

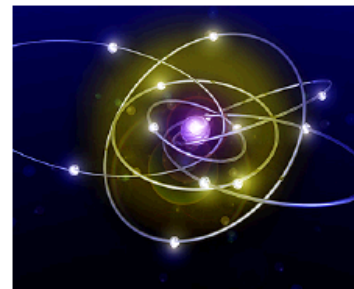
$$\begin{aligned}
 & \frac{1}{2} m v^2 \\
 & \frac{1}{2} m \omega^2 (a + a^\dagger)^2 \quad p = -i \hbar \frac{m \omega}{2} (a - a^\dagger) \\
 & H = \frac{\hbar \omega}{4} (2 a a^\dagger + 2 a^\dagger a) \psi \\
 & = \frac{\hbar \omega}{2} (a a^\dagger + a^\dagger a) \psi \\
 & = \frac{\hbar \omega}{2} (\underbrace{a a^\dagger + a^\dagger a}_{[a, a^\dagger] + 2 a^\dagger a}) \psi \\
 & \psi(1) = \frac{\hbar \omega}{2} (2 a^\dagger a + [a, a^\dagger]) \psi
 \end{aligned}$$

$\rightarrow \hbar \omega (n + \frac{1}{2})$   
 $NB \hat{H} \psi = E \psi$   
 $E = \hbar \omega (n + \frac{1}{2})$

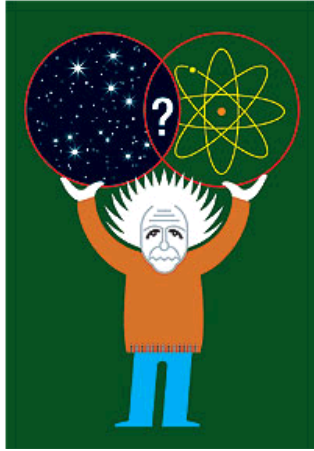
## WHY DO WE NEED QUANTUM MECHANICS?



*Classical mechanics* is the study of the motion of everyday objects in accordance with the general principles first developed by Newton with later modifications by Einstein.



*Quantum mechanics* is a set of mathematical principles that attempts to explain the behavior of atoms and sub-atomic particles.



So, in essence ...

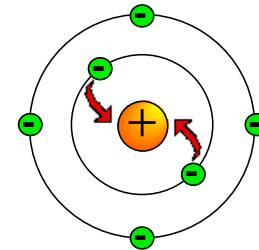
**Classical mechanics** explains the very large

**Quantum mechanics** explains the very small

However, just where one takes over from the other is not well-defined. It is a topic on which there is much current interest since they are not yet compatible and hard to bring together (unify).

The flaws in Newton's concepts are only noticeable when dealing with the very small or the very fast. For everyday objects much larger and much more massive than atoms and much slower than the speed of light, classical physics does a great job.

In the early 20th century experiments produced results that could not be explained by classical physics. For example, the *solar system* picture of an atom, first introduced by Ernest Rutherford in 1911 and modified by Neils Bohr in 1913.

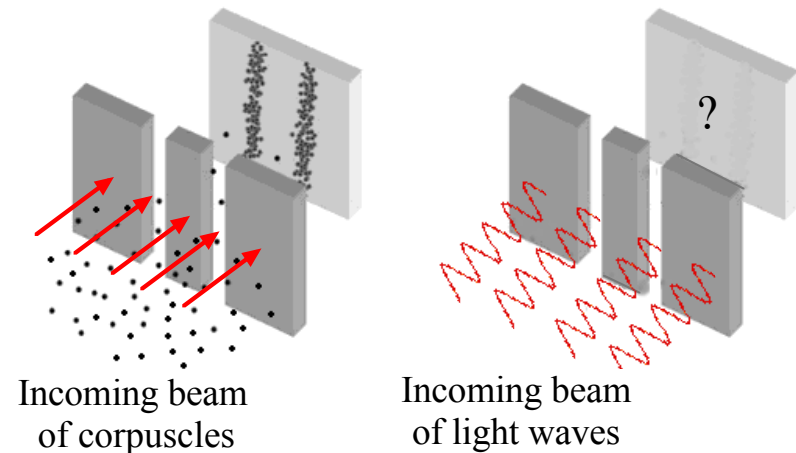


*Physics was in trouble!*

The origin of quantum mechanics is intimately connected to the concept of the wave-particle duality of light:

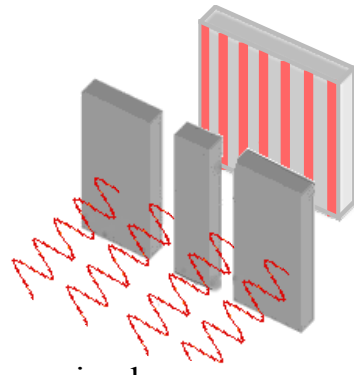
- In the 1680s, Robert Hooke and Christian Huyghens postulated independently that light was composed of *waves*.
- In 1704 in his book *Optiks*, Isaac Newton proposed that light was *corpuscular*, i.e., made up of particles.

### Young's double-slit experiments (1801-3)



In a series of experiments carried out early in the 19th century, Thomas Young sent a beam of light (of a single color) through two closely spaced, narrow slits. If light consisted of particles, one would expect to see only two lines of light on a screen.

*But, what did Young actually observe?*



Incoming beam  
of light waves

Young selected red and blue light from sunlight for his experiments. In both cases he observed a set of equally spaced, bright and dark lines.

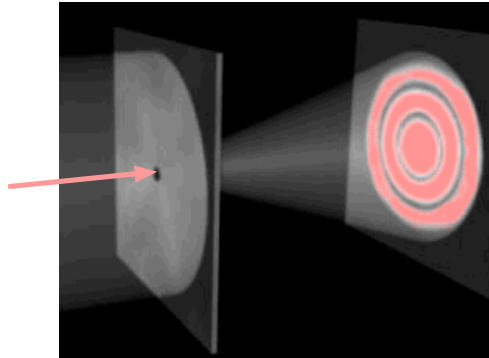
Using a very simple analysis he was able to determine the wavelengths of red and blue light.

