

# BASIC IDEAS of QUANTUM MECHANICS

## I. QUANTUM STATES

Quantum Mechanics is certainly the most bizarre and counter-intuitive theory ever invented/discovered in science. It is so peculiar that an important contingent of its founders (most notably Einstein and Schrodinger) actually rejected it after it was established. And yet it is also overwhelmingly the most successful theory we have ever come up with. For someone unfamiliar with the incredible reach of modern physics, the success of quantum mechanics is hard to grasp. Despite the best efforts of many physicists, it still has no known limits to its application. So far this application extends to physical systems ranging over 47 decades of length scale, from  $10^{-21}$  m (a million times smaller than a proton, and 100 trillion times smaller than an atom) up to  $10^{26}$  m (or  $10^{11}$  light years, the size of the visible universe). This range is almost impossible for us to imagine, and yet it is easily encompassed by the rules of quantum mechanics. In the last 85 years we have seen an astonishing transformation in our understanding of the physical world (with immediate spin-offs to our understanding of chemistry and biology), which has only begun to transform technology, society, and our living standards (the shock is how little quantum phenomena have yet been exploited in the everyday world, but this is certain to change in the next few decades).

On the other hand, this incredibly powerful theory is, in a quite profound way, incomprehensible to us, because of what it seems to say about the nature of physical reality. This has led to enormous confusion and intense debate since the theory was discovered. There is no consensus on how we should view the foundations of the theory - indeed, debate has only intensified in recent years, as experiments have pushed the more counter-intuitive aspects of quantum mechanics into the laboratory. As the well-known physicist Feynman remarked, in his famous "Feynman lectures on physics",

*"We choose to examine a phenomenon which is impossible, absolutely impossible, to explain in any classical way, and which has in it the heart of quantum mechanics. In reality, it contains the only mystery. We cannot make the mystery go away by explaining how it works. We can only tell you how it works."*

R.P Feynman, "Feynman Lectures on Physics, Vol. III" (Addison-Wesley, 1965).

Ironically, Feynman here was talking about quantum superpositions, which are indeed very strange, but which probably do not constitute the strangest feature of quantum mechanics. Many physicists would now agree with Schrodinger that perhaps the most central feature of quantum mechanics, as well as being the strangest, has to be quantum entanglement. In reality we have to see all of these features as part of an integrated whole, whose elements we will take on one by one.

The paradox, for anyone meeting Quantum Mechanics for the first time, is that we should be able to use to such great effect a theory we do not understand. We seem to be in the position of the sorcerer's apprentice, wielding a power beyond our comprehension (with the risk that it may spiral out of our control). Naturally the debate over the foundations of quantum theory has also led to some remarkable philosophical and metaphysical ideas, as well as conclusions about the nature of physical reality that are extremely hard to understand. And yet we will see that even the most extraordinary predictions of Quantum Mechanics are overwhelmingly supported by experiment.

In what follows we take a guided tour through this landscape of ideas. The ideas will be presented in somewhat dogmatic form: just as one needs to learn the rules of chess before playing one's first game, one needs to learn the quantum-mechanical rules before one can appreciate the games that are played with it. The tour is divided into 3 parts. In the present document (part I) we learn what is meant by the idea of a "quantum state", for a physical system, and how these states can be 'added to each other' to produce new quantum states - this is the 'principle of superposition'. The strange character of these states for both simple systems like spins or particles will then be explained. In the document following this (part II), I will explain the even more peculiar "entangled" states that can exist when we have more than one physical system, in which the individual character of each system completely disappear, so that only the properties of the combined system have any meaning. Finally, in the 3rd document in this series (part III), we will look at how all this connected with the physical world, through the very strange idea of 'quantum measurements', which give "probabilities of particular outcomes".

**NB:** Here as elsewhere, I have tried to be comprehensive, perhaps even long-winded, in what follows - if you want a quick summary of the main points, go to the course slides.

## A: PHYSICAL STATES

The first question to address is - what do we mean by the 'state' of some physical system? Our common sense notion of a physical state is based entirely on what physicists call *classical* notions. We immediately find that what is meant by a physical state in quantum mechanics is very different. So we begin by discussing this question, comparing classical and quantum notions of a 'state'.

### A.1: CLASSICAL STATES

By 'classical physics', physicists these days typically mean "everything that is not quantum mechanical". Thus classical physics includes the mechanics and physics of particles and fields, and of spacetime and gravity. A central notion of classical physics is the 'classical state' of some physical system. Now the use of the word "state" here is almost synonymous with the common sense notion of a "state of affairs". We say in ordinary language that at some given time, the world is in some state X, meaning that at this time, all objects in the world are disposed in some specific way, with perhaps some specific set of relationships between them. Inherent in this idea is that this state of affairs is *unique*, ie., that if the world is in one specific state A, it cannot at the same time be in another state B; or that it cannot be in 2 different states at the same time, ie., it cannot be simultaneously in states A and B. In fact what is assumed is that there is a large set of different possible states, which are *all different from each other*, and that the world can only ever be in one of them at any time.

**Examples:** To see what is meant here in the context of classical physics, let's recall how the state of a system is specified in the various different classical theories we have:

(a) For a Newtonian system of  $N$  particles in space, we simply have to specify the state of each particle; the state of the entire world is given one we have done this for all the particles there are. To be precise about this: we must specify simultaneously the positions  $\mathbf{r}_j(t)$ , the masses  $m_j$ , and the velocities  $\mathbf{v}_j(t)$  of all the particles (each one labeled by the index  $j$ , where  $j = 1, 2, 3, \dots, N$ ), at any given time  $t$ . This then specifies the state of the world at time  $t$ . We notice that the quantities  $\mathbf{r}_j(t)$  and  $\mathbf{v}_j(t)$  are *vectors*.

Moreover, using Newton's laws, if we also know the forces acting between all the particles, we can then calculate all these positions and velocities at any other time  $t'$  (where  $t'$  is before or after  $t$ ). This is equivalent to saying that the system evolves deterministically - ie., that by specifying the state at any given time  $t$ , we have also completely determined the state at any other time.

(b) To specify the state of a field like the electromagnetic field, we need to specify the field polarizations at every point in spacetime. Thus, for the EM field, we need to specify, at a given time  $t$ , both the electric field polarization  $\mathbf{E}(\mathbf{r}, t)$ , for all points  $\mathbf{r}$  in space, and likewise for the magnetic field polarization  $\mathbf{B}(\mathbf{r}, t)$  (and both of these are vectors). However, this is not a full description, because we recall that the EM field is connected to the system of charges and currents that generate it, and which it acts upon. Thus a complete description of the state of this system also requires that we specify, at any time  $t$ , the electric charge distribution  $\rho(\mathbf{r}, t)$  (a scalar), and the current distribution  $\mathbf{J}(\mathbf{r}, t)$  (a vector). We see that the specification of the state of a field requires much more information than that of a set of particles, since it requires knowledge of a set of vectors at every point in space (an infinite set of numbers), instead of just specifying the state of a finite set of vectors, two for each particle.

The same remarks are true of the spacetime field in General Relativity - here we not only have to specify everywhere the value of the tensor which describes the field itself, but we also have to specify the disposition of all the mass-energy in the universe (ie., we have to specify the stress-energy tensor as well).

Notice that the state of particles and of fields like the EM field is given by specifying them in space and time - in this sense spacetime is a *receptacle* for particles and for fields, without it necessarily having any separate existence of its own. Of course we then learn in General Relativity that spacetime itself can be thought of as a kind of field. We are free, if we wish, to think of the spacetime field as existing in some higher-dimensional space (which can then be thought of as a receptacle for spacetime). However one of the fundamental discoveries of mathematicians like Gauss and Riemann was that we don't *have to do this*; that we can simply specify a geometry without having to say what higher geometry it may be embedded in.

**Degrees of Freedom:** We can also introduce here the notion of a 'degree of freedom'. Basically this is a way of describing how many different quantities need to be specified in order to completely specify the state of a system. In everyday life we have an intuitive understanding of this notion. Thus, we can specify the shopping purchases made by someone by listing the different items purchased and their prices. Suppose there are  $N$  different items - then we specify the entire shopping list by giving the prices of each. We can then say that there are  $N$  degrees of freedom. It is clear that the more complicated the system we are dealing with, the more degrees of freedom it will have.

Suppose we have a single classical particle existing in 3-dimensional space. Then to specify its state we have to fix 6 different numbers. First, we need to fix the vector  $\mathbf{r}$  describing its position; in ordinary Cartesian coordinates this would mean fixing the  $x$ ,  $y$ , and  $z$  coordinates which specify this. Then we would need to specify the velocity vector  $\mathbf{v}$  of the particle - this means specifying the 3 Cartesian components of this (ie., the magnitude of the velocity in each of the  $x$ ,  $y$  and  $z$  directions). Now notice that in general the particle could have any position and any velocity - thus, each of these 6 numbers could have any value. To specify completely its state in classical mechanics we need to fix all 6 numbers, but in general any of them is quite free to take any value between  $+\infty$  and  $-\infty$ . In this sense we say that the system has '6 degrees of freedom'. It is then clear that a set of  $N$  classical particles has  $6N$  degrees of freedom.

It is equally clear that since we have to specify the state of a field at every point of space, and there is an infinite number of different points in space, then the field has an infinite number of degrees of freedom. In real life we would never be able to do this - this is why, for example, meteorologists 'coarse-grain' their description of all the variables needed to specify the state of the earth's climate at any time (by, eg., measuring the atmospheric pressure and temperature at a finite set of different locations, with the locations specified by some 'grid' of positions on the earth).

The point of view that is adopted here can be described in another way. We see that an important underlying assumption in all of this is what is sometimes called the "reductionist" assumption. This can be described as the assumption that it is possible to reduce the entire description of a physical system to a specification of its microscopic "variables", and the way that these influence each other (ie., 'interact with' each other). Another name for 'variables' is 'coordinates'. Both of these terms simply refer to the quantitative expression of the values of each of the degrees of freedom of the system. We call the variables 'microscopic' because the idea is that we have gone to the most primitive set of variables that exist in the system - we cannot reduce them further to anything else. The entire system is then said to be 'composite', ie., composed or 'built up' from more basic entities, and the most basic entities are described by the microscopic variables. The view that one can do this, that Nature is made up in this way, is called "reductionism". As a concrete set of ideas, and a philosophical view, it really began with Newtonian mechanics (although it is not clear what Newton would have thought of it - he perhaps took a far more provisional attitude to his work than others later did). Here it will often give another name to this philosophical view - I will call it the 'lego block' philosophy, the idea being that Nature is made up from basic building blocks, which themselves are irreducible.

