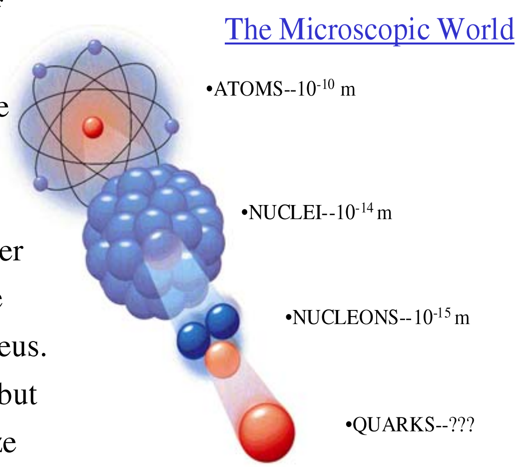
QUANTUM MECHANICS

1. The word "quantum" means packet or bundle. We have already encountered the quantum of light - called photon - in an earlier lecture. Quanta (plural of quantum) are discrete steps. Walking up a flight of stairs, you can increase your height one step at a time and not, for example, by 0.371 steps. In other words your height above ground (and potential energy can take discrete values only).

2. Quantum Mechanics is the true physics of the microscopic world. To get an idea of the sizes in that world, let us start from the atom which is normally considered to be a very small object. But, as you can see, the atomic nucleus is 100,000 times smaller than the atom. The neutron and proton are yet another 10 times smaller than the nucleus. We know that nuclei are made of quarks, but as yet we do know if the quarks have a size or if they are just point-like particles.



3. It is impossible to cover quantum mechanics in a few lectures, much less in this single lecture. But here are some main ideas:
   a) Classical (Newtonian) Mechanics is extremely good for dealing with large objects (a grain of salt is to be considered large). But on the atomic level, it fails.The reason for failure is the uncertainty principle - the position and momenta of a particle cannot be determined simultaneously (this is just one example; the uncertainty principle is actually more general). Quantum Mechanics properly describes the microscopic - as well as macroscopic - world and has always been found to hold if applied correctly.
   b) Atoms or molecules can only exist in certain energy states. These are also called "allowed levels" or quantum states. Each state is described by certain "quantum numbers" that give information about that state's energy, momentum, etc.
   c) Atoms or molecules emit or absorb energy when they change their energy state. The amount of energy released or absorbed equals the difference of energies between the two quantum states.
   d) Quantum Mechanics always deals with probabilities. So, for example, in considering the outcome of two particles colliding with each other, we calculate probabilities to scatter in a certain direction, etc.

4. What brought about the Quantum Revolution? By the end of the 19th century a number of serious discrepancies had been found between experimental results and classical theory. The most serious ones were:

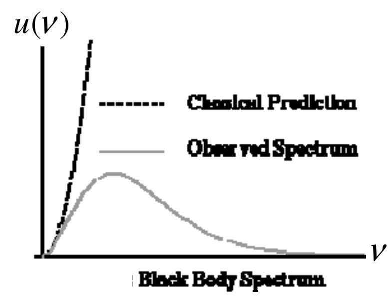
A) The blackbody radiation law

B) The photo-electric effect

C) The stability of the atom, and puzzles of atomic spectra

In the following, we shall briefly consider these discrepancies and the manner in which quantum mechanics resolved them.

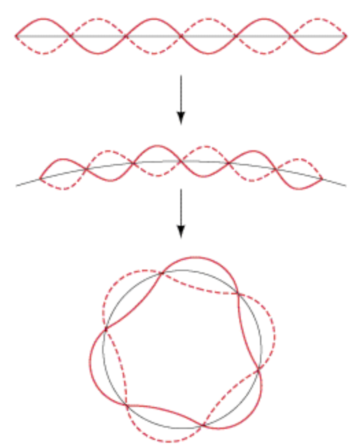
A)Classical physics gives the wrong behaviour for radiation emitted from a hot body. Although in this lecture it is not possible to do the classical calculation, it is not difficult to show that the electromagnetic energy $u(\nu)$ radiated at frequency ν increases as ν^3 (see graph). So the energy radiated over all frequencies is infinite. This is clearly wrong. The correct calculation was done by Max Planck.