According to Young:

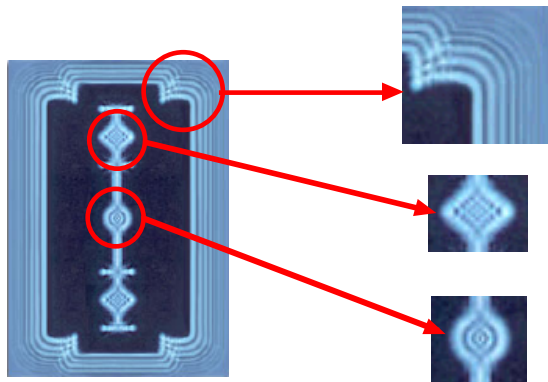
**Red light:**  $\frac{1}{36,000}$  of an inch.

**Blue light:**  $\frac{1}{60,000}$  of an inch.

[http://scientificfingerfood.files.wordpress.com/2014/01/doqpx\\_doubleslit\\_animated.gif?w=604](http://scientificfingerfood.files.wordpress.com/2014/01/doqpx_doubleslit_animated.gif?w=604)



Diffraction from a circular aperture  
(Augustin-Jean Fresnel, 1819).

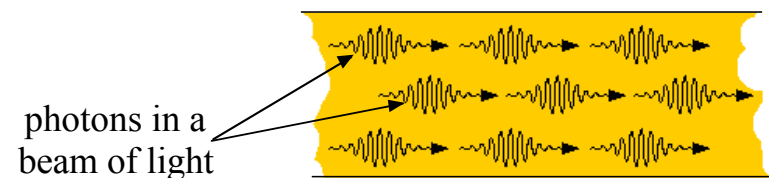


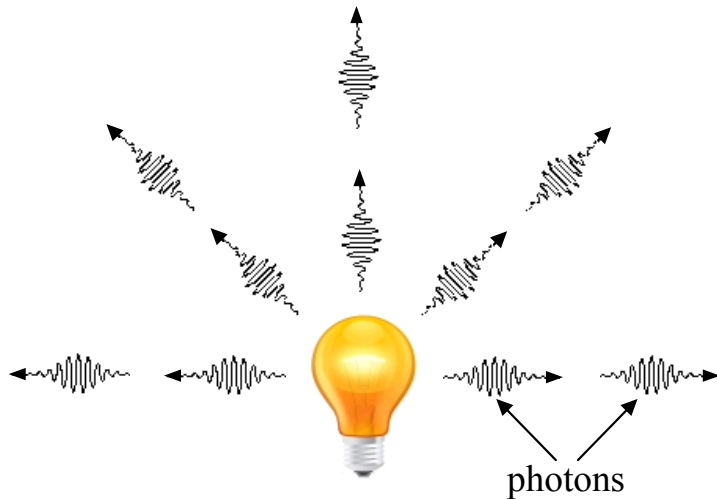
Fringes produced by blue laser light at  
the edges of a razor blade.

*So, light is a wave after all!*

Heh, not so fast ...

- In 1905, Einstein proposed that a light beam was composed of a stream of tiny packets of energy directly related to the wavelength of the light. He referred them as “*das Lichtquant*” (light quanta). In 1926 these packets of energy (particles) became known as *photons*.



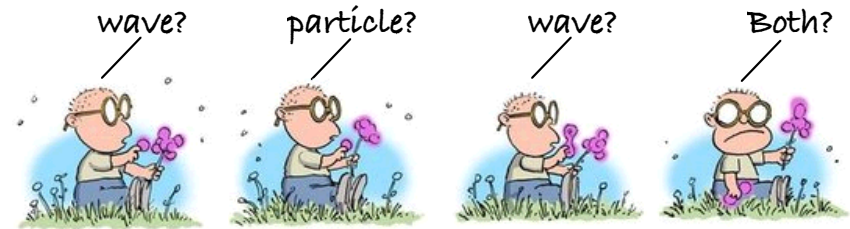


The energy of an individual photon is miniscule, hence the word *quantum* meaning small.

Typically, from a 60W bulb, nearly

200,000,000,000,000,000,000,

i.e., two hundred billion, billion photons are emitted each second!



The dilemma

So, we are forced to accept an uneasy *duality* between wave and particle concepts in explaining the properties of light. Maybe the 1915 Nobel Laureate, William Henry Bragg, had the best solution when he suggested that:

*“Light behaves like waves on Mondays, Wednesdays and Fridays, like particles on Tuesdays, Thursdays and Saturdays, and like nothing at all on Sundays.”*

It was inevitable that someone would ask the question:

*if waves can also be thought of as particles,  
can particles also be thought of as waves?*

*de Broglie's hypothesis (1924)*



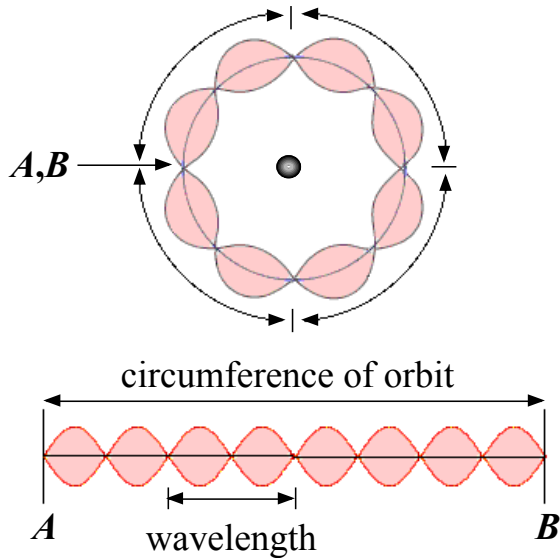
Prince Louis-Victor de  
Broglie  
(1892-1987)  
Nobel Prize in Physics  
(1929)

Louis de Broglie supplied the answer ...  
an emphatic **YES!**

de Broglie was successful almost immediately; he found that particles with finite mass, like electrons, would show wave-like properties with wavelengths directly related to their mass and speed! He called these waves ...