Nowadays in physics we often take for granted that we can specify, at least in principle, *everything* about some physical object or system by giving its state. And the lego block view, that this consists in the specification of all the microscopic variables, is just one exemplar of this idea. This is the view which really underlies classical physics - that any physical system has a definite state, one and one only of many possible states, that these states are all different, and that this state is specified if one can discover the values of all the microscopic degrees of freedom. As a corollary, we see that if we have 2 different physical systems, then they have different degrees of freedom, and that in this sense they are logically and ontologically independent of each other (even if some of the degrees of one system may interact with some of those of the other - as for example in the gravitational interaction).

Now the idea of the 'state' of an object, as an exhaustive description of it, is very old. Thus, recall that Democritus was advocating this idea when he reduced all of Nature (including matter and 'Soul') to his basic atoms; and Aristotle, in a much more explicit way, was trying to do the same when he described the 4 "Causes" of a physical object. However there was a fundamental difference here. The ideas of Democritus were very much in tune with Newtonian ideas. However Aristotle's Causes actually asked for more information than is required by any theory in classical physics. Not only did he demand that one specify (i) the 'Efficient Cause' of the object (which is analogous to the notion of a force in classical mechanics, although of course rather different in detail); (ii) the 'Formal Cause' (analogous to the notion of the state in classical mechanics); and (iii) of the 'Material Cause' (which is analogous to the distribution of different masses in classical mechanics); he also wanted to know the 'Final Cause'. This last notion has no place at all in classical physics - once the definite state of the system has been established, either throughout space at a given time (in Newtonian physics) or throughout spacetime (in relativistic physics) then this is all there is, apart from the forces involved in their dynamics. However, although Aristotle took it for granted that all his Causes existed in space and time, his 'Final cause', in a deterministic classical theory, is completely superfluous. The final state in a classical theory is determined completely by the state at any given time - one then simply lets the Laws of Motion 'unroll', as it were, and the system evolves according to these. In this sense the state of the system is determined at any other time, once it is specified at any particular time, with no need of a 'final cause'.

## A.2: DISCRETE QUANTUM STATES

Quantum states are very different from what we have just seen. In the first place, unlike the states of classical fields or particles, quantum states do not exist in spacetime! This part of quantum Mechanics is quite strange, but at least in the standard framework of quantum mechanics, the states are actually vectors in a space called 'Hilbert space'. To

describe this notion is actually quite difficult without advanced mathematics, but one can get the basic ideas across without having to do this. To do so I will introduce the different kinds of state in quantum mechanics, and the rules governing their behaviour, in the form of a set of rules which I will not initially try to explain in too much detail. You should imagine that I am trying to explain to you the rules of a game, like a chess game only more complicated, which you have never seen before. The best way to do this is not to begin by giving a completely exhaustive description of the rules, which would be quite bewildering, but instead to start off with some simple examples, and build from there.

It turns out that the states of many simple quantum systems are extremely simple in that they require only a small amount of information to describe them completely. The simplest of all are what we call '2-state systems'. Two examples of these are (a) the 'spin' of some elementary particles like electrons, or even of some atoms; and (b) the 'polarization' of a photon, which is the elementary particle associated with light.

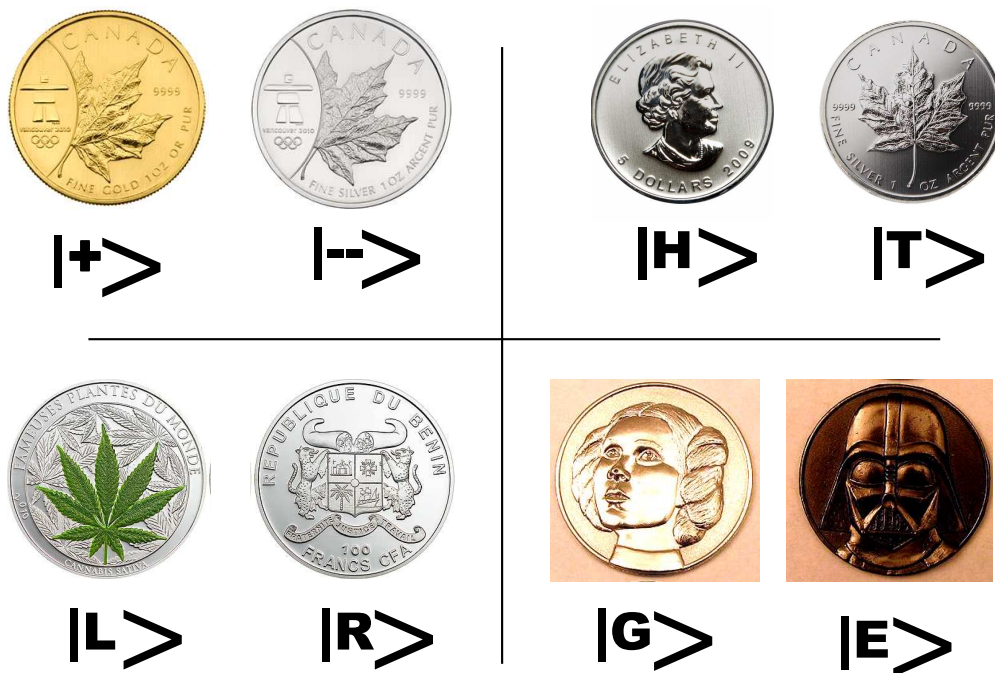


FIG. 1: A set of different '2-state' systems, made from 'quantum coins'. Top left: states  $|+\rangle$  and  $|-\rangle$ ; Top right: states  $|H\rangle$  and  $|T\rangle$ ; Bottom Left: states  $|L\rangle$  and  $|R\rangle$ ; Bottom right: states  $|G\rangle$  and  $|E\rangle$ . For further description see the text.

In fact, almost all of the elementary particles in Nature contain what we can think of as 'internal degrees of freedom', i.e., degrees of freedom associated purely with the particle, and not existing separately from it. And these internal degrees of freedom tend to be associated with discrete quantum states - often just 2 states.

It is illuminating to start with a simple example which is almost frivolous, and which does not exist in the real world - the point here being to make really clear here the difference between classical and quantum states. So we begin with an abstract system where we can avoid any questions about the specific physics we might be dealing with.

**Quantum Coin States:** As noted above, in quantum mechanics we often have internal degrees of freedom which can only take a few discrete values. Let's start by talking about a system which I will call a 'quantum coin'. Now in ordinary common sense life, such a coin could indeed exist in one of 2 states, which in English we usually call 'heads' or 'tails'. To get away from this nomenclature (which originates with older British coins) we will simply talk about '+' and '-' states, and denote them pictorially by the images shown in Fig. 1, top left.

Now the basic idea in classical physics, and in line with common sense, would be that a given coin could be in only one of the 2 states + and -. This is a key requirement of any classical state - a given physical system can only be in one specific state, even though it has available to it an infinity of possible states (through which it can pass as time changes). So, even if we do not *know* what the state of a coin is (it may be hidden underneath a hat, for example, as in a magician's trick), we still assume that it is in one particular state, and one state only.

However in quantum mechanics we have a very strange situation. The first peculiar thing is that we can form what

are called '*superpositions of states*', which in effect add different amounts of the original 2 states, in some proportion. Thus, in terms of the original two state, we cannot say that we are in one or other of these states - in effect, we are in both of them, with some proportion of each. This is of course in complete contradiction with common sense.

The second peculiar thing is that by combining these 2 original states in some proportion, we actually produce another quantum state! Suppose we first add the 2 states + and - in equal proportions, as shown in the top part of Fig. 1. Notice a piece of nomenclature here - to signify that we are dealing with quantum states, we write them in the form " $|+\rangle$ " and " $|-\rangle$ ", ie., we enclose the name of the state in between the symbols " $|$ " and " $\rangle$ ". This nomenclature has a mathematical meaning which you don't need to know about here.

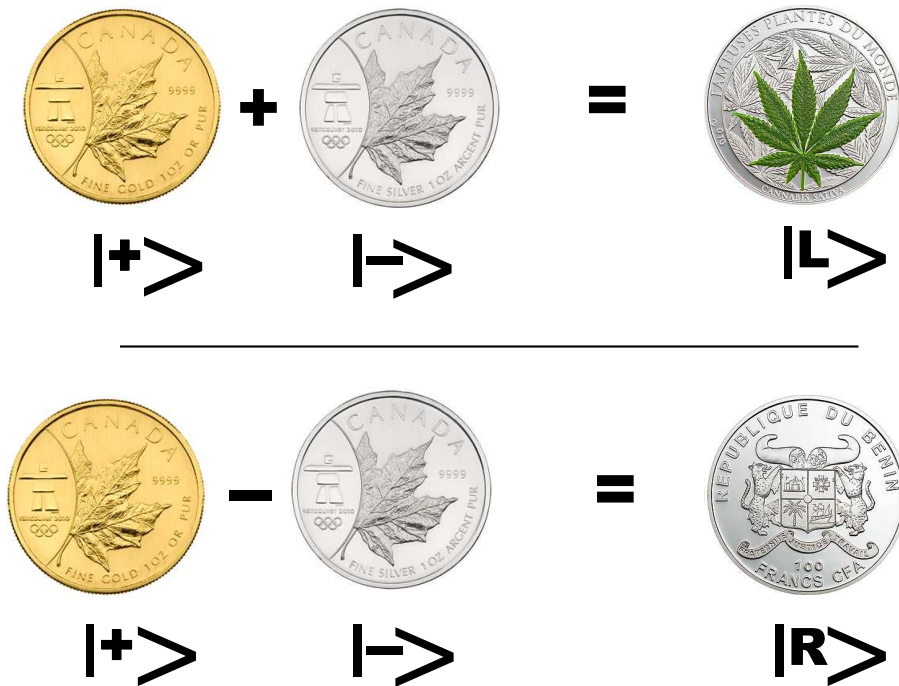


FIG. 2: Illustration of equations (0.1) and (0.2) in the main text. In the top picture we add the states  $|+\rangle$  and  $|-\rangle$  in equal proportions, to get the state  $|L\rangle$ . In the lower picture we subtract  $|-\rangle$  from  $|+\rangle$ , to get the state  $|R\rangle$ . For further description see the text.

Now the key point here is that by adding  $|+\rangle$  and  $|-\rangle$  in equal proportions, we actually get another state which we will call  $|L\rangle$  (you can think of this as signifying 'left', but this is not important). Even more interesting, if instead of adding the 2 states  $|+\rangle$  and  $|-\rangle$ , we subtract one from the other, we get another state, which we call  $|R\rangle$  (where we can think of ' $R$ ' as meaning 'right'). Moreover, just as the + and - states can be thought of as being 'opposite' to each other, so can the  $L$  and  $R$  states, as we will see.

