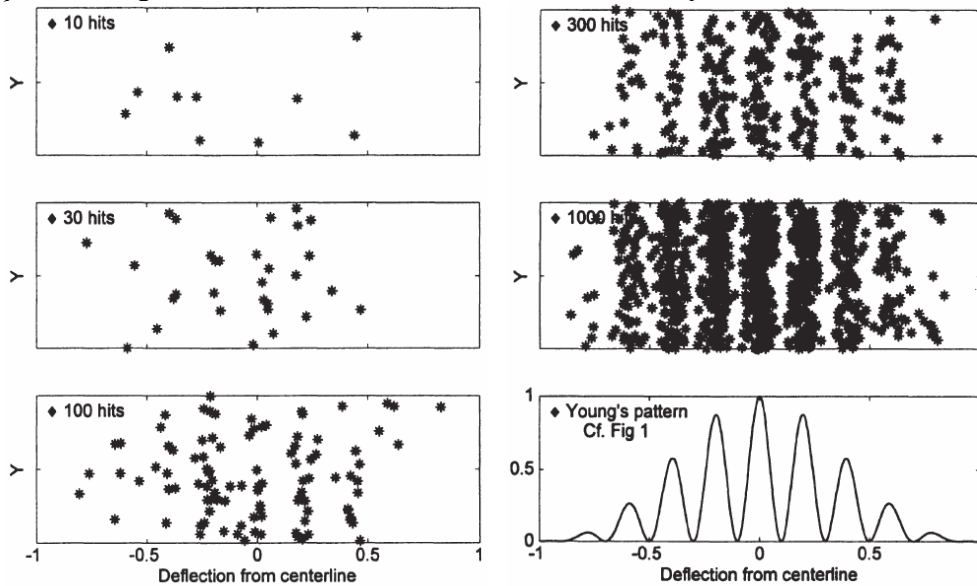


Chapter 8 – Young, Revisited

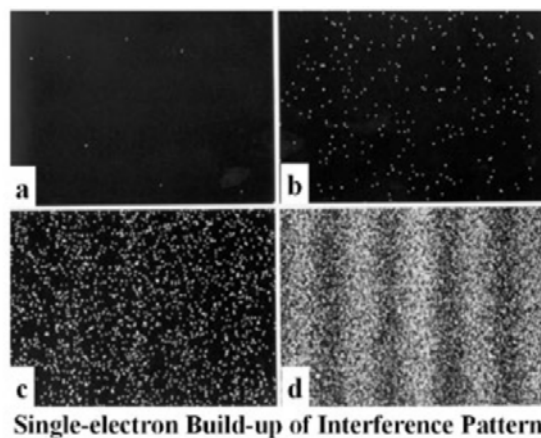
When very sensitive detectors are used to detect smaller and smaller amounts of light, there comes a point when they start registering individual photons. That can be seen in Fig. 8.3, the photos of a woman with differing amounts of exposures.

Much more surprising was this: when Young’s double-slit experiment was repeated by G.I. Taylor in 1909, he was able to detect individual photons... but the individual photons still bunched up in interference patterns even though there were no other photons present to interfere with! In some sense the individual photons are passing through both slits at the same time and interfering with themselves! This is crazy!! But apparently it’s the way the universe works.

That is depicted in Fig. 8.2, and there’s an actual video of the effect posted to the class website.



In fact, *every particle* behaves this same way, not just photons. Here’s the depiction for electrons in the 1989 Hitachi experiment, as given in this article: <https://physicsworld.com/a/the-double-slit-experiment/>



To make matters even more strange, if detectors (“indicators”, as Grometstein calls them) are used to observe which slit the photons or electrons went through, the narrow interference fringes go away and you just get a superposition of two wider bands.

Moral of the story:

Things on a very small scale behave like nothing that you have any direct experience about. They do not behave like waves, they do not behave like particles, they do not behave like clouds, or billiard balls, or weights on springs, or like anything that you have ever seen. –Richard Feynmann, 1963

## Chapter 9 – The Nuclear Atom (1904-1912)

The main topic of this chapter is Ernest Rutherford’s 1910 experiment where he used alpha particles to bombard nuclei, and from the results was able to deduce that the size of a nucleus is around 10 fm, meaning  $10 \times 10^{-15}$  m. Here’s how that went.

Alpha particles are made up of two protons and two neutrons. They have a mass of  $6.64424 \times 10^{-27}$  kg and a charge of  $+2e$ . They are what’s left if you take a helium atom and strip away the electrons, and are often also emitted as independent particles in various radioactive decays. As an alpha particle approaches a nucleus where the positive charge of an atom is concentrated, it experiences a repulsion because both the alpha particle and the nucleus are positively charged. Like charges repel according to Coulomb’s law which governs the electric force between any two charged objects:

$$F = \frac{kq_1q_2}{r^2}$$

- $F$  is the amount of the repulsive force (in N)
- $q_1$  and  $q_2$  are the values of the two charges (in C)
- $r$  is the separation distance between the two charges
- $k$  is the Coloumb force constant, sometimes called “Coloumb’s constant”, and has a value of  $8.988 \times 10^9 \text{ N}\cdot\text{m}^2/\text{C}^2$ . Don’t confuse this with Boltzmann’s constant which was mentioned in Chapter 5 even though both sometimes use the same symbol,  $k$ .