## ***MATTER WAVES.***

His theory had an immediate impact on the structure of atoms. He argued that if an electron in an atom was treated as a wave then the wave had to fit exactly around the nucleus.



When this condition is satisfied, de Broglie said - although he had no proof - a stable orbit is produced so the electrons do not fall to the nucleus. The research formed part of his Ph.D dissertation submitted in 1924 at the University of Paris. Some scholars claim his dissertation is one of the greatest of all time!

- Electron traveling at 1% of the speed of light

Wavelength = 0.00000000024 m.

(0.24 billionths of a meter)

Small but measurable (x-ray). That explains why an electron seems to *act* like a wave.

- Bullet of mass 10g traveling at 2800ft/s

(Typical values for a 0.306 rifle).

Wavelength =

0.000000000000000000000000000000008 m.

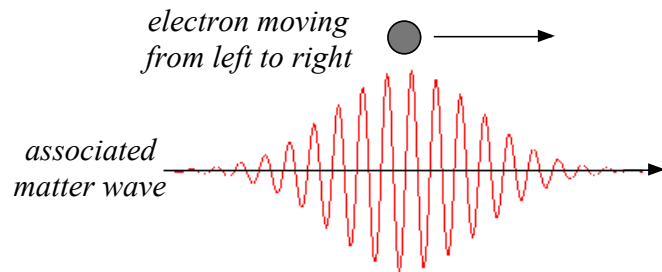
Very small and certainly not measurable. In comparison, the diameter of the nucleus of an atom is

$$\sim 0.0000000000000001 \text{ m},$$

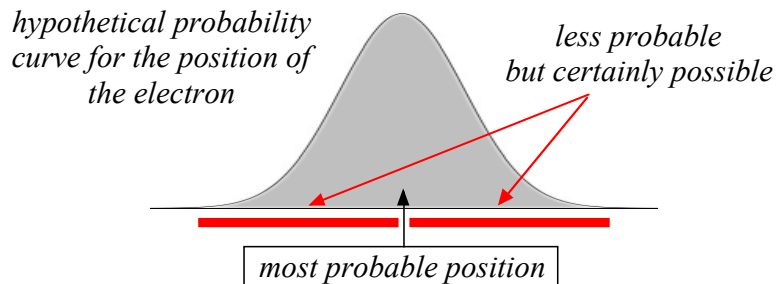
i.e., about 12 billion, billion times larger! That's why a bullet *looks* and *acts* like a particle.



What might a *matter wave* look like? Imagine an electron moving from left to right. We can think of the electron as a *wave packet* ...



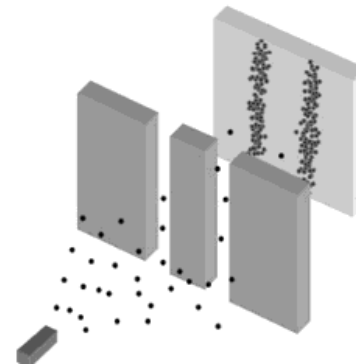
It has a frequency and wavelength just like a wave, but it is localized just like a particle. Classically, we can locate the electron exactly, but if it's a wave, where in the wave is it? The best we can do is to give a probability.



*But are electrons really wave-like?*

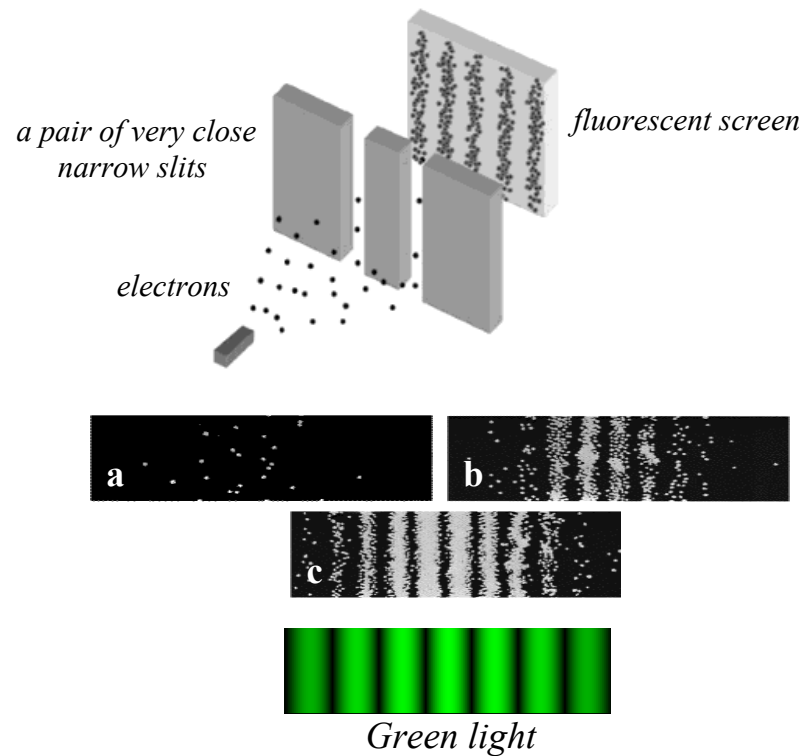
There have been a number of experiments that show that electrons exhibit wave-like properties. Perhaps the most intriguing is the *double-slit experiment*. But, before we go any further, let's ask the question,

*can bullets produce an interference pattern?*



**NO!** ... because their wavelength is so small they act like regular particles.

But with electrons an interference pattern can be seen emerging on a fluorescent screen over time.

