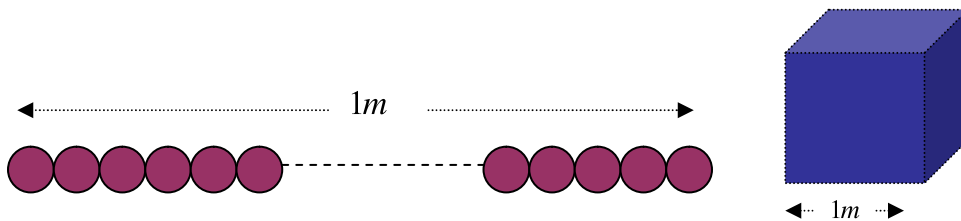


INTRODUCTION TO ATOMIC PHYSICS

1. • About 2500 years ago, the ancient Greek philosopher Democritus asked the question: what is the world made of? He conjectured that it is mostly empty, and that the remainder is made of tiny "atoms". By definition these atoms are indivisible.
 - Then 300 years ago, it was noted by the French chemist Lavoisier that in all chemical reactions the total mass of reactants before and after a chemical reaction is the same. He demonstrated that burning wood caused no change in mass. This is the Law of Conservation of Matter.
 - A major increase in understanding came with Dalton (1803) who showed that:
 - 1) Atoms are building blocks of the elements.
 - 2) All atoms of the same element have the same mass.
 - 3) Atoms of different elements are different.
 - 4) Two or more different atoms bond in simple ratios to form compounds.

2. Avogadro made the following hypothesis : "Equal volumes of all gases, under the same conditions of temperature and pressure, contain equal numbers of molecules". Why? Because we know that pressure is caused by molecules hitting the sides of the containing vessel. If the temperature of two gases is the same, then their molecules move with the same speeds, and so Avogadro's hypothesis follows for ideal gases. The famous number $N_0 = 6.023 \times 10^{26}$ per kilogram-mole is called Avogadro's Number.

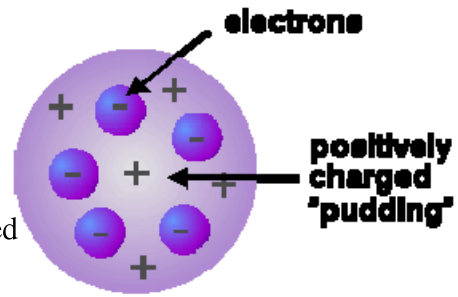
3. Let's get an idea of the size of atoms. Amazingly, we do not need high-powered particle accelerators to do so. Consider a cube of $1m \times 1m \times 1m$. If the radius of an atom is r , then we have $(1/2r)^3$ atoms in the cube. Now in 1kg.atom we have $N_0 = 6 \times 10^{26}$ atoms and each atom occupies a volume $(A/\rho) m^3$, where A = atomic weight and ρ = density.



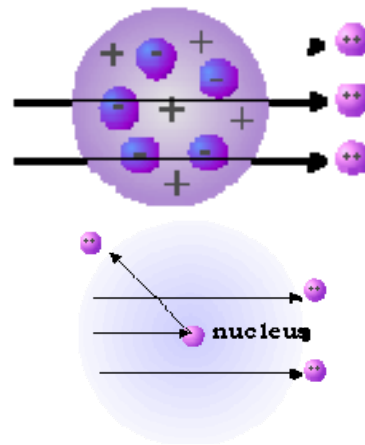
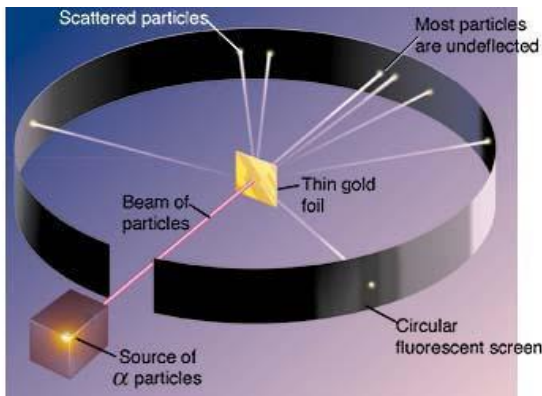
Hence $N_0 = (1/2r)^3 \times A/\rho$. This give $r = \frac{1}{2} \left(\frac{A}{\rho N_0} \right)^{1/3}$. Putting in some typical densities,