This repulsive force creates what can be called an “energy barrier” for the alpha particles, in much the same way that a ramp creates an energy barrier for a skateboarder. Energy comes in two forms, namely kinetic and potential. The equation for the kinetic energy of an object is:

$$KE = \frac{1}{2}mv^2$$

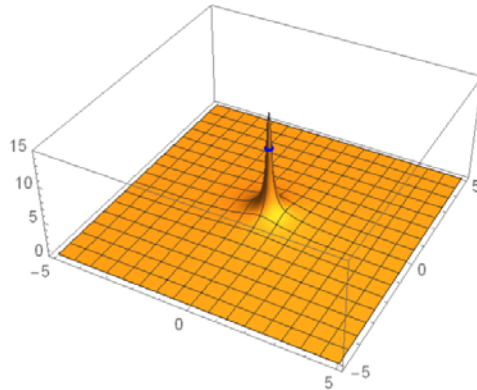
- $m$  is the object’s mass
- $v$  is the object’s velocity

There are also equations for potential energy, but the specific potential energy equation depends on the specific force from which the potential energy arises (in the case, the Coulomb force), so we won’t go into details on that right now.

Back to the skateboarder analogy. In that example, potential energy arises from gravitational force, and the higher up the ramp a skateboarder is the more potential energy she has. As she approaches the ramp, she has kinetic energy. As she rises up the ramp, the kinetic energy is turned into potential energy. The

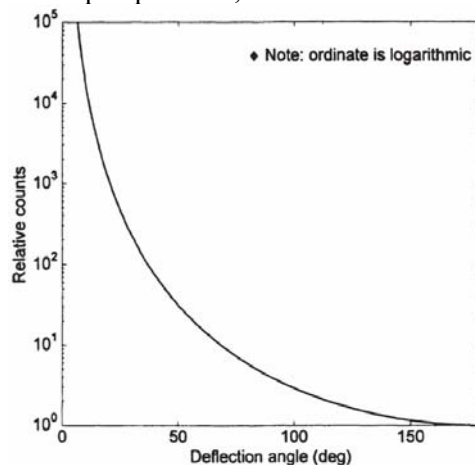
kinetic energy can be reclaimed when she goes back down the ramp, assuming no energy is lost to effects like friction.

In the Rutherford experiment, the potential energy from the nucleus causes the alpha particle to behave like a skateboarder going up a ramp shaped like this (the small blue ring indicates the size of the nucleus):



The *impact parameter* describes the closest distance the alpha particle would get to the nucleus, if it didn't experience any repulsion at all. (The *distance of closest approach*, or DCA, by contrast, is how close the alpha particle *actually* gets to the nucleus.) For large impact parameters the alpha particles won't be deflected much. But with small impact parameters a substantial deflection can occur. For an impact parameter close to zero, the alpha particle can even "go up the ramp" a ways, then turn around and come straight back! With even more energy, the alpha particle can go all the way up the ramp and actually collide with the nucleus.

Here are Rutherford's key results for alpha particles, as summarized in Fig. 9.5:



These experiments disproved J.J. Thomson's "plum pudding" model of the atom which thought the positive charge was spread out rather than gathered into a nucleus. Grometstein estimates (without showing details) that the deflection of an alpha particle by a single plum pudding-type nucleus would have been about  $0.02^\circ$  in a random direction. That means at each nucleus the alpha particles have a 50-50 change of going left or right by about  $0.02^\circ$  (up-down deflections have a similar story). This is analogous to flipping a coin, where at each flip the coin has a 50-50 chance of being heads or tails. Grometstein cites a well-known statistical fact that if you flip a coin 10,000 times, then the coin will probably not go heads *exactly* 5,000 times... but one might reasonably expect the number of heads to be within  $2\sqrt{10,000} = 200$  heads of 5,000. In other

words, the number of heads will likely be  $5,000 \pm 200$ . The square root dependence comes from analyzing random numbers and is common to many statistical events, such as sampling error in election polls. The factor of 2 comes from Grometstein's defining "very likely" to have a precise statistical definition of "within two standard deviations". To summarize the situation: for  $N$  flips the deviation from 50% will very likely be within  $2\sqrt{N}$  flips.

This means that if Thomson's model had been correct, for alpha particles going through a gold foil that is 10,000 atoms thick and with the particles making a  $0.02^\circ$  random deflection at each atom, Rutherford should have seen nearly all of the alpha particles to have deflections less than  $0.02^\circ \times 2\sqrt{10,000} = 4^\circ$ . But that is not at all what Rutherford observed. He saw many deflections at angles larger than that, some at very large angles. Moreover, by increasing the energy of the alpha particles he was able to see the point at which the alpha particles had enough energy to actually penetrate the nucleus, and in that case the number of alpha particles deflected at very large angles (close to  $180^\circ$ , i.e. straight back) was reduced. All of this data when combined with mathematical models beyond the scope of this class resulted in the conclusion that the size of the nucleus is about 10 fm, as mentioned above.