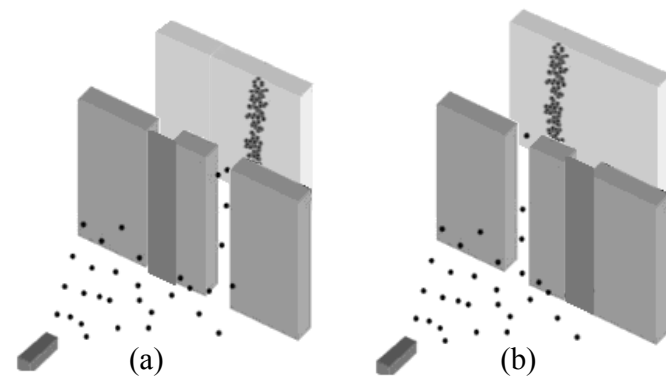


The pattern using electrons looks very similar to those obtained by Young using visible light.

*Proof that electrons can act like waves!*

*Now for some really weird stuff!*

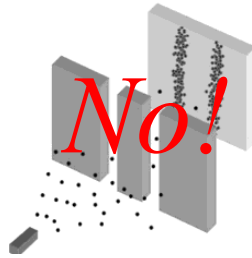
Let's close each slit in turn and accumulate the electrons.



*Clearly, when only one slit is open, an electron can only go through the open slit.*

However, as we have seen, the result with both slits open is not simply a combination of (a) and (b), i.e., two lines, but a multi-line pattern!

Now, let's have both slits open but let only one electron pass at a time. Common sense suggests that each electron must pass through either the left slit or the right slit. So, we imagine that we get just two lines on the screen, one from electrons that passed through the left slit and the other from electrons that passed through the right slit ... *right?*



That is not what we see! So, what does happen? Here's a movie showing how a pattern builds up on a fluorescent screen when electrons are sent through one at a time.



Even though electrons are passed one at a time, an interference pattern emerges!

What does that mean? How does each electron *know* where to go? Can an electron actually pass through both slits at the same time? Does it help us decide if an electron is wave-like or particle-like?

In quantum mechanics objects can have properties that appear to be contradictory, e.g., the wave-like and particle-like properties of an electron. The wave and particle nature of objects can be regarded as *complementary* aspects of a



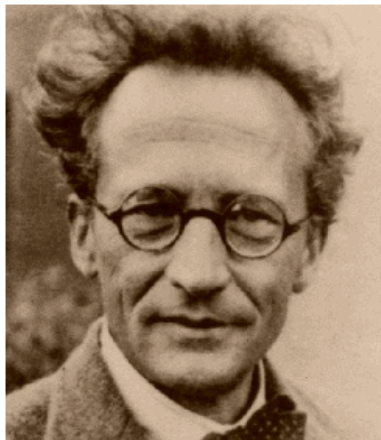
single reality, like the two sides of a coin. An electron can behave sometimes as a wave and sometimes as a particle, but *never both at the same time*, just as a tossed coin may fall *either* heads *or* tails, but never both at the same time!

The complementarity principle is a fundamental concept in quantum mechanics.

In the double-slit experiment, electrons act both as waves and particles. At the slits an electron acts as a wave that passes through both slits\*, which is why we see a multi-line pattern. But, when the electron hits the fluorescent screen it acts like a particle!

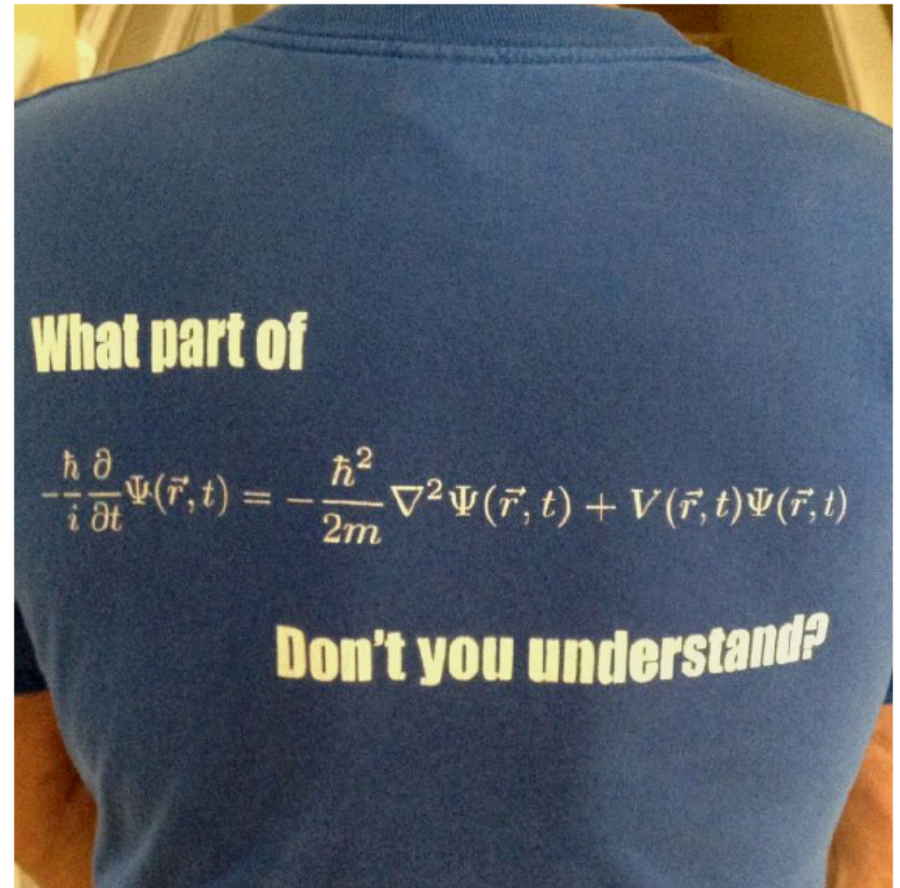
\* That's why the distance between the slits has to be very small.