we find that $r_{Ag} \approx r_{Be} \approx 10^{-10} m$. This shows that atoms are mostly of the same size. This is quite amazing because one expects a Be atom to be much smaller than an Ag atom.

4. Even if you know how big an atom is, this does not mean that its internal structure is known. In 1895 J.J. Thomson proposed the "plum pudding" model of an atom. Here the atom is considered as made of a positively charged material with the negatively charged electrons scattered through it.

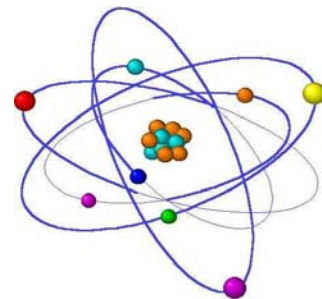


5. But the plum-pudding model was wrong. In 1911, Rutherford carried out his famous experiment that showed the existence of a small but very heavy core of the atom. He arranged for a beam of α particles to strike gold atoms in a thin foil of gold.



If the positive and negative charges in the atom were randomly distributed, all α 's would go through without any deflection. But a lot of backscattering was seen, and some α 's were even deflected back in the direction of the incident beam. This was possible only if they were colliding with a very heavy object inside the atom. Rutherford had discovered the atomic nucleus.

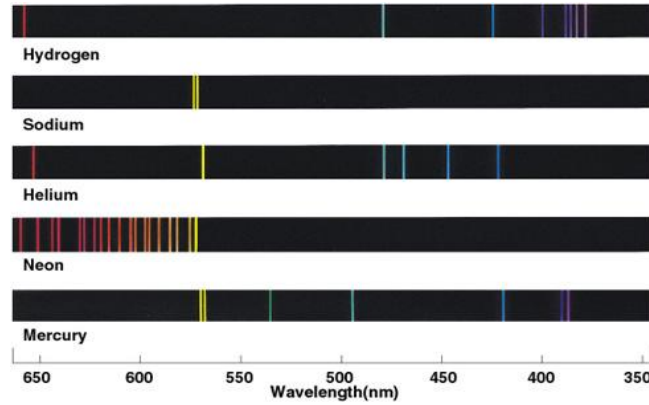
6. The picture that emerged after Rutherford's discovery was like that of the solar system - the atom was now thought of as mostly empty space with a small, positive nucleus that contained protons. Negative electrons moved around the outside in orbits that resembled those of planets, attracted towards the centre by a coulomb force.



7. This sounds fine, but there is a serious problem: we know that a charge that accelerates radiates energy. In fact the power radiated is $P \propto e^2 a^2$, where e is the charge and a is the acceleration. Now, a particle moving in a circular orbit has an acceleration even if it is moving at constant speed because it is changing its direction all the time. So this means

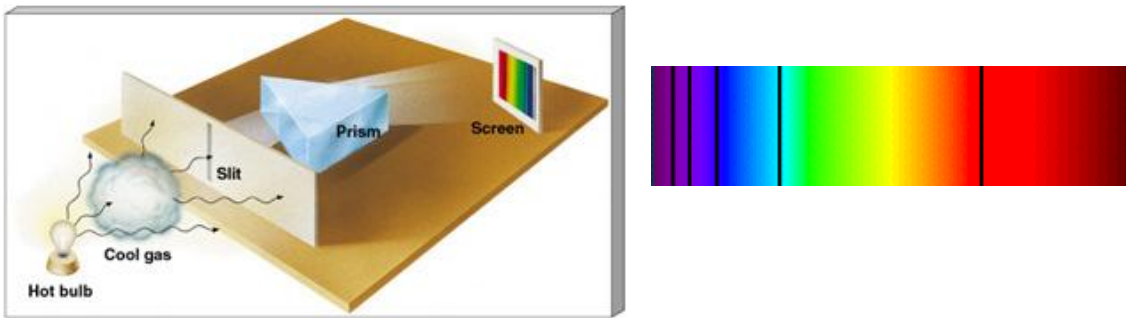
that the electron will be constantly radiating power and thus will slow down, collapsing eventually into the nucleus.