## Chapter 10 – Bohr's Atom (1913-1925)

Rutherford's "solar system" model of the atom, as it came to be known, suffered from two huge flaws. One, it didn't explain the observed atomic spectra. Why are only discrete wavelengths observed? And why those particular wavelengths? Secondly, the laws of electricity and magnetism ("Maxwell's equations") indicated that due to the loss of energy from electromagnetic waves being given off, if an electron were really orbiting a nucleus it would spiral in and collide within 16 picoseconds or so. Bohr proposed an alternate model of the atom to explain these. Bohr's model was a huge break from classical physics and explained some (but not all) features that had been observed. To understand Bohr's model, we must first review the concepts of momentum, angular momentum, and centripetal acceleration.

**Momentum:** The momentum of an object, given the symbol  $p$ , is defined as its mass times its velocity:  $p = mv$ . Its usage in physics is pretty close to its usage in English—the more momentum something has, the harder it is to stop.

**Angular momentum:** The angular momentum of an object, given the symbol  $L$ , is defined as the object's momentum multiplied by a "lever arm" about a central point. For the case of circular motion, the lever arm is just the radius of the circle in which the object is traveling:  $L = mvr$ . Loosely speaking the angular momentum is a measure of how hard it would be to stop something traveling around in a circle.

**Centripetal acceleration:** As per Newton's First Law, objects tend to travel in constant velocity straight-line motion unless acted upon by a force. If an object is traveling in a circle, it must be experiencing a force and hence (from Newton's Second Law) an acceleration... even if its speed is not changing. This type of acceleration is called "centripetal", meaning "center seeking", because the force is constantly deflecting the object towards the center of the circle. It can be shown (but it's beyond the scope of this class) that the amount of acceleration an object must have to move in a circle (radius  $R$ ) at constant speed  $v$  is:

$$a = \frac{v^2}{R}$$

The amount of force required to move the object in the circle is just its mass times that acceleration.

Back to Bohr's model. He proposed three postulates that had no foundation in classical physics... but which seemed to explain the experimental observations related to electrons orbiting their nuclei. They are:

- (1) Angular momentum is quantized. It only exists as multiples of Planck's constant divided by  $2\pi$ , which is given the new symbol  $\hbar$  (pronounced "h bar"). In equation form:  $L = n\hbar$  where  $n$  represents any integer. This means that only certain orbits are possible.
- (2) Electrons in atoms don't follow Maxwell's equations, namely they do not give off radiation as long as they don't switch orbits.
- (3) When an electron does switch orbits, it emits or absorbs a photon to account for the energy difference between the two orbits.

In class we went through the math that combined Bohr's quantized angular momentum with centripetal acceleration caused by the Coulomb force between an electron and a hydrogen nucleus (one proton) to arrive at these two important equations for the orbital radius and orbital energy of electrons in the  $n^{\text{th}}$  orbit in hydrogen atoms. (In these equations  $k$  is the Coulomb force constant.)

$$r_n = \frac{\hbar^2}{kme^2} n^2 = (5.29 \cdot 10^{-11} \text{ meters}) n^2$$

$$E_n = -\frac{k^2me^4}{2\hbar^2} \frac{1}{n^2} = (-13.61 \text{ eV}) \frac{1}{n^2}$$

Success! The energy equation in particular, combined with the third postulate, exactly predicts the known absorption and emission spectral lines of hydrogen atoms. Modified versions of those equations also worked well for other atoms containing only one electron, such as singly ionized helium atoms, doubly ionized lithium atoms, and so forth.

But not total success—the theory couldn't be modified for other atoms, and other special cases such as what happens to atoms in electric and magnetic fields necessitated the creation of other "quantum numbers" besides  $n$  which were required to specify the state of a given electron. These were labeled in *Roots* as  $\ell$ ,  $m_\ell$ , and  $s$ . (Disclaimer: what *Roots* calls  $s$  is often called  $m_s$ .)

We are skipping the Frank-Hertz experiment of 1914, which also helped verify the discrete nature of electron energy levels in atoms.

## Chapter 11 – Compton's Shift (1923)

In addition to the energy of a photon being  $E = hc/\lambda$ , Einstein also proposed that the momentum of a photon is:

$$p = \frac{h}{\lambda}$$

Compton used this to explain his results in a scattering experiment where photons collide with electrons and then go off with a different energy and a different momentum in some other direction.

This type of collision is similar to two billiard balls colliding, which can be analyzed through the principles of conservation of energy and conservation of momentum. Since momentum is a vector quantity, momentum in both  $x$ - and  $y$ -directions is conserved. Suppose a cue ball (labeled C in the figure, but let me call it "ball 1") collides with a target ball (T in the figure, aka "ball 2"), and we measure ball 1's initial velocity ( $v_1$ ) and final angle ( $\alpha$ ). Can we predict these three things? (1) Ball 1's final velocity ( $v_1'$ ). (2) Ball 2's final angle ( $\theta$ ), and (3) Ball 2's final velocity ( $v_2'$ )? Yes we can! We can set up three equations which allow us to solve for those three unknowns. (We will assume both balls have the same mass,  $m$ .)