A method for calculating matter waves and probability curves for electrons in different situations was developed by Erwin Schrödinger in 1921.



Erwin Schrödinger  
1887-1961  
Nobel Prize in  
Physics (1933).

He introduced a “wave equation”, which is now referred to as ***Schrödinger's equation***. His equation has been universally celebrated as one of the most important achievements of the 20th century.



Schrödinger's equation is a favorite 'slogan' on the back of physics student's tee-shirts!

***But ... a word of caution!***

Unlike sound waves or water waves, matter waves are not composed of some material substance. Matter waves are simply measures of probability. So, in principle one cannot be certain what any given particle will do exactly; only betting odds can be given.

Being probabilistic means consecutive measurements of a particular property may produce different results. But, statistically, the outcome of many measurements is predictable.

This limitation represents a breakdown of *determinism in nature*, which Albert Einstein didn't like one bit! It caused him to question the whole concept of quantum mechanics.



In a letter (December 1926) to his friend Max Born arguing against the probabilistic nature of quantum mechanics, he (famously) wrote:

***I, at any rate, am convinced that He [God] does not throw dice.***

On hearing Einstein's argument, Neils Bohr said:

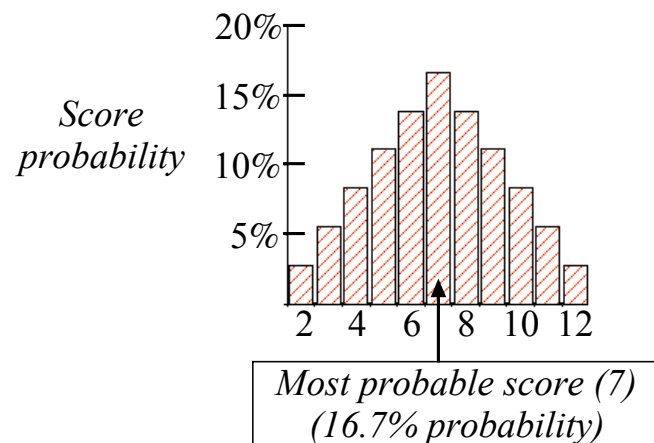
***Einstein, stop telling God what to do!***

As an example, imagine throwing two dice and adding the two scores. If you think of a throw as

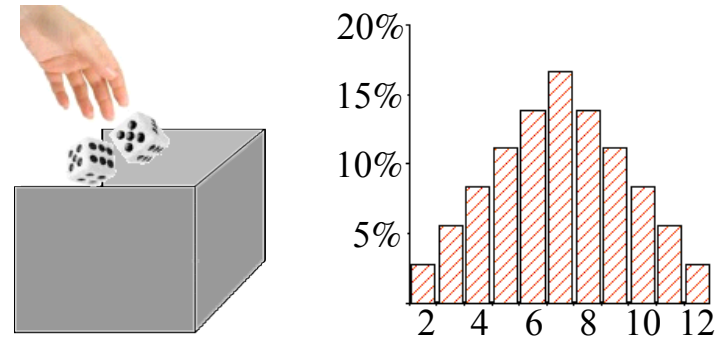


a “measurement”, consecutive scores are uncertain and usually different. But, if the dice are thrown many times, the

overall results are predictable *even though the outcome of an individual throw is not*.



Suppose the two dice are thrown behind a screen so we cannot see the actual score.

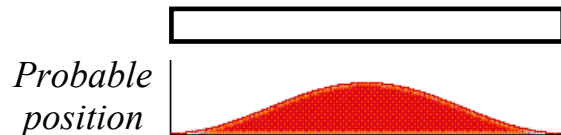


We know what the probability curve looks like, but to find the actual “score”, we have to look behind the screen, i.e., make a *measurement*.

That is what quantum mechanics is all about; we may know what the probability curve looks like, but out of all the possible outcomes, we don’t know which is the actual one, until we make a measurement!

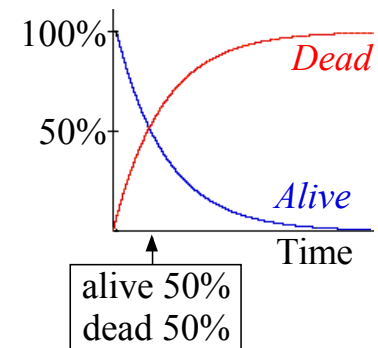


Let's move from dice to the quantum world in a *thought experiment*. We trap an electron in a narrow “tube”. If the electron is free to move back and forth along the tube, the probability curve for the electron's position is a simple curve.



To find its *actual* position we must perform some type of measurement. There is an infinity of positions along the tube but the very act of making the measurement causes the range of possibilities to spontaneously take *one value only*. If we make another measurement we will likely get a different result. *So, the measurement itself determines the outcome.*

This is the **Copenhagen Interpretation**; that all possibilities exist until the measurement is made. The very act of making the measurement collapses all possibilities to a unique answer. But Schrödinger warned against taking that interpretation too literally with his “cat in the box” paradox.



According to the Copenhagen Interpretation the cat could be 50% alive and 50% dead at the same time! Clearly, that cannot be the case.



The probabilistic nature of quantum mechanics also places a fundamental limit on the precision with which certain pairs of physical properties can be simultaneously known. As a consequence, it is not possible to know the value of all the properties of the system at the same time. There is a trade-off; the more precisely one property is measured, the less precisely the other can be controlled, determined, or known.

This is ***Heisenberg's uncertainty principle***.

One such pair is position and speed; the more certain we are of the position of an electron, the less certain we are of its speed.

For everyday (massive) objects like baseballs, the uncertainty is negligibly small. However, on the quantum scale, e.g., electrons, the uncertainties can have significant consequences.

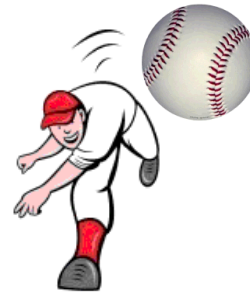


*Why is that?*

Consider the following two simple scenarios ...