Notice how we are treating these quantum states as being like numbers, which we can add and subtract from each other - this is part of the strange set of rules that we are going to learn. In fact it turns out that when we do write down the 'algebra' of these states, what we have shown in the figure can be written like this:

$$\frac{1}{\sqrt{2}} (|+\rangle + |-\rangle) = |L\rangle \quad (0.1)$$

when we sum the 2 states + and - (ie., the top equation in the figure); and when we subtract one from the other, we get instead:

$$\frac{1}{\sqrt{2}} (|+\rangle - |-\rangle) = |R\rangle \quad (0.2)$$

ie., the bottom equation of the figure.

I will explain the origin of the factor  $\frac{1}{\sqrt{2}}$  later on - it is not important for what immediately follows, except in getting the sums right.

Now in fact we can also produce other quantum states of the coins by adding the original states in different proportions. For example, we might try adding them in such a way that the  $+$  state has twice as much weight as the  $-$  state. We would then find that we had a quite different state from either  $|+\rangle$  and  $|-\rangle$ , or from  $|L\rangle$  or  $|R\rangle$ ; in fact it might be something like the state  $|H\rangle$  (where 'H' signifies 'heads'), shown in Fig. 1. I won't go through the algebra here - if I did you would see how by a slightly different combination we could also get the state  $|T\rangle$ , (with 'T' signifying 'tails'), a state which is essentially the opposite to  $|H\rangle$ . And this goes on - by making other combinations we could get the states  $|G\rangle$  and  $|E\rangle$  shown in Fig. 1, and so on.

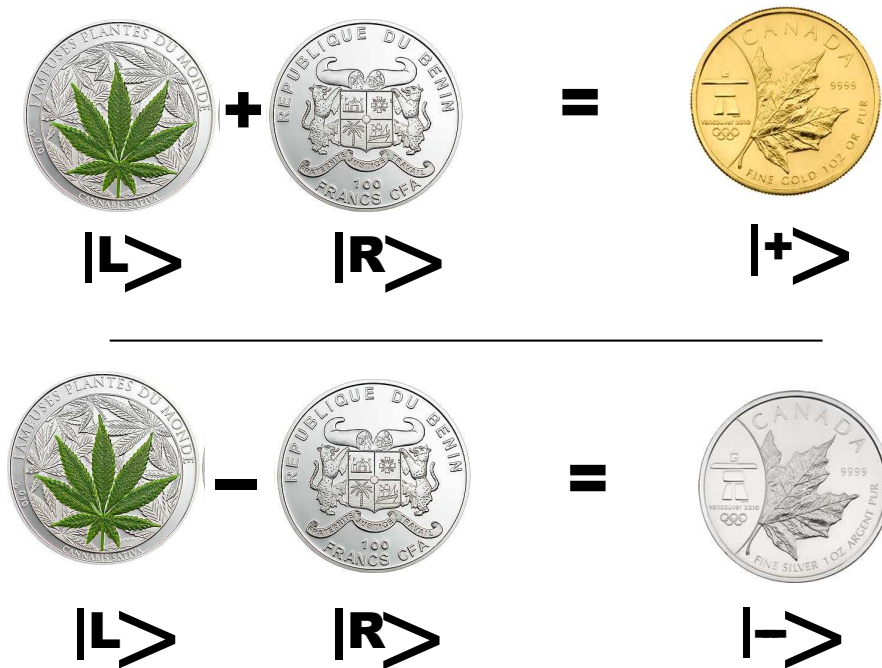


FIG. 3: Illustration of equations (0.3) and (0.4) in the main text. In the top picture we add the states  $|L\rangle$  and  $|R\rangle$  in equal proportions, to get the state  $|+\rangle$ . In the lower picture we subtract  $|R\rangle$  from  $|L\rangle$ , to get the state  $|-\rangle$ . For further description see the text.

However, this is not quite all. Suppose we really take the algebra of these states seriously. Then, going back to our equations (0.1) and (0.2) above, we can either add the two of them together to get

$$\frac{1}{\sqrt{2}}(|L\rangle + |R\rangle) = |+\rangle \quad (0.3)$$

ie., we get back the  $+$  state by adding  $L$  and  $R$ ; and by subtracting (0.2) from (0.1) we also get:

$$\frac{1}{\sqrt{2}}(|L\rangle - |R\rangle) = |-\rangle \quad (0.4)$$

ie., we get back the pair of states  $+$  and  $-$  by superposing the states  $L$  and  $R$  in these two different ways. This result is illustrated in Fig. 3.

We see that we have here a kind of 'quantum democracy' of states: no state is more fundamental than any other! In classical physics, the only meaningful coin states are the heads and tails states - a superposition of these is physically meaningless, a mere game played with symbols. But in quantum physics, we can add states in any proportion to get another state, and then add these others to get back the first ones. In this way we see that we can start with any 'opposite pair' of states, and get to any other such pair - it doesn't matter which pair we start with.

**Quantum Spin States:** Let's now leave this bizarre idea of quantum coins for the moment, and go to something which was discovered at the very beginning of quantum mechanics, back in the 1920's. This is that we can assign what we call a 'discrete quantum number' to all particles in nature, which as called 'spin'. In classical physics, magnetic moments (ie., objects which, like little current loops or small bar magnets, generate a magnetic field) can be oriented



in any direction. However in quantum mechanics, this spin can only take certain discrete values, which in the case of what are called 'spin-1/2' systems, reduces to only two discrete values.

The existence of quantum spin states has been known since the beginning of quantum mechanics, and was demonstrated very quickly in a whole variety of experiments. One of the earliest was the 'Stern-Gerlach' experiment, shown in Fig. 4(a). The basic idea of this experiment is to measure the spin along some particular direction in space, such as the  $z$ -axis (ie., the "up/down" axis); in fact, the magnetic fields in the system are designed to deflect an incoming beam of spins, up or down, by an amount proportional to the component of spin along the  $z$ -axis. Now for a classical spin, orientable in any direction, the component of spin along the  $z$ -direction is completely arbitrary - it can +1 for a spin that happens to be up,  $-1$  for a spin that happens to be down, and any value in between (including zero, for a spin pointed anywhere in the  $xy$ -plane). Thus if we do this experiment for classical spins, we expect the beam of many spins, randomly oriented, to spread out over the whole range between +1 and  $-1$  (see Fig. 4(a), top left). However this is not what happens - in fact it splits into 2 beams, as shown at top right in Fig 4(a), as though only states with spin pointed exactly up or down existed in the beam (ie., the states shown in Fig 4(b)).

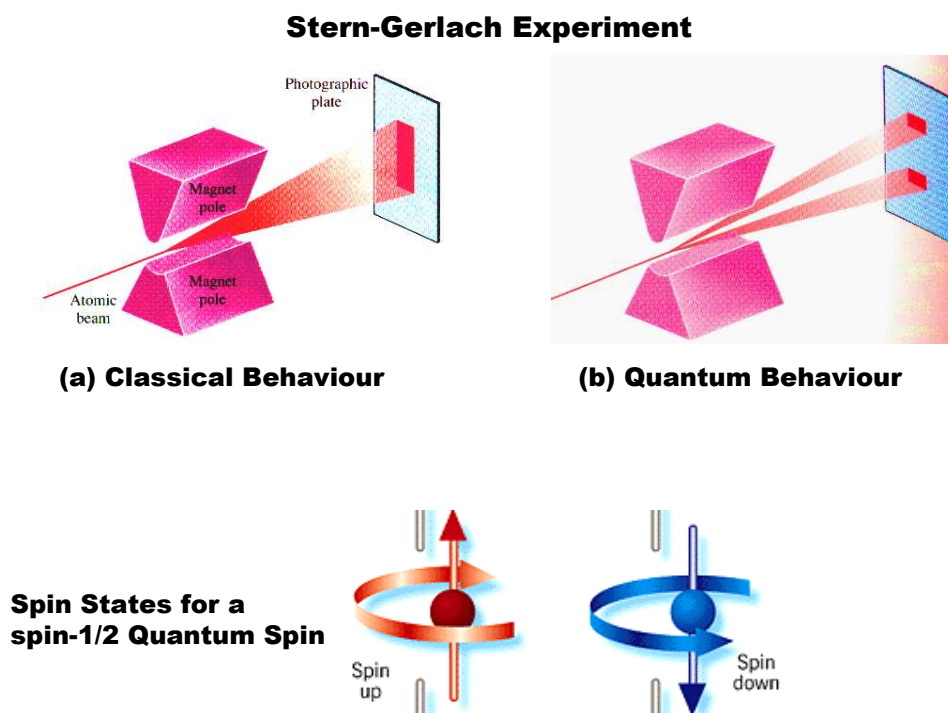


FIG. 4: Spin-1/2 states of a quantum particle. In the top figure we see the Stern-Gerlach set-up, in which a beam of atoms or other particles is sent through a magnetic field configuration which deflects the beam according to the orientation of the spin of the particle. At left is what would happen if the spin could point in any direction - at right is what is actually seen. The lower figure shows what we deduce from this - that the spin can only exist in either the 'up' or 'down' states, along or opposite to the direction of the magnetic field. See text for more details.

Now one might try to argue that somehow the beam had been badly set up, so that in fact there really were only either 'up' or 'down' spins in it. But we can easily show this is not the case - we can, without in any way touching or changing the spins in the beam, rotate the measuring system on its side, so that now it is measuring, say, the  $x$ -component of spin - ie., how much of the spin is pointed in the right/left direction. If the spins were really only up or down, then we would find that the component in the  $x$ -direction was always zero. But this is not what is found - instead, we now find that half of them are oriented left, and half are right!

This apparently totally bizarre situation can be analyzed in exactly the same way as for the 'quantum coins' above. Indeed, the "left" and "right" spins can be written as superpositions of the "up" and "down" spins, in the same way as we saw above. Suppose we call the up and down states  $|\uparrow\rangle$  and  $|\downarrow\rangle$  respectively; and the "right" and "left" states by  $|\rightarrow\rangle$  and  $|\leftarrow\rangle$  respectively. Then in fact we have, by either summing or subtracting one from the other, that

$$\begin{aligned} \frac{1}{\sqrt{2}}(|\uparrow\rangle + |\downarrow\rangle) &= |\rightarrow\rangle \\ \frac{1}{\sqrt{2}}(|\uparrow\rangle - |\downarrow\rangle) &= |\leftarrow\rangle \end{aligned} \tag{0.5}$$

From this we see that if a spin pointing to the right (ie., in a state  $|\rightarrow\rangle$ ) goes through, then it will look as though it is in a superposition of up and down states (of equal weighting).

Moreover, in the same way as before, we can add and subtract these two equations to get the way in which the left and right spins superpose to give up and down:

$$\begin{aligned}\frac{1}{\sqrt{2}}(|\leftarrow\rangle + |\rightarrow\rangle) &= |\uparrow\rangle \\ \frac{1}{\sqrt{2}}(|\leftarrow\rangle - |\rightarrow\rangle) &= |\downarrow\rangle\end{aligned}\quad (0.6)$$

so that if a spin in state  $|\uparrow\rangle$  goes through, then it is in a superposition of up and down states, of equal weighting. We see that the algebra here is just like with the coins.