8. This is not the only thing wrong with the solar system model. If you look at the light emitted by any atom, you do not see a continuous distribution of colours (frequencies). Instead, a spectroscope will easily show that light is emitted at only certain discrete frequencies.

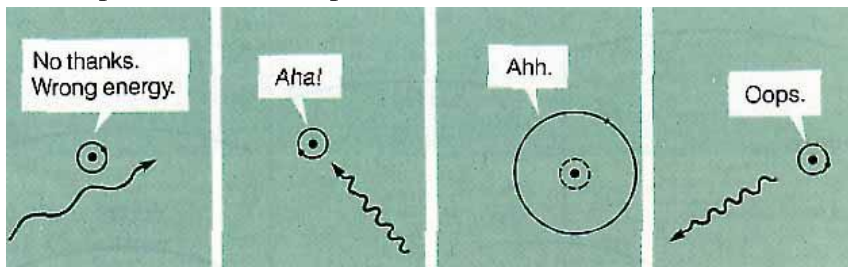


In the above you see the emission spectrum of different atoms.

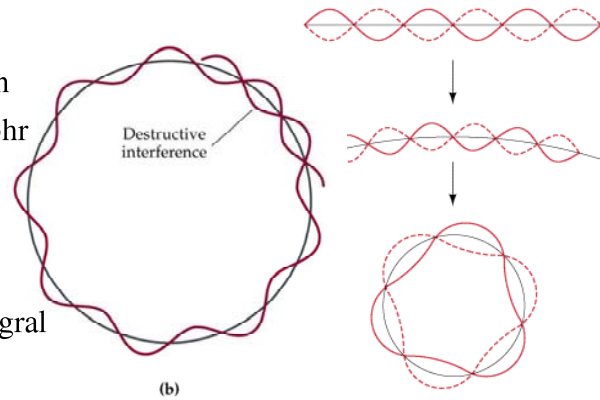
9. Similarly, if white light is passed through a gas of atoms of a certain type, only certain colours are absorbed, and the others pass through without a hindrance.



The above shows the absorption spectrum of a certain atom. The wavelengths for both emission and absorption lines are exactly equal. Classical physics and the Rutherford model have no explanation for the spectrum.



10. Then came Niels Bohr. By this time it was known that electrons had a dual character as waves (De Broglie relation and Davisson-Germer experiment). Bohr said: suppose I bend a standing wave into a circle. If the wavelength is not exactly correct, wave interference will make the wave disappear. So only integral numbers of wavelengths can interfere constructively.

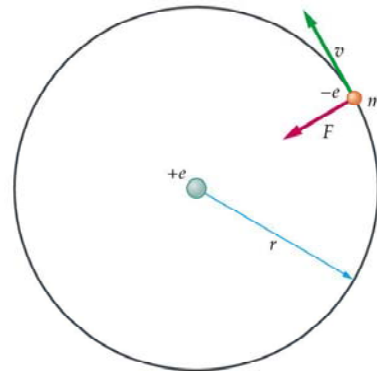


11. Let us pursue this idea further. The electron has a wavelength and forms standing waves in its orbit around the nucleus. An integral number of electron wavelengths must fit into the circumference of the circular orbit. Hence $n\lambda = 2\pi r$ with $n = 1, 2, 3 \dots$. The momentum is $p = mv = \frac{h}{\lambda} = \frac{h}{(2\pi r/n)} = \frac{n\hbar}{r}$. The angular momentum $L = rmv = n\hbar$ is therefore quantized in units of \hbar .