Planck's result is shown above, and it leads to the sensible result that $u(\nu)$ goes to zero at large ν. He assumed that radiation of a given frequency ν could only be emitted and absorbed in quanta of energy $\varepsilon = h\nu$. If the electromagnetic field is thought of as harmonic oscillators, Planck assumed that the total energy of this large number of oscillators is made of finite energy elements $h\nu$. With this assumption, he came up with a formula that fitted well with the data. But he called his theory "an act of desperation" because he did not understand the deeper reasons.

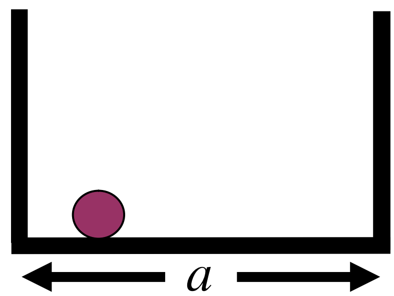
B) I have already discussed the photoelectric effect in the previous lecture. Briefly, Einstein (1905) postulated a quantum of light called photon, which had particle properties like energy and momentum. The photon is responsible for knocking electrons out of the metal - but only if it has enough energy.

C) Classical physics cannot explain the fact that atoms are stable. An accelerating charge always radiates energy if classical electromagnetism is correct. So why does the hydrogen atom not collapse? In 1921 Niels Bohr, a great Danish physicist, made the following hypothesis: if an electron moves around a nucleus so that its angular momentum is $\hbar, 2\hbar, 3\hbar, \cdots$ then it will not radiate energy. In the next lecture we explore the consequences of this hypothesis. Bohr's hypothesis called for the quantization

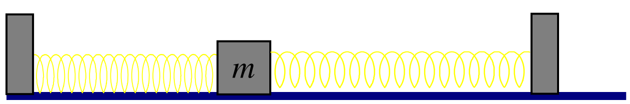


of angular momentum. If the electron is regarded as a De Broglie wave, then there must be an integer number of waves that go around the centre. Of course, this is not proper quantum mechanics and cannot be taken too seriously, but it definitely was a major step in the ultimate development of the subject. Even if one's understanding was imperfect, it was now possible to understand why atoms had certain energies only, and why the light radiated by atoms was of discrete frequencies only. In contrast, classical physics predicted that atoms could radiate at any frequency.

5. One consequence of quantum mechanics is that it explains through the uncertainty principle the stability of the atom. But before talking of that, let us consider a particle moving between two walls. Each time it hits a wall, a force pushes it in the opposite direction. There is no friction, so classically the particle just keeps moving forever between the two potential walls. In QM the uncertainty of the particle's position is $\Delta x = a$ and so, from $\Delta x \Delta p \geq \hbar/2$, we have $\Delta p\, a \approx \frac{\hbar}{2}$. From this we learn that the kinetic energy $\frac{(\Delta p)^2}{2m} \approx \frac{\hbar^2}{8ma^2}$. This is telling us that as we squeeze the particle into a tighter and tighter space, the kinetic energy goes up and up!