One thing we have not yet said anything about here is how we describe the motion of the spin through real space (the spin is, after all, attached to a particle which is moving in space). This question is discussed later on, when we come to deal with quantum states in space (section 1.A.3).

**Photon Polarization States:** Another important 2-state degree of freedom is the analogue of spin for photons (ie., the particles of light). This is called the photon polarization, and we can see it most clearly if we look at what in classical electromagnetism is called 'circular polarization'. In a circularly polarized light wave, the direction of the electric field rotates around the wave as we travel along it (see Fig. 5(b)).

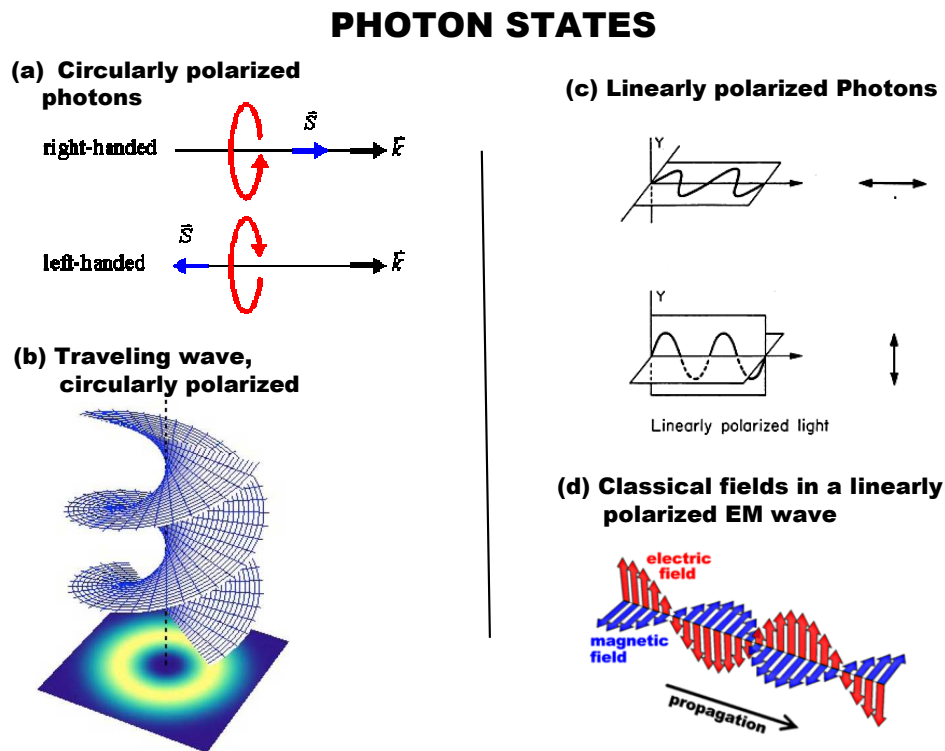


FIG. 5: Photon states. In (a) we show the clockwise and anticlockwise states - the polarization vector  $\mathbf{S}$  is directed either parallel or anti-parallel to the direction  $\mathbf{k}$  of light propagation. In (b) we see the corresponding direction of electric fields as one travels along the beam. In (c) we show the electric field for vertical and horizontal linearly polarized states; and in (d) we see how both the electric and magnetic fields vary along a linearly polarized EM wave. See text for more details.

Now for a quantum photon state, this corresponds to having the 'spin' of the photon pointing along the wave, either parallel or antiparallel to it depending on whether the field is rotating clockwise (right-handed) or counter-clockwise (left-handed) as we travel along the wave (see Fig. 5(a)). Sometimes these 2 photon states are just labeled as  $|+\rangle$  and  $|-\rangle$ ; alternatively they are named  $|R\rangle$  and  $|L\rangle$ .

You might wonder what happens if we superpose these 2 states. The answer is that we get *linearly polarized* states, of the kind we already saw when dealing with the polarization of EM waves. Let's imagine a photon traveling along



the  $x$ -direction, and 2 such states, one polarized vertically and the other in the horizontal plane (see Fig. 5(c)). We will label these states as  $|\uparrow\rangle$  and  $|\leftrightarrow\rangle$ . Then the result of doing the superpositions is just

$$\begin{aligned}\frac{1}{\sqrt{2}}(|L\rangle + |R\rangle) &= |\uparrow\rangle \\ \frac{1}{\sqrt{2}}(|L\rangle - |R\rangle) &= |\leftrightarrow\rangle\end{aligned}\tag{0.7}$$

and of course by superposing the states  $|\uparrow\rangle$  and  $|\leftrightarrow\rangle$  we can get back the two circularly polarized states. Again, we see the same 'quantum democratic' algebra at work, of making one set of states from another, with none of them being regarded as any more fundamental than the other.

Just as with spins, the discussion of the 2-state properties of photons does not exhaust their properties, for photons also propagate in real space. Actually the quantum properties of photon propagation are rather easy to understand. We recall that in the classical picture of EM waves, a wave of wavelength  $\lambda$  has a frequency  $\nu$ , ie., there are oscillations of the electric and magnetic fields at any point in space through which the wave passes; the frequency is then given by  $\nu = c_o/\lambda$ , where  $c_o$  is the velocity of light, since then  $\nu$  waves pass each second. Now in quantum mechanics, we actually find again a frequency  $\nu$  of oscillation of the electric and magnetic fields at a given point in space, associated now with a photon of wavelength  $\lambda$ , but there is an extra ingredient - the energy of the photon is given by a specific amount, given by  $E_\nu = \hbar\nu$ , where  $\hbar \sim 10^{-34}$  Js is 'Planck's constant'. Thus we say that the photons come in 'packets' or 'quanta' of energy, such that the energy is proportional to the frequency - higher frequency (ie., shorter wavelength) photons have higher energy. We shall return to this property of photons many times. Note that, just as with 2-state photon polarizations, we are at liberty to make a photon which is in a superposition of 2 or more *different* frequency states (ie., of different wavelengths). Natural 'white light' is in fact typically composed of an enormous number of different photons, with a continuous spectrum of different frequencies - and many of these photons will also be in superpositions of states of different frequency.

**Summary for Discrete states:** What have we seen so far, with these different examples of 2-state systems? Well, let us first recall that in classical physics, we assumed that any given physical system can be understood in terms of its degrees of freedom, its 'microscopic variables'; and that if we specify the values of all of these, we have completely specified the physical state. A system can exist in one and only one state at any time, and if we change the values assigned to the variables, we automatically have a different state. We have now seen that things are rather different with quantum systems - for although we can assign a definite state to a physical system, this state can be decomposed into a 'sum over' a number of other states (for systems with 2 degrees of freedom, it can be decomposed into a sum over 2 states). Moreover, this decomposition can be done in many different ways. Thus, in a real sense, there is a kind of 'quantum democracy' at work here - any quantum state can be decomposed, in a specific way, into a "superposition of other states", so that no given state is any more fundamental than any other - they can all be constructed from each other.

What has been done here is only the beginning. First, we have not yet explored what happens when we try to make a *composite* quantum system (ie., a system like a Hydrogen atom, composed of 2 particles); this will be done in the 2nd document in this series, where we see that the answer is very strange indeed. Second, we have not explained how it is that in the world of common sense that we experience, we see systems in one definite state, not in some superposition. To put it another way: "if all states are on an equal level, then what determines which ones we see?" This 2nd question is actually rather important, since many situations arise in which, because of some symmetry in the situation, no one state is favoured over any other (for example, they may all have equal energies). Then typically the system will 'spread out' into all of them, ie., go into a superposition of all of these states.

We will answer this 2nd question at several points in what follows; first when we come to the dynamics of Quantum states (see section B.2 below), and then when we talk about one of the most peculiar aspects of quantum mechanics, viz., the link between quantum states and what we see and experience, through what are called 'quantum measurements' (see part III of this series of documents).

## B: QUANTUM STATES in SPACE

Not all quantum states are discrete - indeed, many of them have an infinite number of degrees of freedom. Consider, for example, physical systems which are extended in space, like traveling particles. In classical physics, these can exist over a continuous range of different positions, or having a continuous range of different possible velocities. The simplest example is a single particle - in a 3-dimensional space, it has 6 degrees of freedom, and the particle will typically evolve in time, changing the values of its 6 microscopic variables as it goes along. So then - what are the quantum states for these systems like? We will see that they are quite different - in fact, the degrees of freedom for

a single particle are infinite in number, and the way we describe them makes the single-particle system look instead like a field.

We will separate our answer to this question into two parts. First, we will ask - what do the states look like in space? We will see that they look like waves; and when they are confined to some region of space, they organize themselves in 'standing waves', ie., waves frozen in place. This is what will be described immediately below. The second question is - how do they move in time? This will be dealt with in section B.2 below - but the short answer, is, again, that they move like waves.

Before we start, let us recall some of the characteristic properties of waves and wave propagation. These of course were first discussed in real detail by Huyghens, and we have already seen them in our discussion of optics and electromagnetic waves. We have seen that waves can be delocalized in space, and travel through it. Moreover, 2 different waves can 'interfere', ie., when moving through each other, their amplitudes add and reinforce each other where the wave crests meet, or where the troughs meet (constructive interference); but if a crest from one wave meets a trough from the other, then they cancel each other, and the result is no amplitude at all (destructive interference). All of this is familiar in the propagation of water waves, sound waves, and of course EM waves.

In cases where waves are trapped, they will organize themselves so that their amplitude is zero outside the region where they are allowed, and they will then propagate around inside the allowed region, reflecting off the boundaries. Typically one sees multiple waves traveling around inside such a closed region (think of a swimming pool with many waves moving around, interfering with each other as they meet). However one can also set up a standing wave in such a confined space - in such a wave, oscillations occur in time, but the wave does not move. We can think of a standing wave as one on which 2 equal waves move in opposite directions through each other, in such a way that the pattern of nodes (areas where the wave amplitude goes to zero) and maxima (where the amplitude goes to a maximum) do not move. The most obvious example of this you are likely to see in everyday life is on the strings of a musical instrument.

### B.1: BOUND STATES in SPACE

Having said all of this, let us start by first looking at how quantum states will behave in situations where the physical system of interest is confined to some region of space. In physics we call such states 'bound states', because they are bound to this region. For this to happen, the potential energy of the system must be lower in this region than it is outside. We call this region a 'potential well' (because a graph of the potential energy looks like a well). Since any object wants to lower its potential energy as much as possible, it will try to settle to the bottom of the well if it can. In classical mechanics it can do so - the potential energy is converted to kinetic energy (ie., the particle accelerates towards the direction of the bottom of the potential), and then if it can dissipate this kinetic energy as friction, it will end up in the bottom of the potential well. In what follows we begin by recalling some examples of potential wells and their effects in classical mechanics. We then look at the quantum states for some model potential wells; and then focus on one very important example, that of the electrons bound to an atomic nucleus. Finally, we look at a uniquely quantum phenomenon, called 'quantum tunneling', which involves *escape* from a potential well.