Conservation of energy:

$$\frac{1}{2}mv_1^2 = \frac{1}{2}mv_1'^2 + \frac{1}{2}mv_2'^2$$

Conservation of momentum in the x-direction:

$$mv_1 = mv_1' \cos \alpha + mv_2' \cos \theta$$

Conservation of momentum in the y-direction:

$$0 = mv_1' \sin \alpha - mv_2' \sin \theta$$

Going through quite a bit of algebra from those three equations we arrive at the answers to our three questions above:

- (1)  $v_1' = v_1 \cos \alpha$
- (2)  $\theta = 90^\circ - \alpha$
- (3)  $v_2' = v_1 \sin \alpha$

The situation with a photon colliding with a stationary electron is quite similar. We just need to use the equations for energy and momentum of a photon which we know, and Einstein's equation that relates energy and momentum of a high speed electron, which we don't know but which I don't especially care that you know. Since the photon loses energy in the process it is shifted to higher wavelength. If one sets up three equations again and goes through the math (beyond the scope of this class), then one can arrive at Compton's equation which relates the new photon wavelength ( $\lambda'$ ) to the original wavelength ( $\lambda$ ):

$$\lambda' = \lambda + \frac{h}{mc}(1 - \cos \alpha)$$

In the equation,  $m$  is the mass of the electron and  $\alpha$  is the scattering angle of the photon. This equation exactly matched Compton's experimental data for how the wavelength shifted as a function of angle  $\alpha$ , and could only be derived by viewing photons as particles very similar to electrons.

## Chapter 12 – A Princely Postulate (1924)

It had been established through experiments such as Young's double-slit experiment, G.I. Taylor's follow up with single photons, the photoelectric effect, and Compton scattering, that light displayed both particle and wave aspects. De Broglie took this one step farther and said that *everything* displays both particle and wave aspects. Specifically, the wavelength  $\lambda$  of a "particle" (or any object with mass) is given by the same exact same equation that Einstein proposed for photons, where  $p$  is momentum and  $h$  is Planck's constant:

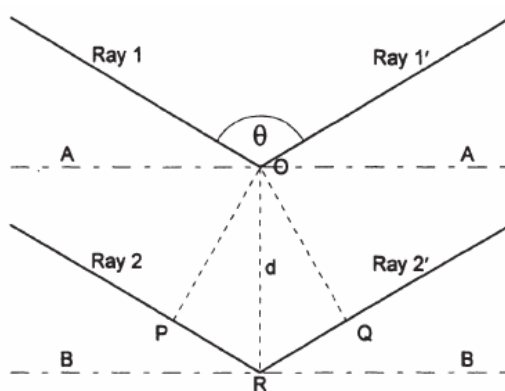
$$\lambda = \frac{h}{p}$$

For macroscopic objects this equation predicts tiny wavelengths, and so their wave nature is never observed. But for particles such as electrons, this predicts wavelengths that are long enough to have real effects on the electrons' behavior... for example, being able to see interference fringes in the double-slit experiment done with electrons as mentioned in Chapter 8.

Another case where the wave nature of electrons was unambiguously observed was in diffraction by crystals, where a beam of x-rays (or later, electrons) is sent towards a crystal and scattering from the planes of atoms in the crystal causes bright diffraction spots to occur at specific angles which can be determined from Bragg's law:

$$n\lambda = 2d \cos \frac{\theta}{2}$$

Here  $n$  is the diffraction "order", typically a small integer,  $\lambda$  is the wavelength of the x-rays (or electrons),  $d$  is the spacing between planes of atoms, and  $\theta$  is the diffraction angle as defined in this figure (Fig. 12.2):



Although the equation was developed by Bragg in 1912 for use with x-rays, in 1927 Davisson and Germer found that electrons diffracted in exactly the same way, with the appropriate wavelength given exactly as predicted by de Broglie's equation. One can also modify de Broglie's equation which relates wavelength to momentum, to an equation that relates wavelength to kinetic energy ( $KE$ ), like this:

The definition of  $KE$  gives an equation for velocity  $v$ :

$$KE = \frac{1}{2}mv^2 \rightarrow v = \sqrt{\frac{2KE}{m}}$$

Plugging that  $v$  into the definition of momentum gives an equation for  $p$  in terms of  $KE$ :

$$p = mv = m \sqrt{\frac{2KE}{m}} = \sqrt{2mKE}$$

Equating that  $p$  to the momentum in de Broglie's equation gives us a useful equation that relates  $\lambda$  to  $KE$ :

$$\frac{h}{\lambda} = \sqrt{2mKE}$$

De Broglie's equation, though powerful and borne out by experiment, is incomplete, in that it doesn't explain *how* or *why* electrons act as waves, nor how to reconcile the concept with other experiments in which electrons seem to act as particles. De Broglie's "matter waves" as we can call them, aka the particle "wave functions", are given the symbol  $\psi$  (Greek letter psi).

## (Chapter 13 – skipped)

### Chapter 14 – Inventing the Wave Equation (1926) – part 1

Schrödinger's equation is the heart of quantum mechanics. His equation gives more insight into what the wave function of a particle is, and allows one to calculate  $\psi$  for a given environment which is characterized by a particle's potential energy (which I will call  $PE$  but which *Roots* calls  $U$ ). We will study this chapter in four parts.