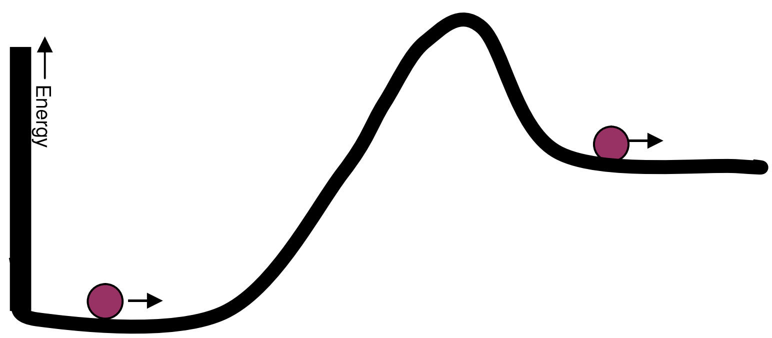
6. The story repeats for a harmonic oscillator. So imagine that a mass moves in a potential of the type shown below, and that its frequency of oscillation is ω. Classically, the lowest energy would be that in which the mass is at rest (no kinetic energy) and it is at the position where the potential is minimum. But this means that the body has both a



well-defined momentum and position. This is forbidden by the Heisenberg uncertainty principle. A proper quantum mechanical calculation shows that the minimum energy is actually $\frac{1}{2}\hbar\omega$. This is called the zero-point energy and comes about because it is not possible for the mass to be a rest. The oscillator's other energy states have energies $\frac{1}{2}\hbar\omega, \frac{3}{2}\hbar\omega, \frac{5}{2}\hbar\omega, \frac{7}{2}\hbar\omega, \cdots$ We say that the energies are quantized. This is completely impossible to understand from classical mechanics where we know that we can excite an oscillator to have any energy we want. Quantized energy levels are indeed what we observe in so many physical systems: atoms, rotating or vibrating molecules, nuclei, etc.

7. We can understand from both the previous examples why the hydrogen atom does not collapse even if the electron does not have any orbital angular momentum around the proton. The uncertainty principle essentially forces the electron to stay away from the proton - if it tried to get too close, the kinetic energy would rise enormously because $\Delta x \Delta p \geq \hbar / 2$ says that if Δx becomes small then Δp must become big to compensate.

8. Quantum mechanics predicts what is called "tunneling" of particles through a potential barrier. Again, we shall use the uncertainty principle but this time the energy-time one. Imagine a particle that moves in a potential of the shape shown below. Suppose it does not have enough energy to go over the peak and on to the other side. In that case, we



know from our experience that it will just keep oscillating - moving first towards the hill and then down again, etc. But quantum mechanically, it can "steal" energy ΔE for a time Δt and this may be enough to surmount the hill. Of course, the particle must respect $\Delta E \Delta t \geq \hbar / 2$ so the time is small if it needs a large amount of energy to cross over. Again, I have given only a rough argument here, but in quantum mechanics we can do proper calculations to find tunneling probabilities.

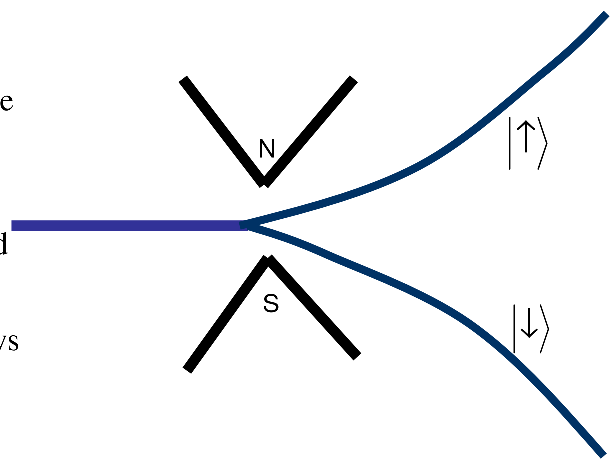
9. Without tunneling our sun would go cold. As you may know, it is powered by hydrogen fusion. The protons must somehow overcome electrostatic repulsion to get close enough so that they can feel the nuclear force and fuse with each other. But the thermal energy at the core of the sun is not high enough. It is only because the tunneling effect allows protons to sometimes get close enough that fusion happens.