12. Now let us suppose that the electron moves in an orbit of radius r when it has $L_n = n\hbar$. Equilibrium demands that the centrifugal force be equal to the

coulomb attraction: $\frac{mv_n^2}{r} = k \frac{e^2}{r^2}$. From $v_n = \frac{n\hbar}{mr_n}$

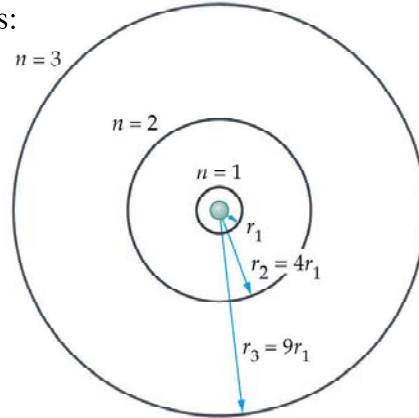
we find that the radius $r_n = \left(\frac{\hbar^2}{mke^2} \right) n^2$.



- For $n = 1$ the electron orbit which is closest to the nucleus, $r_n = a_0 \equiv 0.53 \times 10^{-8} \text{ cm}$ (this is called the Bohr radius).
- For higher n , $r_n = a_0 n^2$. The atom becomes huge for $n \approx 100$, the so-called Rydberg atom. Such atoms are of experimental interest these days.
- Note that the speed of the electron is smaller in orbits farther from the nucleus, $v_n = \frac{ke^2}{n\hbar}$. As n becomes very large, the electron is very far out and very slow.
- In the above $n = 0$ is strictly not allowed. As you can see, none of the formulae make any sense for this case. The minimum angular momentum that the electron can have is \hbar . (In proper quantum mechanics the minimum is $0\hbar$ and this is a big difference with the Bohr model of the atom).

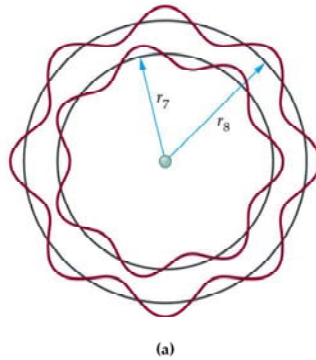
13. We can compute the energies of the various orbits:

$$\begin{aligned}
 E &= K + U = \frac{1}{2}mv^2 + U \\
 &= \frac{1}{2}\left(\frac{ke^2}{r}\right) - \frac{ke^2}{r} = -\frac{ke^2}{2r} \\
 \text{Hence, } E_n &= -\left(\frac{ke^2}{2}\right)\left(\frac{mke^2}{\hbar^2}\right)\frac{1}{n^2} \\
 &= -\left(\frac{mk^2e^4}{2\hbar^2}\right)\frac{1}{n^2} = -\frac{13.6 \text{ eV}}{n^2}
 \end{aligned}$$



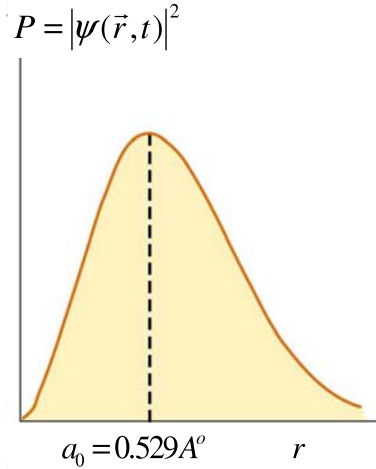
14. In the Bohr model, electrons can jump between different orbits due to the absorption or emission of photons. Dark lines in the absorption spectra are due to photons being absorbed, and bright lines in the emission spectra are due to photons being emitted. The energy of the emitted or absorbed photon is equal to the difference of the initial and final energy levels, $h\nu = E_f - E_i$. The picture below shows the electron in the $n = 7$ and $n = 8$ levels. The photon emitted has $h\nu = E_8 - E_7 = -13.6\left(\frac{1}{8^2} - \frac{1}{7^2}\right) \text{ eV}$.