Schrödinger's equation involves derivatives. The derivative of a function is a function in its own right whose value at each point describes the slope of the original function. It's given the symbol  $D$ : the derivative of the function  $f$  is labeled  $D(f)$ . A region of  $f$  that is sloping upwards will have a positive derivative. A region that is sloping downwards will have a negative derivative. A region which is flat will have a derivative equal to zero. The derivative of the derivative is called the "second derivative" of a function, and given the symbol  $D^2(f)$  (the 2 doesn't mean squared, it means two sequential derivatives). For some additional assistance on the concept if needed, see the video and simulation given in the warmup exercise:

- <https://www.youtube.com/watch?v=rAof9Ld5sOg>
- <https://phet.colorado.edu/en/simulation/legacy/calculus-grapher>

Since sines and cosines are so important when discussing waves, we need to know what their derivatives and second derivatives are. The results are as follows (side note:  $\sin kx$  is shorthand for  $\sin(kx)$  to avoid using so many parentheses; similarly for  $\cos kx$ ):

$$\begin{aligned}D(\sin kx) &= k \cos kx \\D(\cos kx) &= -k \sin kx \\D^2(\sin kx) &= -k^2 \sin kx \\D^2(\cos kx) &= -k^2 \cos kx\end{aligned}$$

If the sine or cosine function has an amplitude different than 1, then just multiply the derivative by the amplitude as well, e.g.:  $D(5 \sin kx) = 5k \cos kx$ , etc.

We therefore have an equation for both sine and cosine waves that looks like this:

$$D^2(f) = -k^2 f$$

That's called a "differential equation", meaning an equation that involves derivatives (which are also sometimes called "differentials"). Unlike regular equations which you solve for *values* of  $x$ ,  $y$ , etc., differential equations are typically used to solve for *functions*. What's more, sine and cosine functions (and sines and cosines added together) are the *only* functions that will solve that particular differential equation. So, for example, if you arrive at an equation that looks like  $D^2(f) = -49f$ , the only functions that are solutions to the equation will be:  $\sin 7x$ ,  $\cos 7x$ , with any amplitudes you like, or any of those functions added together.

In the last chapter we saw that the wavelength of a particle with mass  $m$  was related to its kinetic energy according to:  $\frac{h}{\lambda} = \sqrt{2mKE}$ . Since the wavenumber  $k$  is defined in terms of the wavelength according to  $k = 2\pi/\lambda$ , one can put that equation in terms of  $k$  instead of  $\lambda$ :

$$k = \frac{\sqrt{2mKE}}{\hbar}$$



To create his equation, Schrödinger said that the differential equation for sines and cosines given above, namely  $D^2(f) = -k^2f$ , should hold for matter waves of a given kinetic energy  $KE$  as long as we use the  $k$  value appropriate for the given kinetic energy in a given region of space:

$$D^2(\psi) = -\frac{2m}{\hbar^2} KE \psi$$

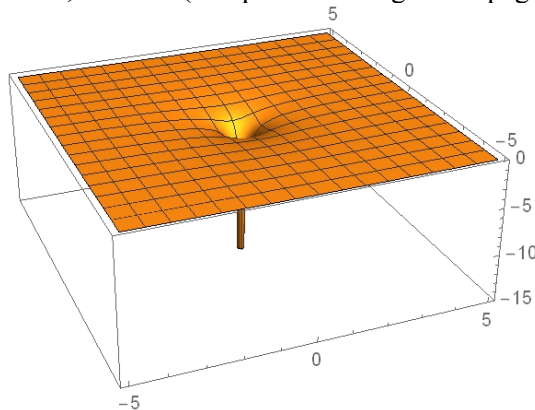
Since total energy  $E_{tot}$  is conserved, kinetic energy will increase and decrease as a particle moves through regions of different potential energy, so we can put the equation in terms of the total energy and potential energy like this, using  $KE(x) = E_{tot} - PE(x)$ :

$$D^2(\psi) = -\frac{2m}{\hbar^2} (E_{tot} - PE(x)) \psi$$

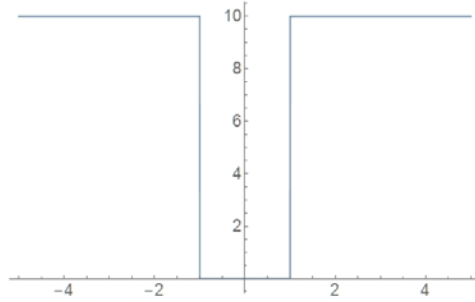
This is Schrödinger's equation, which we could expand to describe functions of  $x$ ,  $y$ , and  $z$ , rather than functions of  $x$  alone (but we won't). It is a differential equation that allows one to solve for the wave function  $\psi$  of a particle, given the potential energy landscape it finds itself in (which relates closely to the forces acting on the particle).  $\psi$  is a function of  $x$ , so I could have written it as  $\psi(x)$ . And actually, for a given potential energy function, Schrödinger's equation often predicts *multiple* possible wave functions, which we call different possible “states” or “energy states” of the particle. For each possible wave function, the equation also allows one to calculate the total energy of the state in a manner that we will see in the next section.