**Bound States in a Potential Well:** There are many different kinds of potential well in Nature, all of them causing an object in the well to be attracted to the lowest part of it. There are many examples in Nature of this sort of thing; some examples are:

(i) a negatively charged electron near a positively charged proton (ie., the constituents of a Hydrogen atom). In this case the attractive interaction between them means that the electron has lower potential energy when it is near the proton - in fact, as we already saw in discussing the Coulomb interaction, the energy of the electron is given by  $V(r) = -ke^2/r$ , where  $r$  is the distance between the 2 particles. Here  $e$  the electric charge, and  $k$  a constant. A similar example is that of a particle of mass  $m$  in the attractive gravitational field of another mass  $M$ ; they then each find themselves in a gravitational potential well, with now  $V(r) = -GmM/r$ . Both of these potential wells have energy going like  $-1/r$ , a shape you have seen in our discussion of electricity and gravitation. The big difference is that the electric force is much stronger, so that the potential well is much deeper. In classical mechanics, if a mass orbiting the sun can get rid of its kinetic energy (eg., by friction with gas in space) it will eventually spiral down to the bottom of the potential well, ie., into the sun.

(ii) A ball-bearing in a cup - here the attractive gravitational force of the earth means the ball-bearing is at a lower potential energy at the bottom of the cup (indeed, its potential energy is just proportional to its height  $z$ ; so that  $V(z) = mgz$ , where  $m$  is the mass of the ball-bearing, and  $g$  is a constant). So we can think of the region of the cup as forming a potential well, and the walls of the cup a potential barrier - if the ball-bearing gets enough energy to go over the cup rim, it will then fall because it finds a region of lower potential energy on the other side. A similar example is a pendulum with a ball of mass  $m$  swinging at the end of a string. Again, the potential energy is at its lowest when the pendulum ball is at its lowest, and the energy is proportional to the height of the ball, ie.,  $V(z) = mgz$ .

In quantum mechanics things are very different.

In Fig. 6(a) we show both the energies and the 'wave-functions' of bound states in a specific kind of potential well. This is the so-called "square well" potential. In this potential, the walls are infinitely high, ie., it would cost an infinite energy to surmount them. This means that they are impenetrable - the system is completely trapped. The figure on the left shows a set of states labeled by the 'quantum number'  $n$ . The lowest state, with  $n = 0$ , has the lowest energy, not far above the floor of the potential. Note, however, that this energy is *not zero*. We say that this is the 'ground state'  $|\psi_0\rangle$  of the particle, and its energy is  $E_0$ , which is the ground state energy. Another name commonly used for this energy is the zero point energy. The shape of this state  $\psi_0(x)$  - what is called the 'wave-function' for this state, as a function of the position  $x$  - is also shown. It is at a maximum value in the centre, falling to zero at the sides.

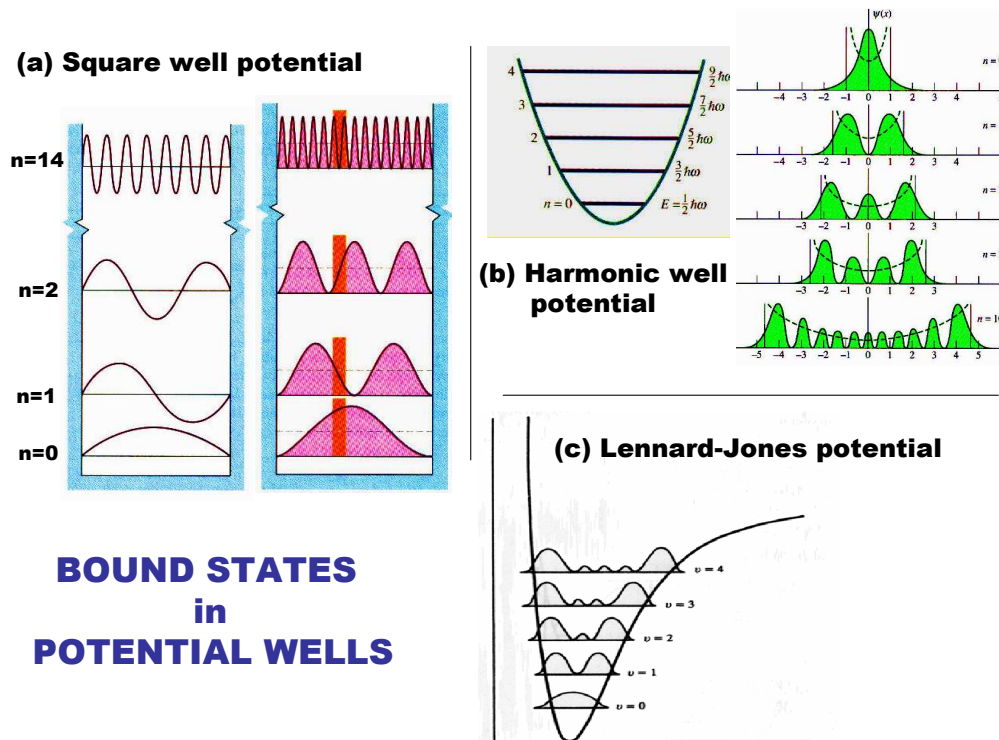


FIG. 6: Bound states of quantum particles. In (a) we show at left, the bound states and energies of a particle in a 'square well', with the wave functions shown at heights corresponding to their energies; and at right we show the 'probability density' function  $P(x)$  for a particle in the box to be found at position  $x$ . In (b) we show, at left, the potential for a 'harmonic oscillator' potential well, along with the energies of the lowest bound states; and at right we see the probability densities  $P(x)$  for these same states. Some of the bound states of an electron around a nucleus are shown. In (c) we show the Lennard-Jones potential well, along with the probability densities for the lowest energy states. See text for more details.

Also shown here on the left are some of the higher energy states in this potential well - they are labeled in order of their energies, so that the next one up is  $|\psi_1\rangle$ , and so on. We notice that (a) the higher wave functions  $\psi_n(x)$  have more and more oscillations in them, and that (b) they have higher and higher energies. In fact, for the square well (but not for other forms of potential well) the energies actually obey the following rule:

$$E_n = \frac{\pi^2 \hbar^2}{mL^2} (n+1)^2 = (n+1)^2 E_0 \quad (0.8)$$

What this equation is saying is that the energy  $E_n$  goes up as the square of the number of oscillations, so that  $E_n \propto (n+1)^2$ . This is because the number of oscillations in the trapped wave is actually equal to  $n+1$ . Now what does this equation mean? Notice first that the lowest energy  $E_0$ , the ground state energy, has some value (given by  $E_0 = \frac{\pi^2 \hbar^2}{mL^2}$ , in fact). We say that this ground state has no "nodes" in it - ie., no points inside the box where it goes to zero. We are fitting a single "half-wave" inside the box. But the higher states have more and more nodes - the  $n=1$  state (the lowest 'excited state' has 1 node, in the middle; the  $n=2$  state, or 2nd excited state, has 2 nodes; and so on). By putting more and more nodes in the states, we are forcing them to have a shorter and shorter wavelength,

and more and more oscillations inside the well, and therefore they have a higher and higher energy. What the equation is then saying is that the energy  $E_n$  is equal to a constant  $E_o$  times the square of the number of nodes. Later one we will see why it has this form, but for now we just want to see what are the implications of the form.

Finally, in the right hand part of Fig. 6(a), we see what is called the 'probability density' function  $P(x)$  for the same states. We will discuss this whole idea in more detail later on, but suffice it to say here that the probability density is a curve which tells us the probability we will find the particle at some place, and in fact it is given by the *square* of the wave-function itself. Thus, even though the wave function can be negative, the probability density is always positive. We notice that  $P(x)$  also oscillates more and more as we go to higher energy states. Roughly speaking, it costs a lot of energy to make a wave-function change quickly.

Now a square well potential is physically completely unrealistic - it implies the existence of infinite forces at the walls, to keep the particle from crossing them, and an infinitely high energy outside the box, whose origin would be very hard to explain. However, immediately to the right of this picture, in Fig. 6(b), we see another potential well, the so-called 'harmonic oscillator well', with a set now of equally spaced energies for the different states, and for which on the right, some of whose probability densities are shown. Again, the lowest energy state  $|\phi_o\rangle$ , with energy  $E_o$ , has a wave-function  $\phi_o(x)$  and a probability density with the fewest oscillations, and as we go up to higher energy states, there are more and more oscillations. Notice that these wave-functions do not abruptly fall to zero at their edges, but rather trail out into the 'forbidden' higher energy regions. Moreover, the energies of the states now rise linearly with  $n$ , ie., we have roughly that  $E_n \propto (n + 1)$ , instead of  $(n + 1)^2$  as we saw for the square well potential - this is because higher energy states can spread out more, so their wavelength does not get shorter as quickly as those in the square well. Actually the harmonic oscillator is a potential that gives a very realistic description of many physical systems - for example, it describes the energy of an oscillating system such as a spring, or a pendulum when it is making small oscillations about its lowest point.

Finally, let us go to Fig. 6(c), where we address an obvious question that we can ask about bound states, viz.: what happens if a particle has enough energy to escape a potential well - what then do the energies and wave-functions look like? Fig. 6(c) shows the states of a particle in a well of finite depth, in what is called a 'Lennard-Jones' potential. As one climbs up the eigenstates of ever higher energy, the particle gets closer and closer to the energy at which it ought to be able to escape. We can see that these higher energy states have a finite amplitude and probability density ever further from the region of low energy, and in fact, when they do get to the 'threshold' where they are at the top of the potential well, the wave-functions and probability densities begin to spread off to infinity - the particle becomes 'unbound' at these energies. Below, we will look more at these unbound states. Note that the Lennard-Jones potential actually provides an approximate description of the force between 2 simple atoms - it is attractive at long distances, but then becomes strongly repulsive if they try to get too close - and at an optimum distance, it is at a minimum.

To summarize - in the classical Newtonian mechanics of particles, the particles, once they have 'fallen into' a potential well, can never get out unless they are given enough extra energy to do so. However they can occupy any classical state inside the well - they can be in any position inside, and have any velocity (provided the velocity is not high enough to allow them to escape). However quantum states are very different. Only certain 'wave' states are allowed, ones that 'fit into' the potential. And these states can only have certain discrete energies. Thus we have what is called the '*quantization*' of energies - the limitation of the energies to certain discrete values. Notice that this quantization is arising because the states look like waves - waves do exactly the same thing, as one sees in looking at the possible oscillation shapes, or 'standing waves', of a guitar string.