$$h\nu = E_8 - E_7 = -13.6\left(\frac{1}{8^2} - \frac{1}{7^2}\right) \text{ eV}$$



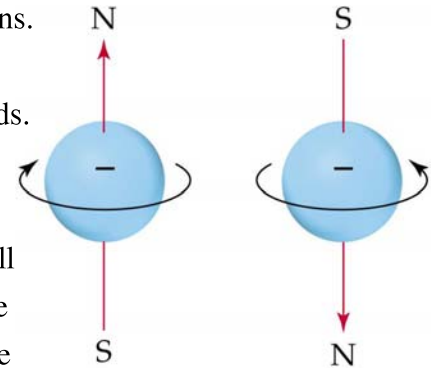
15. The Bohr model gave wonderful results when compared against the hydrogen spectrum. It was the among the first indications that some "new physics" was needed at the atomic level. But this model is not to be taken too seriously - it fails to explain many atomic properties, and fails to explain why the H atom can exist even when the electron has no orbital angular momentum (and hence no centrifugal force to balance against the Coulomb attraction). It cannot predict all the lines observed for H, much less for multi-electron atoms such as Oxygen. The real value of this model was that it showed the way forward towards developing quantum mechanics, which is the true physics of the world, both microscopic and macroscopic. I have discussed some elements of QM in the last lecture, in particular the wavefunction $\psi(\vec{r}, t)$ of the electron.

16. Quantum mechanics gives a picture that is quite different from the solar-system model. We solve the "Schrodinger Equation" to find the wavefunction $\psi(\vec{r},t)$, whose square gives the probability of finding the electron at the point \vec{r} . In the lowest energy state, the electron can be viewed as a spherical cloud surrounding the nucleus. The densest regions of the cloud represent the highest probability for finding the electron.



- The principal quantum number $n = 1, 2, 3 \dots$ determines the allowed energy levels. An electron can only have energy $E_n = -\frac{13.6}{n^2}$ eV. Miraculously this is the same result as in the Bohr model.
- The orbital angular momentum is determined by the number l , and $L = \sqrt{l(l+1)}\hbar$. Allowed values of l are, $l = 0, 1, 2, 3 \dots, n-1$.
- The magnetic quantum number m_l determines the projection (or component) of the vector angular momentum \vec{L} on to any fixed axis, $L_z = m_l \hbar$. Allowed values are, $m_l = -l, \dots, -2, -1, 0, 1, 2, \dots, l$.

17. Electrons can be thought of as little spinning balls of charge. All electrons spin at the same speed (more accurately, their spin angular momentum is the same and equals $\hbar/2$). An electron can spin in only one of two possible directions. When charges move around in a circle, that constitutes a current. As you know, currents give rise to magnetic fields. This is why electrons are also little magnets that interact with other magnets. Now go back to the Stern-Gerlach experiment described in the previous lecture, and you will understand better why the electrons were deflected by the applied magnetic field. Now that we have learned that the electron has spin, we can describe the two spin states by giving the "magnetic" quantum number m_s where $m_s = -\frac{1}{2}, \frac{1}{2}$. These two states have the same energy except when there is some magnetic field present.



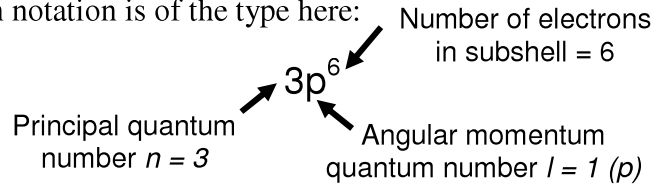
18. States (or orbitals) having $l = 0, 1, 2, \dots$ are called s,p,d, \dots . The s-states are spherical. As n increases, the s-orbitals get larger and the wavefunction is larger away from the nucleus.