## Chapter 14 – Inventing the Wave Equation (1926) – part 2

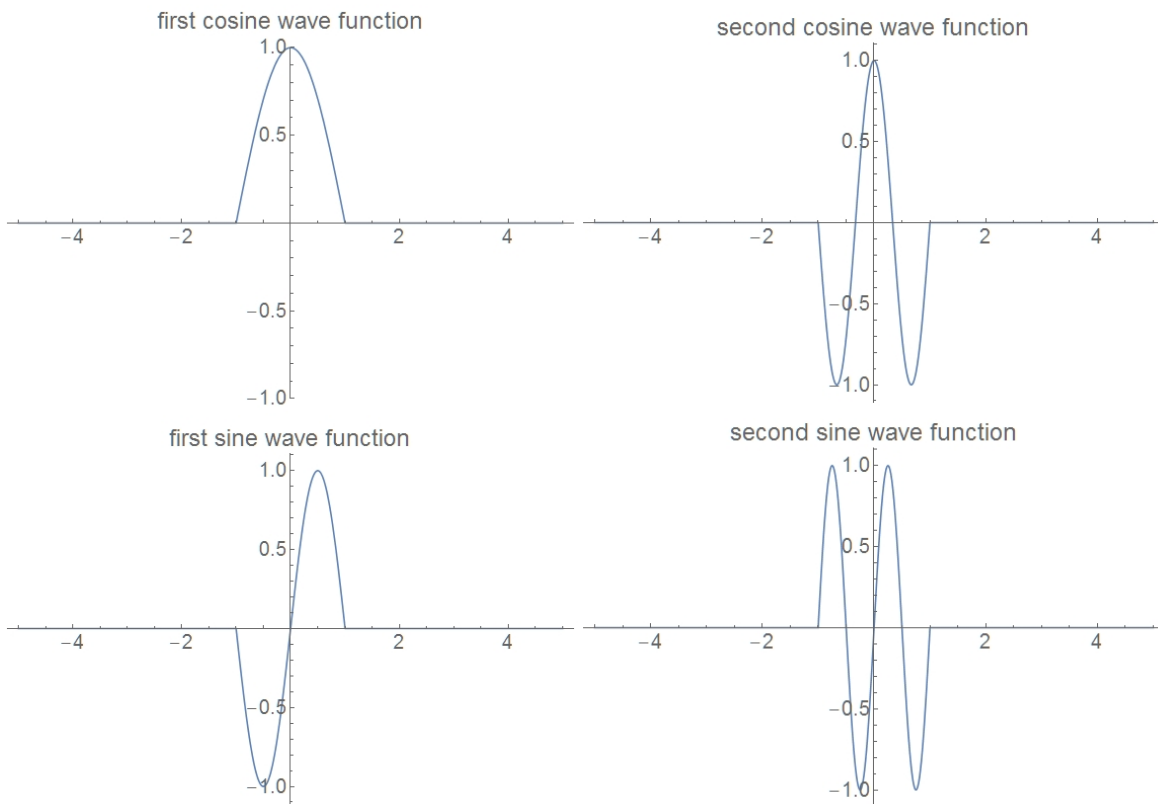
Now that we have the equation, we need to focus on what it tells us. If we want to predict the possible states of an electron in an atom, we would need to solve the Schrödinger equation for the potential energy of an electron in the environment of a nucleus. This is essentially just the opposite of the potential of an alpha particle near a nucleus, since electrons have a negative charge and alpha particles have a positive charge. The potential creates a well, like this (compare to the figure on page 3 of this document):



However, that problem is too hard to solve. So we will create a model, which looks like the following but with the sides going up to infinity instead of only to 10; also the sides of the well in this model are at  $+d$  and  $-d$  instead of at  $+1$  and  $-1$  as the figure shows. It's called an “infinite square well”:



Given this potential energy,  $\psi$  for the electron is zero outside the well because the sides of the well form a barrier that it cannot overcome. Inside the well the potential energy  $V(x)$  is zero, so Schrödinger's equation becomes  $D^2(\psi) = -\frac{2m}{\hbar^2} E_{tot} \psi \dots$  and we already know what the solutions are to this differential equation! They are just sine and cosine functions, like  $\sin kx$ ,  $\cos kx$ , or combinations. Since the wave function inside the well must go to zero at the boundaries in order to match up with the wave function outside the well, that puts a condition on what values of  $k$  are allowed. This results in a set of allowed wave functions that seems very similar to the standing waves we saw earlier in the semester. Specifically, the first four look like this:



If we shift the origin to be at the left hand side of the well instead of the middle (which doesn't affect the physical situation at all), the sines and cosines can be summarized as a set of sine functions like this, where  $n$  is the number of the state which in this case matches the number of antinodes in the corresponding  $\psi$ :

$$\psi_n = \sin \frac{n\pi x}{2d}$$

In other words, the first allowed wave function is  $\psi_1 = \sin \frac{\pi x}{2d}$ , the second one is  $\psi_2 = \sin \frac{2\pi x}{2d}$ , etc. These allowed wave functions are called the *eigenfunctions*.