Finally, as we will discuss below in more detail - quantum states differ from classical states in one other crucial respect. Even if they are bound, and have too little to escape over the top of the barrier around a potential well, they may still escape if the potential barrier is lower on the other side. They can then 'leak through the barrier to the other side, and escape away from the potential well. This phenomenon is called "quantum tunneling", and is extremely important for the understanding of many physical systems - we will discuss it more below.

**Summary - Superpositions of Discrete States:** It should now be fairly obvious that a 2-state system is just a special case of a more general situation in which one can form superpositions of  $N$  states. The natural way to do this is by taking a set of discrete bound states. And indeed there is nothing to stop us from making such superpositions. Actually, since these states do not move around inside the potential well, and they each have a specific energy, we given them a special name. They are called 'eigenstates', or 'stationary states'; and their energies are sometimes called the 'eigenenergies'. And from these different bound states, we can construct any state inside the potential well, simply by adding together (ie., *superposing*) various proportions of the different eigenstates. At this point you may find it easier to see how we can write this down mathematically. Suppose we give a name to each of the eigenstates, calling them  $\phi_n(x)$ , where the label  $n$  can take any value, from 1 to  $N$  (ie., we can have  $n = 1$ , or  $n = 2$ , etc.). And suppose we give the name  $\Psi(x)$  to some arbitrary quantum state for the particle in the potential. Then what we

saying that we can write an *arbitrary* quantum state inside the potential well in the form

$$\Psi(x) = \sum_n c_n \phi_n \quad (0.9)$$

You should not be afraid of this equation - all it says is that the wave-function  $\Psi(x)$ , which is some shape in space  $x$ , can be written as the sum of (this is what the symbol  $\sum_n$  means, literally 'the sum over the labeling index  $n$ ') a set of different eigenfunctions  $\phi_n(x)$ , with different coefficients (ie., weighting factors)  $c_n$ .

The 2-state system is the simplest possible case of this superposition - for then we just have  $\Psi = c_1\phi_1 + c_2\phi_2$ . All of the states for the different 2-state systems we saw above are like this.

Note that these various features of the state superpositions (that we can define a set of 'stationary states' for inside an enclosure, and that these states can then be added together to make some arbitrary waveshape) are features you have seen many times in everyday life. When we analyze the sound of somebody's voice, or the sound of a violin, into its spectrum (ie., its different frequency components) all we are doing is analyzing it into the different eigenstates of vibration - these are then added in various proportions to hear the sound that is produced. Likewise waves on the water in, eg., a swimming pool or a lake, are also superpositions of all the different eigenstates of water waves in these enclosures. And when you look at some arbitrary shape of a string tethered at each end (like a guitar string), you are looking at a shape which can be constructed by adding together the various basic eigenstates of oscillation of the string - and in fact these look exactly like the states shown in Fig. 6(a) for the square well potential.

## B.2: EXAMPLES of BOUND STATES in NATURE

The above discussion of bound and/or discrete states was a little abstract; Fig. 6 is just a set of simple models, which help to illustrate the main features of bound quantum states. In order to gain some intuition, and to see how utterly central all this is to our understanding of Nature, we will look at 2 different examples. These examples are chosen for their relative simplicity - in fact Nature is choc-a-block with examples, ranging from nucleons bound together inside a nucleus, to atoms and electrons in a solid or liquid, to various kinds of particles in a star or even a black hole. But from the 2 examples below we can extract some very general features.

**Electronic States in an Atom:** In Fig. 7 we show the bound states of an electron around a proton. These 2 particles attract each other via the Coulomb interaction, and so we expect the electron to form bound states around the much heavier proton - this is how a Hydrogen atom is formed.

However, these electronic states are a lot more complicated than the ones we have just been looking at, because they are now in 3 dimensions. We call the various shapes that we get 'electron wave-functions' or 'electron clouds', and they come in all shapes and sizes, some of which are shown in the pictures in Fig. 7(a) and 7(b). These pictures actually show the magnitude of the probability density for each of these states. The states of lowest energy are concentrated around the protonic nucleus - the lowest energy state of all (called the  $n = 1$ , or '1s' state) is a spherical cloud very close to the nucleus.

In Fig. 7(c) we also show the energies of some of these states, and possible transitions between them. The very lowest state, the  $n = 1$  state or 'ground state', is at an energy of  $-13.58 \text{ eV}$ ; this means that its energy is  $13.58 \text{ eV}$  lower than the energy of a 'threshold state', ie., one that can just escape from the atom (NB: an 'eV', or 'electron volt', is a measure of energy we have already seen in classical EM - it is the energy change experienced by an electron when it changes its electric potential by one Volt). To get a feeling for these numbers, note that a photon of red light, with wavelength  $\sim 7000 \text{ \AA}$ , or  $7 \times 10^{-7} \text{ m}$ , has an energy  $\sim 1.7 \text{ eV}$ , and a photon of blue light, with wavelength  $\sim 4000 \text{ \AA}$  (ie.,  $4 \times 10^{-7} \text{ m}$ ), has an energy of roughly  $3 \text{ eV}$ . The energy required to excite an  $H$  atom from its ground state to a state just at the threshold (ie., to *ionize* it) is thus over 4 times larger than this, and corresponds to the energy of a photon in the far ultraviolet, or wavelength less than  $1000 \text{ \AA}$ . From what was said previously about the relation between energy and frequency for photons, you can also find out the frequencies of these photons of light - they are actually very high.

There is actually an infinite number of bound states, labeled by  $n = 1, 2, 3, \dots, \infty$ , but the separation in energy between them gets smaller and smaller as  $n$  increases. For an electron to actually make a physical transition between one of these states, it has to either receive energy to go up to a higher state, or emit energy, to descend to a lower state. The energy emitted or absorbed is just the difference in energy between the 2 states. This is normally accomplished by interactions between the electron and light, in which a photon of the right energy is emitted or absorbed - a process which is of course of key importance, for it is the quantum version of the interaction between EM waves and electric charges that we saw in discussing EM fields.

There are many things that one can say about what is shown in Fig. 7 (which of course describes the bound states for the simplest possible atom). Three key points to notice here are:

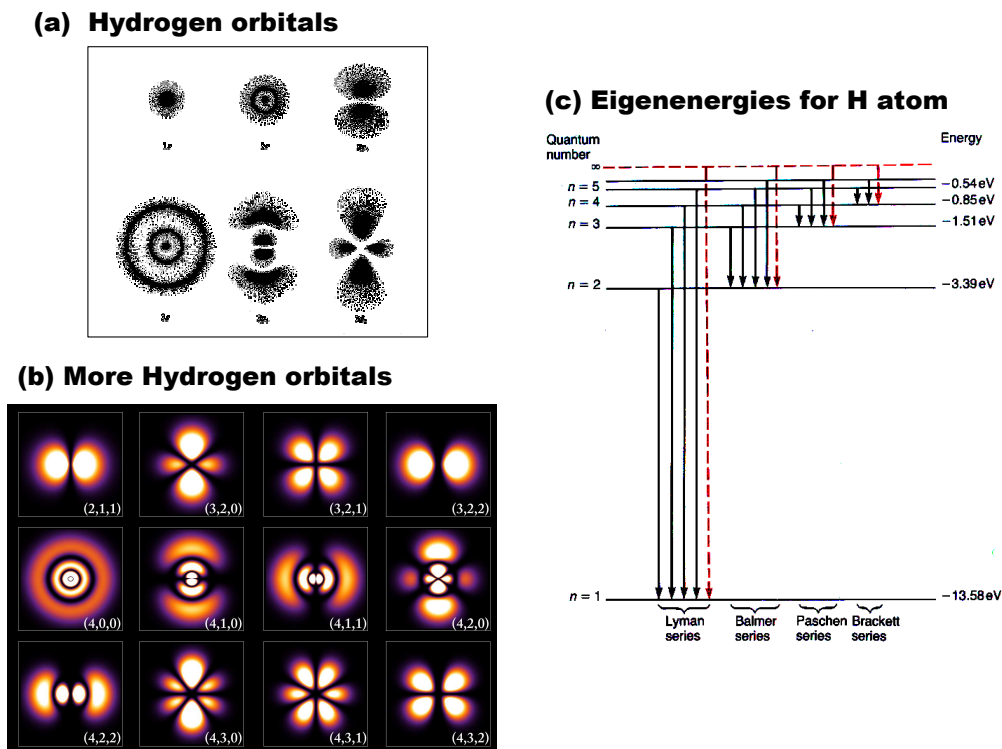


FIG. 7: The bound states for an electron in the attractive Coulomb field of a proton (the Hydrogen atom). In (a) we see the probability densities in 3-d space for some of the lowest energy states (with high density shown dark); and in (b) we see probability densities for some of the higher energy states (with high probability shown light). In (c) we see some of the energy levels, along with possible transitions between the states having different energies, and the sequence of spectral lines these correspond to. See text for more details.

(i) The electron states of lowest energy are concentrated near the proton. This is exactly what we would expect, because by being close to the proton they are in a region of very low potential energy. Notice also that these lowest energy states have few or no oscillations in their shape. Higher energy states are further away from the proton, and show more and more oscillations. Again, this is what we would expect from what we have seen in the bound state models already discussed above.

(ii) the shapes are essentially those of 'standing waves' around the proton. However, because we are 3 dimensions, these waves not only oscillate as a function of the distance away from the proton (ie., they show 'radial oscillations' like spherical ripples, around the proton), but they also oscillate as we move in a path around the proton, ie., they show oscillations as a function of angle.

(iii) There are of course many possible transitions between the states. Physicists have given some of the sequences of transitions names, in order to classify them. Those transitions between all the different 'excited' bound states and the ground state form a series called the Lyman series. However one can also have the set of all transitions between the first excited state (ie., the  $n = 2$  state) and all higher states; this is called the Balmer series. Two other series, involving transitions between either the  $n = 3$  or  $n = 4$  states, and all other bound states, are also shown in Fig. 7(c). The key feature to note here is that only certain discrete energies are allowed for these transitions, ie., the exact difference in energy between some pair of eigenstates.

