tag{16}$$

Note that this TOTAL RELATIVISTIC ENERGY has the irreducible value $E_0 = mc^2$ when the particle is at rest (momentum = zero). This should ring a bell. To separate the KINETIC ENERGY $K$ from the total relativistic energy we just subtract off $E_0$.

It turns out [Don't you love that phrase?] that de Broglie's relation (1) *is relativistically correct!* Thus we can still use it to calculate the total energy even if the confined particle is ultrarelativistic or massless. In fact, any particle acts pretty much like a photon at high enough momentum, where we can ignore $m^2c^4$ in comparison with $p^2c^2$, in which case the formula simplifies to $E = pc$ or (for our ultrarelativistic particle in a box)

$$E_n = \frac{nhc}{2\ell}. \qquad (17)$$

### 24.3.1 Black Holes

As long as we're being relativistic, why not go all the way? Suppose a very lightweight particle is in orbit around a very heavy mass $m$, attracted only by gravity. A simple application of Newton's Second Law yields the ORBITAL VELOCITY

$$v_{\rm orb} = \sqrt{\frac{Gm}{r}}. \qquad (18)$$

Taking this at face value, what happens when $v_{\rm orb} \to c$? For a given $m$, there is a radius called the SCHWARZSCHILD RADIUS

$$R_S = \frac{Gm}{c^2} \qquad (19)$$

for which anything close to the mass cannot maintain its orbit without exceeding the speed of light. Since this is impossible [I am being really sloppy and glib now, but the conclusion is qualitatively correct] once anything gets inside that radius it falls in the rest of the way and never comes out. Even light. Hence the term, "BLACK HOLE". Any mass $m$ has its $R_s$; but usually the *density* of a given lump of matter is not high enough to place sufficient $m$ inside a given $r$ to cause a black hole to form.

### 24.3.2 The Planck Length

An exception is the overly confined particle. Even a massless photon, if confined to a small enough region, will have such an enormous energy of confinement [from Eq. (17)] that its *effective mass*

$$m_{\rm eff} = \frac{nh}{2\ell c}. \qquad (20)$$

(from $E = m_{\rm eff}c^2$) will be big enough to make $\ell$ smaller than the Schwarzschild radius! Using $m_{\rm eff}$ in the formula (19) for $R_S$ and setting $\ell = R_S$ gives an approximate formula for the PLANCK LENGTH

$$\ell_P = \sqrt{\frac{hG}{c^3}}. \qquad (21)$$

If you try to confine any particle (even a photon) to a region smaller than $\ell_P$, it will cause a gravitational collapse into a black hole. *I.e.* you can't do it. This is where quantum mechanics is certain to break down. Want to do some leading edge Physics theory? Quantum gravity is a good place to start.

By the way, the above handwaving derivation simply explains why you can't *confine a particle* to a prison of dimensions smaller than the Planck length. It says nothing about restrictions on an *empty* prison, nor does it make any claims about any "grainyness" of spacetime. If there is such quantization of space and time, you will have to construct a different argument for its existence. People do. But hey, this is weird enough!