The energy of each state can be found by plugging the equation for  $\psi$  back into the Schrödinger equation  $D^2(\psi) = -\frac{2m}{\hbar^2} E_{tot} \psi$  and using what we know about second derivatives of sine functions:

$$\begin{aligned} \text{Schrödinger equation with } \psi \text{ plugged in: } & D^2 \left( \sin \frac{n\pi x}{2d} \right) = -\frac{2m}{\hbar^2} E_{tot} \left( \sin \frac{n\pi x}{2d} \right) \\ \text{Evaluate the second derivative: } & -\left( \frac{n\pi}{2d} \right)^2 \left( \sin \frac{n\pi x}{2d} \right) = -\frac{2m}{\hbar^2} E_{tot} \left( \sin \frac{n\pi x}{2d} \right) \end{aligned}$$

The negative signs and the sine functions cancel, giving us:

$$E_{tot} \text{ of } n^{\text{th}} \text{ state} = \frac{n^2 \pi^2 \hbar^2}{8md^2}$$

(This is also the kinetic energy of the  $n^{\text{th}}$  state, since for this particular model the potential energy in the well is defined to be zero.)

For an electron in a well going from  $-0.5$  nm to  $+0.5$  nm, the energies of the lowest four states are:

$$\begin{aligned} E_1 &= 0.376 \text{ eV} \\ E_2 &= 1.504 \text{ eV} \\ E_3 &= 3.384 \text{ eV} \\ E_4 &= 6.016 \text{ eV} \end{aligned}$$

These energies are called the *eigenenergies*. For this model, they don't really match the energies of electrons in any atoms, although they are the right order of magnitude... **HOWEVER if one uses the actual potential energy instead of our simplistic model one, and the full 3-dimensional version of the Schrödinger equation, the resulting energies for an electron in a hydrogen atom exactly match the observed ones.** The wave functions are the "atomic orbitals" that many students learn in chemistry classes (to be technical, the orbitals are the wave functions squared, not just  $\psi$ ).

The Schrödinger equation as given here doesn't have any time dependence. Schrödinger modified the equation to predict what the wave functions will do as time passes (in fact it's possible he did the version that includes time first and then this version second), and found that the wave functions oscillate at a frequency  $f$  that is related to the energy of each state, according to:

$$f = \frac{E_{tot}}{h}$$

which looks very similar to Einstein's equation for photons, although the frequency in the equation means something different. For photons, it's the frequency of the electromagnetic wave that the photons are part of, i.e. the oscillation of the electric and magnetic fields that produce the wave, which when quantized give you photons. For electrons (and other particles with mass) it's the frequency of oscillation of the wave function itself, which as we will see in the next two sections involves complex numbers.

## Chapter 14 – Inventing the Wave Equation (1926) – part 3

The wave function  $\psi(x)$  is an indication of where the particle is located. In 1926 Max Born gave the more specific interpretation that  $|\psi(x)|^2$ , when properly normalized, indicates the *probability* of finding a particle at the given point  $x$ . This is one of the key principles of quantum mechanics. So  $|\psi(x)|^2$  is really the measurable quantity, not  $\psi(x)$  itself. This is good, because Schrödinger found the oscillating parts of the wave functions involve complex numbers which can't correspond to "real" quantities (pun intended). But when you take the magnitude of the wave function squared, as indicated by absolute value signs in  $|\psi(x)|^2$ , you end up with a purely real function.

The proper normalization involves making sure that the total probability indicated by  $|\psi(x)|^2$  is 100%. That generally requires calculus so we won't do that, we will just assume that if an eigenfunction is given to us, it has already been normalized. As a side note, the infinite square well wave functions given on the previous page have not been normalized, but we don't really need them for anything except their general shapes so it's OK.

The Schrödinger equation predicts that particles can be in a *quantum superposition* of eigenfunctions. A superposition state is when two or more eigenfunctions are added together in some ratio such as

$$\psi(x) = C_1\psi_1(x) + C_2\psi_2(x) + C_3\psi_3(x) + \dots$$

The superposition state must be normalized so that the squares of the coefficients add up to 1 (since the wave function squared gives the probability):  $C_1^2 + C_2^2 + C_3^2 + \dots = 1$ . If they don't add up to 1 in that manner, then you must normalize them by dividing all coefficients by the square root of the sum of the squares—and then the squares of the coefficients will add up to 1 and will indicate the percentage that the superposition is in each of the states 1, 2, 3, etc. When normalized, the expected energy of the superposition state is given by a weighted average of the energies of the eigenstates,  $E_{tot} = C_1^2 E_1 + C_2^2 E_2 + C_3^2 E_3 + \dots$ . In other words, each state that's part of the superposition contributes its coefficient squared towards the total energy of the state.

Back to complex numbers. More background on complex numbers is available at these links which were provided in the reading assignment/warmup exercise:

- <https://www.youtube.com/watch?v=T647CGsuOVU> - Imaginary Numbers Are Real Part 1
- <https://www.youtube.com/watch?v=2HrSG0fdxLY> - Imaginary Numbers Are Real Part 2
- <https://www.youtube.com/watch?v=N9QOLrfeKNC> - Imaginary Numbers Are Real Part 3
- <https://www.youtube.com/watch?v=DThAoT3q2V4> - Imaginary Numbers Are Real Part 4
- <https://www.youtube.com/watch?v=65wYmy8Pf-Y> - Imaginary Numbers Are Real Part 5
- [https://www.youtube.com/watch?v=z5IG\\_6\\_zPDo](https://www.youtube.com/watch?v=z5IG_6_zPDo) - Imaginary Numbers Are Real Part 6
- <https://www.youtube.com/watch?v=YHvR8siLiD0> - Imaginary Numbers Are Real Part 7
- <https://www.youtube.com/watch?v=sKtIoBAuP74> - Euler's Identity