10. Quantum mechanics is all about probabilities.What is probability? Probability is a measure of the likelihood that an event will occur. Probability values are assigned on a scale of zero (the event can never occur) to one (the event definitely occurs). More precisely, suppose we do an experiment (like rolling dice or flipping a coin) N times where N is large. Then if a certain outcome occurs n times, the probability is $P = n / N$.

11. The simplest system for discussing quantum mechanics is one that has only two states. Let us call these two states "up" and "down" states, $|\uparrow\rangle$ and $|\downarrow\rangle$. They could denote an electron with spin up/down, or a switch which is up/down, or an atom which can be only in one of two energy states, etc. Things like $|\uparrow\rangle$ were called kets by their inventor, Paul Dirac.

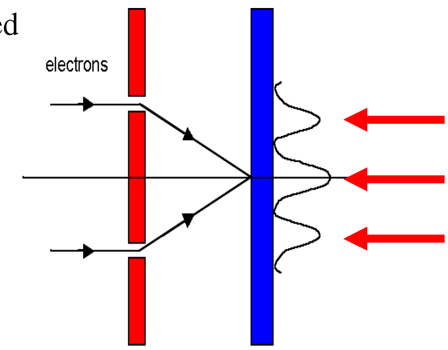
For definiteness let us take the electron example. If the state of the electron is known to be $|\Psi\rangle = \sqrt{\frac{2}{3}}|\uparrow\rangle + \sqrt{\frac{1}{3}}|\downarrow\rangle$, then the probability of finding the electron with spin up is $P(\uparrow) = \frac{2}{3}$, and with spin down is $P(\downarrow) = \frac{1}{3}$. More generally: $|\Psi\rangle = c_1|\uparrow\rangle + c_2|\downarrow\rangle$ denotes an electron with $P(\uparrow) = |c_1|^2$ and $P(\downarrow) = |c_2|^2$. This means that if we look at look at a large number of electrons N all of which are in state $|\Psi\rangle$, then the number with spin up is $N|c_1|^2$ and with spin down is $N|c_2|^2$. We sometimes call $|\Psi\rangle = c_1|\uparrow\rangle + c_2|\downarrow\rangle$ a *quantum state*, and c_1 and c_2 *quantum amplitudes.*

12. The Stern-Gerlach experiment illustrated here shows an electron beam entering a magnetic field. The electrons can be pointing either up or down relative to any chosen axis. The field forces them to choose one of the two states. That the beam splits into only two parts shows that the electron has only two states. Other particle beams might split into $3, 4, \cdots$



13. If a_1 and a_2 are the amplitudes of the two possibilities for a particular event to occur, then the amplitude for the total event is $A = a_1 + a_2$. Here a_1 and a_2 are complex numbers in general. But the probability for the event to occur is given by $P = |A|^2 = |a_1 + a_2|^2$. In daily experience we add probabilities, $P = P_1 + P_2$ but in quantum mechanics we add amplitudes: $P = |a_1 + a_2|^2 = a_1^* a_1 + a_2^* a_2 + a_1^* a_2 + a_2^* a_1 = P_1 + P_2 + a_1^* a_2 + a_2^* a_1$. The cross terms $a_1^* a_2 + a_2^* a_1$ are called interference terms. They are familiar to us from the lecture on light where we add amplitudes first, and then square the sum to find the intensity. Of course, if we add all possible outcomes then we will get 1. So, for example, in the electron case $P(\uparrow) + P(\downarrow) = |c_1|^2 + |c_2|^2 = 1$. Note that amplitudes can be complex but probabilities are always real.

14. Let us return to the double slit experiment discussed earlier. Here the amplitude for an electron wave coming from one slit interferes with the amplitude for an electron wave coming from the other slit. This is what causes a pattern to emerge in which electron are completely absent in certain places (destructive interference) and are present in large numbers where there is constructive interference. So what we must deal with are matter waves. But how to treat this mathematically?