As an example, in major league games, a radar gun is used to measure the speed of a pitch but it has a negligible effect on the direction or speed of the ball.

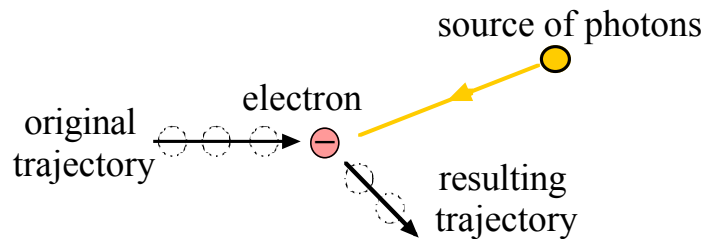
*Actual case ...*



If this is the uncertainty in speed, the uncertainty principle tells us that the minimum uncertainty in position is

$0 \cdot 00000000000000000000000000000004$  m,  
which is billions and billions of times smaller  
than the size of an atom ( $\sim 0\cdot0000000006$  m)!  
Well, you can't measure that, especially for a  
moving baseball! So, as a batter, you'll never  
notice the uncertainty in position.

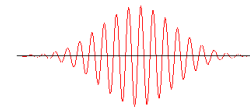
But, in the quantum world that is not the case. When a high energy photon bounces off an isolated atom or electron, it causes them to change direction and speed.



This makes it impossible to measure precisely the position and speed at the same time *as they have been affected by the measurement itself*. All we can do is measure position and speed within a certain range of *uncertainty*.

### *Actual case ...*

What's the uncertainty in position for an electron traveling at 1% of the speed of light?



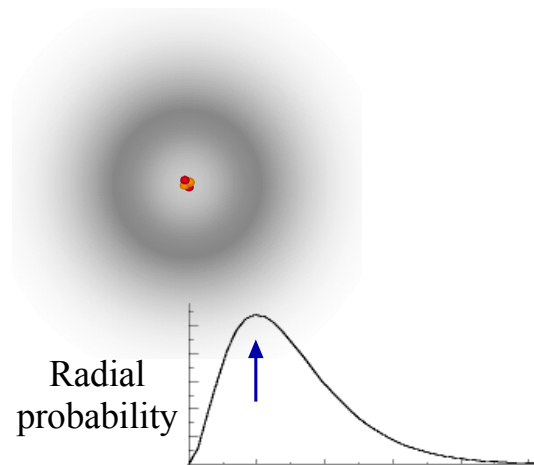
Let's assume we can measure the speed of the electron with the same uncertainty as the baseball, i.e., 0.3%. Then, the uncertainty principle tells us that the minimum uncertainty in position is

0.000000006 m,

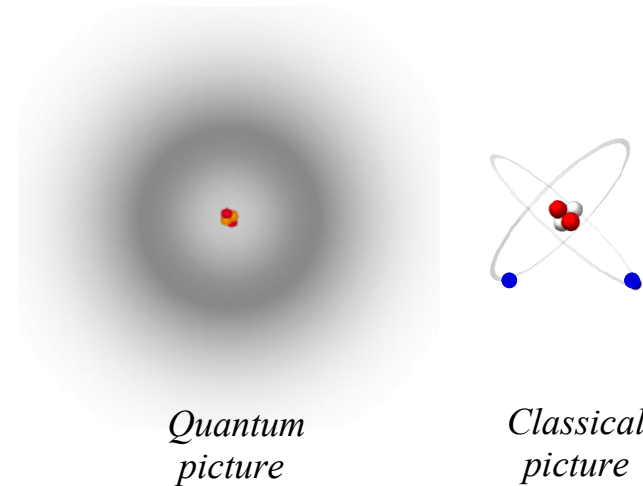
which is about 10 times the size of an atom.

Since the uncertainty is bigger than the size of an atom, we cannot tell precisely where in an atom such an electron is located!

So, where are the electrons located in an atom?  
We can use Schrödinger's equation to help us discover the *probability of where they are located*. We find the electrons form a “fuzzy cloud” around the nucleus.



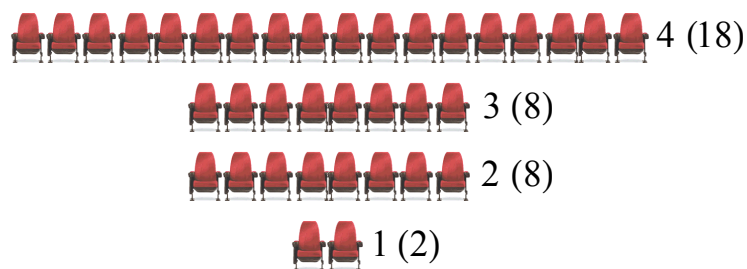
The density of the fuzzy cloud, represents an indication of the probability of where electrons are located; the darker regions indicate greater probability.



The quantum picture of an atom is completely different compared with the classical picture, prior to the advent of quantum mechanics.

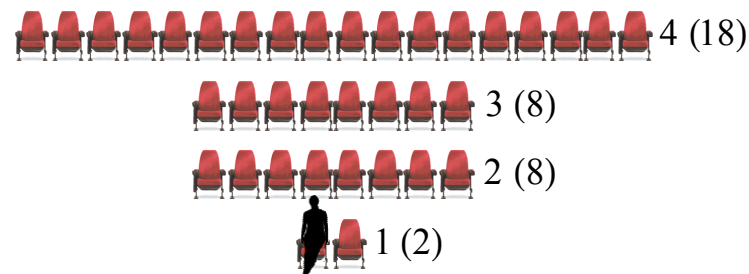
*What else does Schrödinger's Equation  
tell us about atoms?*

It helps us understand the Periodic Table!