The main points from the first seven videos are as follows:

1. Imaginary numbers are a useful mathematical construct which can help solve problems that involve real situations.
2. Imaginary numbers lie on an axis that in some sense is perpendicular to the real number line, and hence complex numbers (numbers which have both a real and an imaginary part) can be thought of as points in a plane.
3. One can represent those points in polar form, with a magnitude and an angle. For a given complex number  $z$  which has real part  $x$  and imaginary part  $iy$ , the magnitude is given by (via the Pythagorean theorem)  $|z| = \sqrt{x^2 + y^2}$  and the angle can be found through some trigonometry.

- Multiplying together two complex numbers has a geometrical interpretation, namely the angles of the two numbers add together and the magnitudes multiply.

The point of the last video was to help you understand Euler's equation,  $e^{ix} = \cos x + i \sin x$ . Through a little bit of thinking about where the point  $(\cos x, \sin x)$  lies in the complex plane, one can conclude that the complex number  $e^{ix}$  has a magnitude of 1 and an angle of  $x$ . Therefore multiplying by  $e^{ix}$  causes a rotation of  $x$  radians or degrees (depending on what angular units you're using) without changing the magnitude of the number. Multiplying by  $e^{-ix}$  causes a rotation of  $-x$  radians or degrees.

How do complex numbers relate to wave functions? When I previously said that a wave function oscillates at frequency  $f = \frac{E_{tot}}{h}$ , I didn't mean the wave function just oscillates up and down in amplitude. If it did that, at most times the wave function squared would not be normalized, i.e. there wouldn't be a 100% chance of finding the particle somewhere. What really happens, is that each eigenfunction oscillates according to  $e^{-i\omega t}$ , where the angular frequency  $\omega$  of a state is given by  $\omega = 2\pi f = 2\pi \left(\frac{E}{h}\right) = \frac{E}{\hbar}$ . By Euler's formula  $e^{-i\omega t}$  is  $\cos \omega t - i \sin \omega t$ . Multiplying by this factor gives rise to sinusoidal oscillations in time, in both the real and the imaginary parts of the wave functions, but because they are out of phase with each other the normalization condition of  $|\psi|^2$  is maintained. That can be seen since  $e^{-i\omega t}$  has magnitude of 1, so regardless of time it doesn't change the magnitude of  $\psi$ .

For superposition states, each eigenfunction component oscillates at its own particular frequency given by its own particular energy, like this:

$$\psi(x, t) = C_1\psi_1(x)e^{-i\omega_1 t} + C_2\psi_2(x)e^{-i\omega_2 t} + C_3\psi_3(x)e^{-i\omega_3 t} + \dots$$

where  $\omega_1 = E_1/\hbar$ ,  $\omega_2 = E_2/\hbar$ ,  $\omega_3 = E_3/\hbar$ , etc.

By the way, the complex number nature of the wave function and how eigenfunctions oscillate in time is referred to in passing in *Roots* and depicted in one figure but without the (hopefully helpful) added detail that I have provided.

To sum up some of the major points of this and the previous section:

- Potential wells have special solutions called eigenfunctions.
- Each eigenfunction represents a state with a different energy.
- Eigenfunctions have both real and imaginary components.
- Those real and imaginary components oscillate at frequencies that depend on the energies of the given state.
- The magnitude squared of the wave function is a probability function describing where the particle is likely to be.
- Particles can be in superposition states that contain different amounts of two or more eigenfunctions; in that case the state as written as a sum of eigenfunctions with different coefficients (normalized so the squares of the coefficients add up to 1).
  - The squares of the coefficients indicate the probability of being in each of the eigenstates.
  - Each eigenfunction oscillates at its normal frequency but the state as a whole does not oscillate at any one frequency.

All of those points can be demonstrated with this wonderful PhET simulation called "Quantum Bound States": <https://phet.colorado.edu/en/simulation/legacy/bound-states>

## Chapter 14 – Inventing the Wave Equation (1926) – part 4

The final section of Chapter 14 involves a scenario where electrons are shot at a potential “barrier”, which is the opposite of a potential well. The scenario can be demonstrated with this equally wonderful PhET simulation called “Quantum Tunneling and Wave Packets”, if you set the potential to a few different values as specified in the warmup instructions:

<https://phet.colorado.edu/en/simulation/legacy/quantum-tunneling>

Some key observations:

- A wave function is made up of a real and an imaginary component, each of which can have spatial oscillations (see Fig 14.4).
- A wave function traveling in a region with a flat potential energy will gradually spread out (see Fig. 14.5).
- A wave function which impacts a barrier will split into two parts: a part that travels through the barrier and a part that gets reflected off the barrier. The two parts represent probabilities that the wave will transmit or reflect. (See Fig. 14.6.)
- If the barrier is sufficiently large, the part that transmits will be very small, essentially zero (see Fig. 14.7).
- The reflected portion can interfere with the incoming wave, resulting in spatial oscillations in not only  $\psi$  but also  $|\psi|^2$  (see Figs. 14.7 and 14.8).