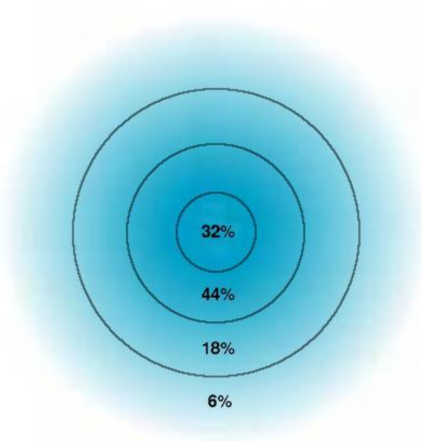
15. The above brings us to the concept of a "wave function". In 1926 Schrödinger proposed a quantity that would describe electron waves (or, more generally, matter waves).

- The wavefunction $\Psi(x,t)$ of a particle is the amplitude to be at position x at time t.

- The probability of finding the particle at position x between x and $x+dx$ (at time t) is $|\Psi(x,t)|^2\, dx$. Since the particle has to be somewhere, if we add up all possibilities then we must get one, i.e. $\int_{-\infty}^{+\infty} |\Psi(x,t)|^2\, dx = 1$.

- $\Psi(x,t)$ is determined by solving the "Schrodinger equation" which, unfortunately, I shall not be able to discuss here. This is one of the most important equations of physics. If it is solved for the atom then it tells you all that is possible to know: energies, the probability of finding an electron here or there, the momenta with which they move, etc. Of course, one usually cannot solve this equation in complicated situations (like a large molecule, for example) and this is what makes the subject both difficult and interesting.

16. For an electron moving around a nucleus, one can easily solve the Schrodinger equation and thus find the wavefunction $\Psi(x,t)$. From this we compute $|\Psi(x,t)|^2$, which is large where the electron is more likely to be found. In this picture, the probability of finding the electron inside the first circle is 32%, between the second and first is 44%, etc.



QUESTIONS AND EXERCISES

Q.1 Compare the size of the kinetic energy of a particle confined to a distance which is of the size of:

a) A grain of salt (1mm).

b) An atom

c) A nucleus

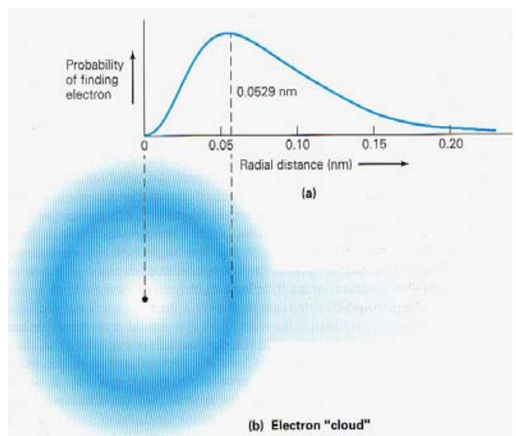
Give your answer only in terms of ratios of b/a and c/a.

Q.2 The probability of death in an accident is 1.5% and the probability of injury is 35%. How many people are killed in 1000 accidents? Injured? Not injured or killed?

Q.3 In the double slit experiment, what would you see if one slit is closed? Why does the interference require both slits to be open at the same time?

Q.4 Suppose a particle that can move only between $x = 0$ and $x = a$ has wavefunction $\Psi(x) = N \sin \frac{\pi x}{a}$. What is the value of *N*? [Hint, the particle has to be somewhere!]

Q.5 Classically we are used to a picture of the atom as a small solar system in which the electron orbits the nucleus. But quantum mechanically this is not true. Instead, the electron is distributed as a cloud around the centre. Where the cloud is most dense, chances of finding the electron are greatest. Now look at the graph and picture at the right.



a) Does the atom have a definite size? If not, can you say anything at all about it?

b) This particular state of the electron is such that it is symmetrically distributed, independent of angle. In this case, can the electron have non-zero angular momentum?

c) If the answer above is "no", then why does the electron not fall into the positively charged nucleus?