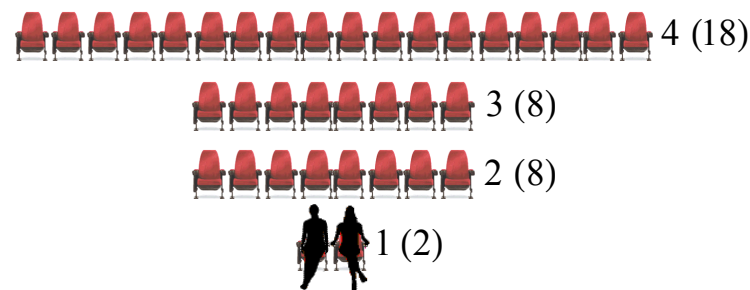


An “empty atom” is like an empty auditorium with rows (called “*shells*”) and seats (called “*states*”) where electrons can reside. However, there is a fixed number of seats in each row, i.e., 2 in row 1, 8 in row 2, etc.

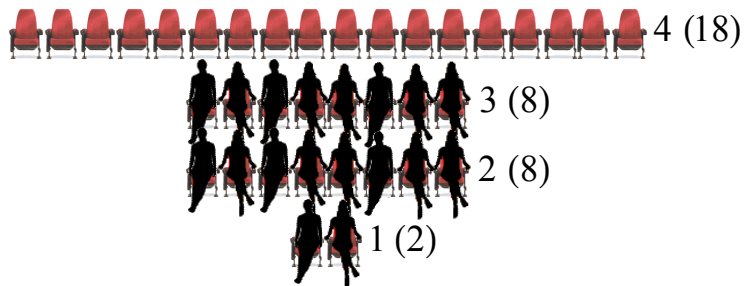
Now let us gradually fill the auditorium (*atom*) with people (*electrons*).



This represents an atom of hydrogen (1 electron).



This is the next element, helium (2 electrons).



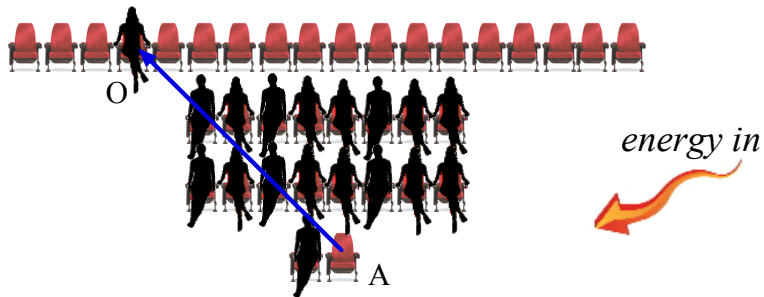
Now put 18 people (*electrons*) in the auditorium (*atom*). Note that no two people (*electrons*) can occupy the same seat (*state*)! So, when one row is filled, a new row is started. This is a fundamental property of quantum mechanics, i.e., no two electrons in an atom can exist in the same state. It is called the *Pauli exclusion principle*.

This picture represents an atom of the element argon (18 electrons).

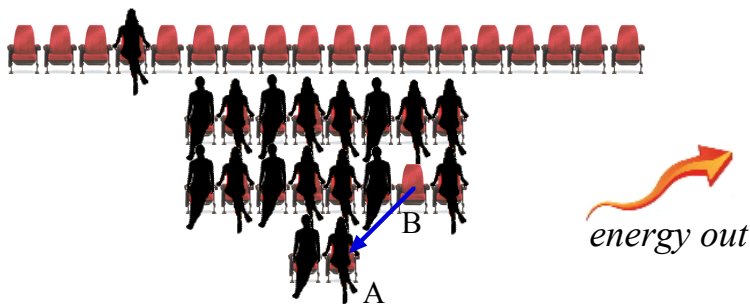
In this way, Schrödinger was able to build and explain the arrangement of chemical elements in the Periodic Table.

The Periodic Table of the Elements																		He																	
1 H Hydrogen 1.01																		2 He Helium 4.00																	
3 Li Lithium 6.94		4 Be Beryllium 9.01														5 B Boron 10.81		6 C Carbon 12.01		7 N Nitrogen 14.01		8 O Oxygen 16.00		9 F Fluorine 18.99		10 Ne Neon 20.18									
11 Na Sodium 22.99		12 Mg Magnesium 24.31														13 Al Aluminum 26.98		14 Si Silicon 28.09		15 P Phosphorus 30.97		16 S Sulfur 32.07		17 Cl Chlorine 35.45		18 Ar Argon 39.95									
19 K Potassium 39.10		20 Ca Calcium 40.08		21 Sc Scandium 44.96		22 Ti Titanium 47.87		23 V Vanadium 50.94		24 Cr Chromium 52.00		25 Mn Manganese 54.94		26 Fe Iron 55.85		27 Co Cobalt 58.93		28 Ni Nickel 58.69		29 Cu Copper 63.55		30 Zn Zinc 65.39		31 Ga Gallium 69.72		32 Ge Germanium 72.61		33 As Arsenic 74.92		34 Se Selenium 78.96		35 Br Bromine 79.90		36 Kr Krypton 83.80	
37 Rb Rubidium 85.47		38 Sr Strontium 87.62		39 Y Yttrium 88.91		40 Zr Zirconium 91.22		41 Nb Niobium 92.91		42 Mo Molybdenum 95.94		43 Tc Technetium 98.91		44 Ru Ruthenium 101.07		45 Rh Rhodium 102.91		46 Pd Palladium 106.42		47 Ag Silver 107.87		48 Cd Cadmium 112.41		49 In Indium 114.82		50 Sn Tin 118.71		51 Sb Antimony 121.76		52 Te Tellurium 127.60		53 I Iodine 126.91		54 Xe Xenon 131.29	
55 Cs Cesium 132.91		56 Ba Barium 137.33		57 La Lanthanum 138.91		58 Ce Cerium 140.12		59 Pr Praseodymium 140.91		60 Nd Neodymium 144.24		61 Pm Promethium 144.91		62 Sm Samarium 150.36		63 Eu Europium 151.96		64 Gd Gadolinium 157.25		65 Tb Terbium 158.93		66 Dy Dysprosium 162.50		67 Ho Holmium 164.93		68 Er Erbium 167.26		69 Tm Thulium 168.93		70 Yb Ytterbium 173.04		71 Lu Lutetium 174.97			
87 Fr Francium 223.02		88 Ra Radium 226.03		89 Ac Actinium 227.03		90 Th Thorium 232.04		91 Pa Protactinium 231.04		92 U Uranium 238.03		93 Np Neptunium 237.05		94 Pu Plutonium 244.06		95 Am Americium 243.06		96 Cm Curium 247.07		97 Bk Berkelium 247.07		98 Cf Californium 251.08		99 Es Einsteinium 252.08		100 Fm Fermium 257.10		101 Md Mendelevium 258.10		102 No Nobelium 259.10		103 Lr Lawrencium 260.10			