19. In the world we are used to, we can always tell apart identical particles (same mass, charge, spin,...) by simply watching them. But in QM, their identities can get confused and identical particles are indistinguishable. Suppose that A and B are particles that are identical in every possible way, and we exchange them. Of course, the probability of finding one or the other must remain unchanged. In other words, $|\Psi(1,2)|^2 = |\Psi(2,1)|^2$, where 1 and 2 denote the positions of the first and second particles. But something very interesting happens now because either one of two possibilities can be true: $\Psi(1,2) = +\Psi(2,1)$ or $\Psi(1,2) = -\Psi(2,1)$. Particles obeying the first are called *bosons*, while those obeying the second are called *fermions*. What if we bring two fermions to same point in space? Then: $\Psi(1,1) = -\Psi(1,1)$. This means that $\Psi(1,1) = 0$! In other words, two identical fermions will never be at the same point or in the same quantum state. This is the famous Pauli Exclusion Principle.

20. Let us apply the Pauli Exclusion Principle to the multi-electron atom where each electron has the quantum numbers $\{n, l, m_l, m_s\}$. Only one electron at a time may have a particular set of quantum numbers. Now for some definitions:

- Shell - electrons with the same value of n
- Subshell - electrons with the same values of n and l
- Orbital - electrons with the same values of n , l , and m_l

Once a particular state is occupied, other electrons are excluded from that state. The electron configuration is how the electrons are distributed among the various atomic orbitals in an atom. A common notation is of the type here:



21. Building the shell structure of multi-electron atoms through $n = 4$ using the Pauli Principle.

n	Possible Values of l	Subshell Designation	Possible Values of m_l	Number of Orbitals in Subshell	Total Number of Orbitals in Shell
1	0	1s	0	1	1
2	0	2s	0	1	4
	1	2p	1, 0, -1	3	
3	0	3s	0	1	9
	1	3p	1, 0, -1	3	
	2	3d	2, 1, 0, -1, -2	5	
4	0	4s	0	1	16
	1	4p	1, 0, -1	3	
	2	4d	2, 1, 0, -1, -2	5	
	3	4f	3, 2, 1, 0, -1, -2, -3	7	

QUESTIONS AND EXERCISES

Q.1 Using Avogadro's number, find the number of molecules in:

- a) 1 gram of oxygen ($A = 16$).
- b) 1 gram of lead ($A = 208$).

Q.2 What would the value of the principal quantum number n have to be for a hydrogen atom to be 1 cm in radius? Why do we never see atoms this big, even though the formula for radius allows it?

Q.3 The energy levels of the H atom are given by $-\frac{13.6}{n^2} eV$. Why the minus sign? This is actually an important point and you should go back to the lecture on electric potential to see why this is so.

Q.4 Using the table provided in point 21 above, find the allowed electron configurations for the following atoms: Li, Be, C, N, O.

Q.5 Plot the function $P(r) = r^2 e^{-r^2/a_0^2}$ against ρ , where ρ is the distance measured in units of a_0 , $\rho = r/a_0$. Answer the following questions:

a) At what value of r does $P(r)$ have a maximum?

b) If we define the average value of r as $\langle r \rangle = \frac{\int_0^\infty dr r P(r)}{\int_0^\infty dr P(r)}$, evaluate $\langle r \rangle$. Why is it sensible to call this an average value?

Q.6 The diagram on the right shows transitions between different levels of a hydrogen atom.

- a) What is the minimum energy required to excite the atom?
- b) What is the minimum energy required to knock an electron completely out?
- c) If more energy was supplied than in the part b above, what would happen?
- d) How would your answer to a and b above change if we considered a helium ion instead (2 protons instead of one)?