These sequences of transitions were known well before Quantum Mechanics - they showed up in the spectra of stars and of either glowing hot gases, or in cold gases illuminated by white light. The radiation emitted by a hot gas (like a star) is coming precisely from transitions in which an excited atom loses energy by emitting a photon at one of the allowed energies. This is known as an emission spectrum - it consists of a set of bright lines at different precise frequencies in the spectrum of the starlight. But starlight also contains dark lines - these arise because light from a very hot region of the star's surface then passes through colder gas. The colder gas can then absorb light at certain allowed frequencies (see Fig. 8(a)). What are these frequencies? They depend of course on what are the atoms in



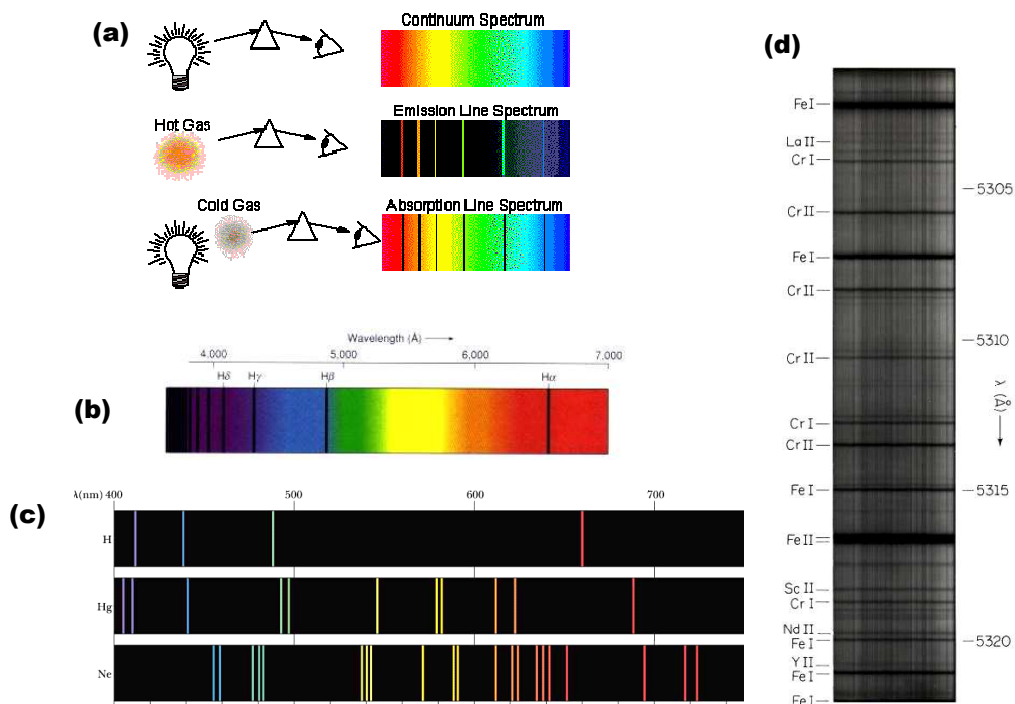


FIG. 8: Some aspects of light spectra. In (a) we show how a continuous spectrum (ie., 'white light') can be produced by some 'black body', how a hot gas will produce a set of emission lines, and how white light passed through a cold gas will give a set of absorption lines. In (b) we see the absorption spectrum of cold  $H$  gas, in the visible light regime (wavelengths between 4000-7000 Å). In (c) we compare the emission lines from hot gases of  $H$ ,  $Hg$  and  $Ne$  (the latter two being used in lamps). Finally in (d) we look at a very small section of the visible absorption spectrum (for wavelengths roughly between 5300-5320 Å) for light emitted from the sun - the ionic species responsible for some of the lines are indicated. See text for more details.

the gas doing the emitting or the absorbing. But in all cases the allowed frequencies are given by the fundamental relationship  $\nu_{nm} = \epsilon_{nm}/\hbar$ , where the energy  $\epsilon_{nm}$  is just the difference in energy between the 2 atomic states involved:

$$\epsilon_{nm} = \hbar\nu_{nm} = E_n - E_m \quad (0.10)$$

In other words, all possible pairs of levels can be involved. The resulting absorption spectrum for  $H$  is in the range of visible light shown in Fig. 8(b). We see only a few lines - this is because most of the transitions take place in either the ultraviolet (for high-energy transitions) or the infrared (for the large number of low-energy transitions). Only transitions in the energy range from roughly 1.7-3 eV are in the visible light range.

Now the energy level structure of the  $H$  atom is actually quite simple - there is only one electron involved. All other atoms contain many electrons and the number of possible transitions can be very large indeed. For this reason the spectra of the heavier elements are usually much richer (see Fig. 8(c)); and the spectrum of each element is quite different from the others, so that this spectrum acts as a 'fingerprint' for the element concerned. Moreover what one sees in the spectrum will depend on temperature, because if the temperature is very high (ie., there is a lot of thermal energy around), many atoms will be in the higher energy levels, and so the emission from these levels will be much stronger. We see that the spectrum of a gas can tell us a great deal about it - what chemical species are in the gas, and at what temperature.

When we come to the spectrum of a star, the spectra are often extremely complex - in the spectrum of the sun, for example, over 100,000 lines have been identified (see Fig. 8(d)). However with a lot of work, it is possible to identify which elements these come from. In fact we can do a lot more - we can tell what state the elements are in (whether they are in atomic form, or if they are ionized, ie., with one or more electrons missing), and also what temperature they are at, what the gas density is, etc...and if there are any molecules, we can also see these. The result is that we know in incredible detail what is the chemical composition of the sun, and of millions of other stars, and at what temperature the various chemical species are found in them. More details on this topic are found in the course slides.

**Chemistry: Electronic States in Molecules:** The hydrogen atom that we just looked at above is the simplest chemical system that exists in Nature (unless you could ionized Hydrogen, ie., an H atom stripped of its electron - this of course leaves nothing but the nucleus, ie., a proton). But what happens when we try to put atoms together? We know that these form molecules, but how? This was one of the great mysteries about the world around us before the discovery of Quantum Mechanics - how on earth did we get such a variety of materials and substances in Nature? It was easy to say that the different elements somehow mixed together to make 'composites' that were more complicated, but this is really just a kind of 'bla-bla' scenario - lots of talk, but no detail on how this is supposed to happen, why certain structures form and not others, why each one has the properties it does, and so on. This is the subject of Chemistry - how to explain the bewildering array of molecules in Nature, their structures and properties, their energetics, the transformations taking them from one to another (ie., chemical reactions), and so on.

Let's first remind ourselves of what is involved in understanding chemistry. In Fig. 9(a) we show a simple molecule, the ethene or "ethylene" molecule. This is formed from 2 Carbon atoms and 4 Hydrogen atoms, with chemical formula  $C_2H_4$ . The 2 images at the top of Fig. 9(a) show some of the electron clouds for the molecule, both before the 2 Carbons join (at left), and after they join (at right); and just below we see the "ball and stick" representation of the molecule, which is a simple way of seeing how the different atoms in the molecule are arranged. In the top left image of Fig. 9(a) we see what we might think of as 2 separate  $CH_2$  ions; each of the Carbons has various electrons clouds sticking out (the  $sp_2$  and the  $p$  orbitals) as well as having already binded to itself 2 Hydrogens. But how is this binding accomplished? On the right-hand side of Fig. 9(a), we see how things look when the 2 C ions have joined - there are no more electron orbitals sticking out; in fact the orbitals from each C ion have now joined to form what are called 'double covalent bonds', which bind then together and give us the whole  $C_2H_4$  molecule. The 'double bond' structure is indicated by the double lines between the C atoms, in the ball-and-stick picture.

A more complicated and rather illuminating example is shown in Fig. 9(b). This is the 'benzene' molecule, with formula  $C_6H_6$ . In the 19th century the structure of this molecule was considered to be something of a mystery until the chemist *Kékulé* discovered the solution, which is shown in ball-and-stick form on the left hand image of Fig. 9(b) (according to legend, *Kékulé* discovered this structure as a consequence of a dream, in which he saw a 'fire dragon' eating its own tail). Now we can imagine 2 different ball-and-stick structures, depending on which C atoms are linked by double bonds and which ones by single bonds - each of these is associated with a quantum state, and we call these 2 states  $|1\rangle$  and  $|2\rangle$  respectively. If we now look at the real space images showing where the C electron clouds are in one or other of these structures, we find that they are as shown in the upper colour image in the right-hand part of Fig. 9(b) - they are all sticking out perpendicular to the ring. However this is not actually what the benzene molecule looks like, at least in its lowest energy 'ground state'. The actual ground state is

$$|\Psi_o\rangle = \frac{1}{\sqrt{2}}(|1\rangle + |2\rangle) \quad (0.11)$$

ie., a superposition (called a 'hybridization' by chemists) of the two states. The distribution of the electron clouds for this superposition or hybrid is shown in the lower right colour image of Fig. 9(b); we see that the electron orbitals associated with the C atoms have now actually spread out and joined into rings, situated on either side of the benzene plane. This looks like a nicer and more symmetric picture - but why does it do this, and indeed, why do the orbitals merge in this way, in this kind of chemical bonding?

In Fig. 9(c) we show a 'toy model' which is able to explain the main mechanism at work here. We show 2 potential wells, each containing a particle of mass  $m$ . The only difference between these 2 wells is that they do not have the same spatial extent - one of them is wider than the other. However the effect on the energy levels of the bound states is very interesting and important - we see that by widening the wells, we actually *lower the energy levels*. Why is this? We can see what is going on if we look again at the lowest energy bound state (the ground state) in, eg., the square potential well in Fig. 6(a). This ground state has a wavelength given by roughly twice the size of the binding potential, ie., the width of the potential well. Now if we try and 'squash' the wave, to make it fit into a smaller length, we simply shorten the wavelength. The effect of doing this can be seen very simply, just by looking at the higher excited states in the same potential well - we see that we actually increase the energy. In fact, we can see that the next excited state, with half the wavelength, has an energy 4 times higher, and the next excited state, with one-third the wavelength of the ground state, has an energy 9 times higher. The general relationship is then that the energy of the state  $E \sim 1/\lambda^2$ . From this we can see that if we confine a system to a length scale  $L$ , then its ground state energy must go like  $E_o \sim 1/L^2$ . Actually, the complete equation reads as follows:

$$E_o \sim \frac{\hbar^2}{2mL^2} \quad (0.12)$$

so that we also see that if we increase the mass  $m$  of the particle, we also lower the ground state energy.