Because of its widespread applicability in both physics and chemistry, Schrödinger's equation created a revolution in the physical sciences.

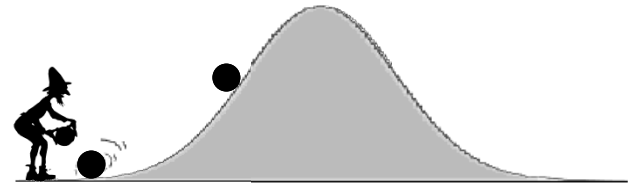


Like people, an electron can move to an empty seat (*state*). To make the move from  $1A \rightarrow 4O$  requires that energy be put *into* the atom.



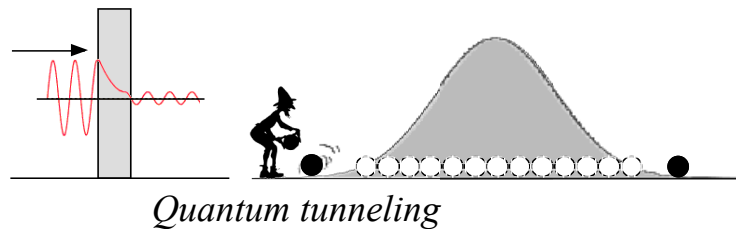
Now seat (*state*) 1A is vacant, it can be filled by one of the other people (*electrons*), e.g.,  $2B \rightarrow 1A$ . In this case, the atom *gives out* energy, such as light, or an x-ray.

*More weird stuff ...*



If you want to roll a ball over a hill, the ball must have enough energy to get to the top. If it doesn't have enough energy, it will roll back before getting to the top, so it cannot reach the other side. If we think of the hill as a *barrier*, then the ball can only reach the other side if it has enough energy to overcome the barrier.

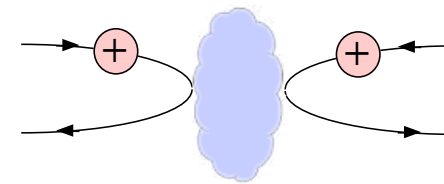
But, in a quantum system that is not necessarily the case!



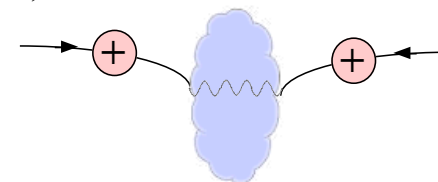
Electrons can overcome a barrier and reach the other side even though they have less energy than the height of the barrier! The process is called *quantum tunneling* and, depending on the energy of the electron, it can occur through barriers up to a few atoms thick (a few billionths of a meter).

Although a quantum phenomenon, it has a number of important macroscopic physical applications, e.g., it is fundamental to the operation of certain semiconductor devices such as tunnel diodes and tunnel junctions.

A nuclear fusion reaction that takes place in the Sun is the combining of two protons to form deuterium. The protons must get very close to each other for the reaction to occur.



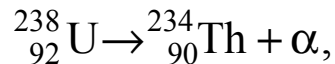
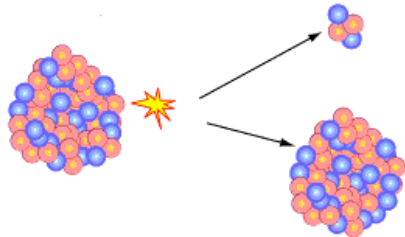
Protons strongly repel each other and the interior temperature of the Sun (about 15 million °C) does not provide enough energy to overcome the repulsion barrier between them (about 16 billion °C is required).



In order for the fusion reaction to take place, the protons “tunnel” through the repulsion barrier.



Another example of quantum tunneling is radioactive decay. In the decay of uranium,



alpha-particles ( $\alpha$ ) do not have enough energy to simply “jump” out of the uranium nucleus. They have to overcome a barrier, so, they must *tunnel out* from the nucleus!

Radioactive nuclei have half-lives that vary from fractions of a second to billions of years. The half-life is a measure of the probability (i.e., the difficulty) of tunneling.

So, to answer the original question,

*Why do we need quantum mechanics?*

*I offer the following answers.*

Newton’s equations and Einstein’s relativity explain the properties of macroscopic objects. But quantum mechanics is essential for understanding and quantifying ...

- the growth and properties of the universe after the Big Bang,
- the structure and properties of atoms,
- the microscopic and macroscopic properties of solids such as metals and semiconductors,
- the arrangement and properties of atoms at surfaces,
- the structure and stability of molecules,
- ...

*And some final words ...*

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**EINSTEIN ATTACKS  
QUANTUM THEORY**

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**New York Times**  
May 4, 1935.

*I think I can safely say that nobody  
understands quantum mechanics.*

Richard Feynman,  
The Character of Physical Law (1965).

*Quantum mechanics makes absolutely no  
sense.*

Sir Roger Penrose, FRS.

*Very interesting theory - it makes no sense  
at all.*

Groucho Marx.