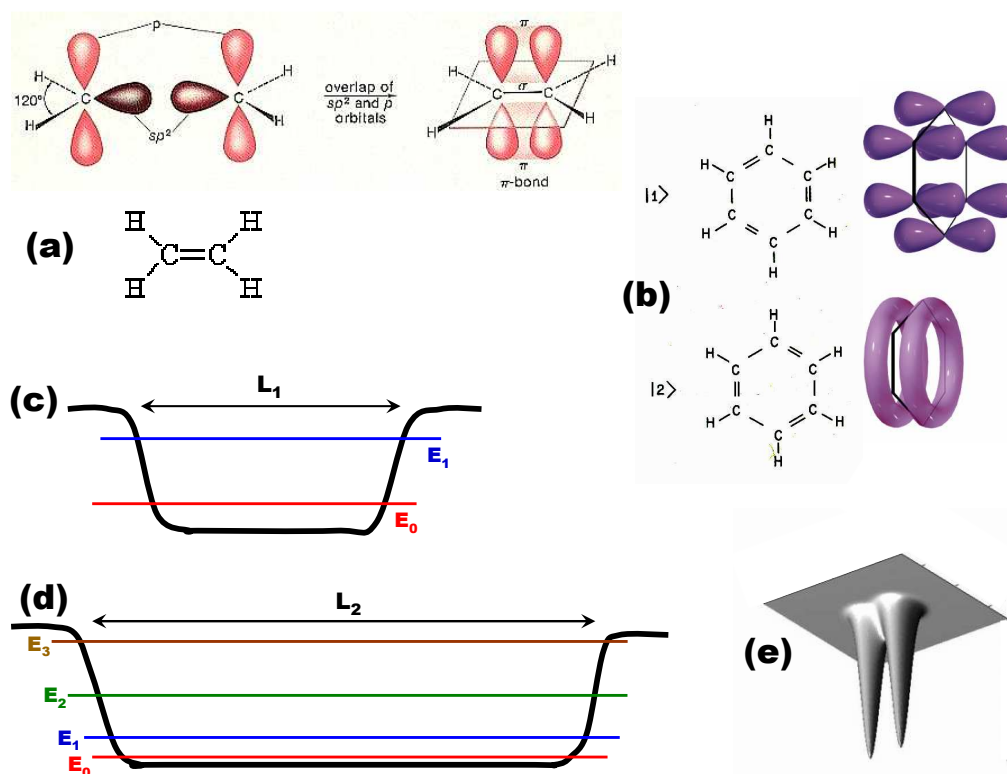


FIG. 9: Chemical bonding in Nature. In (a) we show the Ethene molecule  $C_2H_4$  - the left top image shows the C electron clouds before the 2 inter-Carbon bonds are formed, and the right top image shows it after the molecule has formed. The arrangement of atoms in a 'ball-and-stick' notation is also shown. In (b) we show the benzene molecule  $C_6H_6$ ; at left we shown the 2 states in ball-and-stick notation, which then 'hybridize' to form the molecule. The unhybridized form is shown in the image at top right, the hybridized ground state is shown at lower right. In (c) and (d) we show the lowest energy levels for 2 different potential wells differing only in their spatial extent (they have widths  $L_1$  and  $L_2$  respectively). In (e) we see the double attractive potential well acting on an electron, produced by 2 H nuclei close to each other.

I won't give any kind of justification of this equation here (nor will I expect you to be able to derive it), but we will use it immediately below. Let's first see how it explains chemistry. Suppose we bring 2 atoms together - to make it simple we can imagine we have 2 H atoms. Before they come together, each atom has one electron bound to the H nucleus (a proton) by a strong electrostatic attraction, giving the usual single potential well. In fact the radius of the H atom is very small - only about  $0.5\text{\AA}$  (here  $1\text{\AA}$ , called "1 Angstrom", is a length of  $0.1\text{ nm}$ , ie.,  $10^{-10}\text{m}$ ). Thus the H potential well is very narrow. Now if we bring 2 nuclei close to each other, we get a 'double well' potential, shown in Fig. 9(e), formed by the 2 protons together. The following things then occur:

(i) each of the electrons that are bound to their respective proton can now spread its electron cloud over both potential wells. This is very important - it allows the electrons to greatly lower their energy, by the mechanism we have just discussed. It also means that the new ground state of the electrons has a quite different shape from the ground state they have when in a single isolated H atom - now the ground state envelops the 2 nuclei. This new electron cloud can be thought of, roughly, as a kind of 'joining' of the clouds that exist around each isolated atom - it is in fact the shape of the chemical bond.

(ii) by having part of their electron clouds between the 2 protons, they 'screen' the normally repulsive force between these protons - instead of each proton seeing the repulsive force of the other, they instead see the electrons situated between them, towards which they are attracted.

The main result here is that the system has a much lower energy when the electrons are allowed to spread out and cover the pair of atoms. This is the key to chemical bonding - that the electrons can lower their energy by spreading out, and thereby forming a link between different atoms. And if we look at any of the huge variety of molecules in Nature, we see that their structures are largely determined by this simple consideration. The wave-function of the electron adapts itself, by making superpositions of different states, so that it can spread out and lower its energy as much as possible. And, just like the H atoms, there will be lots of higher energy states associated with the electrons

in each molecule, which we can probe in exactly the same way as we did with the H atom, ie., by using spectroscopy, and looking for the absorption and emission lines. Every molecule and every ion has its own unique pattern of energy levels, and hence its own spectral signature, which allows it to be identified, whether it be in a lab on earth, or in a far distant quasar. It is for this reason that we know far more about the constitution and structure of the stars, than we will ever know about what is happening only a hundred km below our feet.

## B.2: UNBOUND STATES in QUANTUM MECHANICS

It is of course a matter of common experience that many physical systems are not bound or 'trapped' at all, but are free to move around. Objects moving in space have a great deal of freedom (although they may actually be trapped in a large volume - thus, eg., the earth seems to move freely in space, but it is actually confined to move in the region of the inner solar system, by the deep gravitational potential well of the sun). And of course photons spend most of their time flying freely through space. So how does quantum mechanics treat these 'unbound' or almost unbound systems?

The answer, as noted already at the beginning of this section, is that the unbound quantum states move like waves. We have seen much of this behaviour already, in looking at the dynamics of waves in optics and EM theory. Just as in the case of EM waves, water waves, or sound waves, we expect the waves representing the quantum states to be refracted, diffracted, etc., and to show interference effects. There are also other effects we did not discuss in the sections on EM theory, which turn out to be of key importance for quantum systems - most notable amongst these is 'quantum tunneling'.

In what follows I briefly describe the main characteristics of the wave-functions and wave propagation for quantum particles moving through space.

**Propagation of Quantum Superpositions in Space:** The interesting and important thing I want to do here is to give you an intuitive grasp of what is going on, and in fact a large part of this intuition was already given by Huyghens, way back in the 17th century. The key point here is that in ordinary space, we can think of quantum states propagating in space like waves. And, as Huyghens pointed out, a good way to think about the propagation of any wave is to think in terms of the propagation of 'wavelets' from every point on a wavefront. If we start with some wavefront, of some shape, then the subsequent time evolution of the wave can be thought of as arising from the emission, from every different point on this wave front, of a little 'wavelet'. Then, later on, the new wavefront will be produced by adding together all the little wavelets.

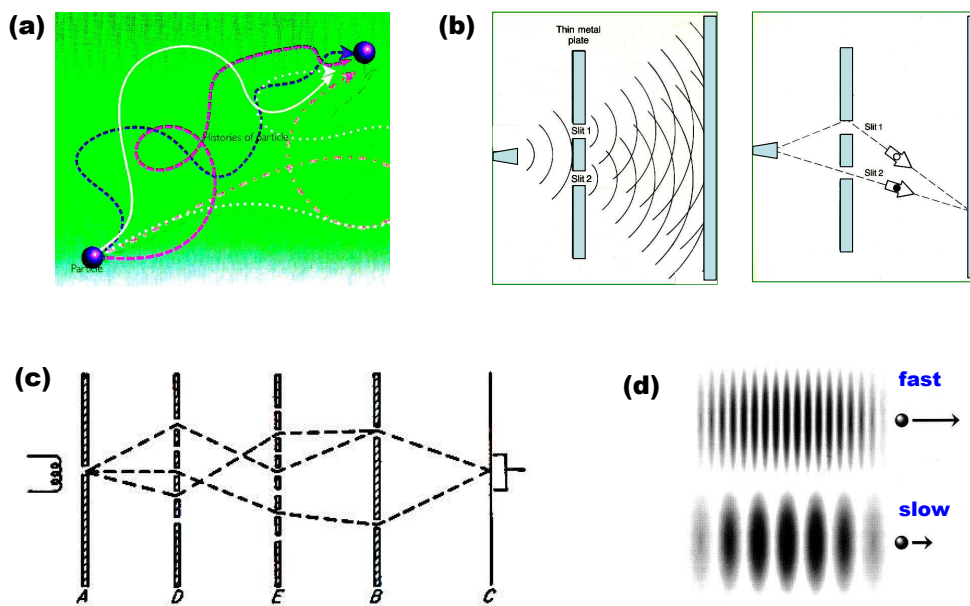
Some 20 years after the discovery of quantum mechanics, Feynman (in his PhD work) found another way of doing this which was equivalent but much more graphic. Instead of starting off by talking about the propagation of waves, he began by discussing the propagation of particles - he imagined that if a quantum particle is at some point  $\mathbf{r}$  in space at some time  $t$ , then immediately afterwards it can go off in any direction along some path, and that its actual time evolution will be obtained by adding together all possible such paths, with a weighting factor for each one. *However*, the weighting factor for each path is actually given by a wave amplitude - essentially this weighting factor oscillates along the path. Thus when one adds up all the paths, some paths contribute more than others, because some of them add together constructively (the wavefronts are synchronized and so add together), whereas others add destructively (a wavefront for one coincides with a 'trough' for another, and we say that the 2 waves are 'out of phase' with each other).

The basic ideas here are illustrated in Fig. 10. In Fig. 10(a) we see how a particle propagates in free space, by following literally all possible paths between 2 points. In Fig. 10(b) we see the wave picture again, of propagation of a particle through a 2-slit arrangement. In the language of paths, the particle can go along any one of the paths that takes it through one or other of the slits, and when we sum over all of these paths, we see that we can think of it as going through both slits simultaneously. Now the key is that because it travels along the paths like a wave, we can think of the paths radiating out from each slit like a wave - and then we recover the familiar wave interference for the 2-slit experiment, that we have already seen for classical light waves. So the result of Feynman, that if we sum all paths coming out of, eg., slit 1, considered here as a small almost 'point-like' radiator, the sum looks just like a wave radiating out from slit 1. The remarkable thing is then that the Feynman and the Huyghens constructions are actually mathematically equivalent - the Huyghens construction is just allowing propagation from all points along the wavefront. But the Feynman construction is much more direct, because it graphically illustrates the idea that in its motion, a quantum state will attempt to find a way to every other state that is accessible to it, ie., to explore all possible superpositions of the available states.

Moving now to Fig. 10(c), we look at a generalization of the 2-slit experiment, where the particle goes through a sequence of 'gates', and can pick any one of a number of paths through the different gates. We can think of the particle 'choosing' at any point which gate it will next go through, or, when following a continuous path, which way it will go next. The essence of quantum superposition is then that it will not just pick on or other of the choices - it

will pick ALL of them simultaneously. The remarkable thing is, again, that the net result is that the quantum state ends up propagating like a wave from each one of these slits, spreading out across every region it can.

Finally, we can ask: what happens if we finally remove all of these slits? Then we just get a propagating wavefront, as Huyghens said so long ago. This is shown in Fig. 10(d); we see 2 different waves, with different wavelengths and of course different frequencies, propagating along in some direction.



### “SUM OVER PATHS” and QUANTUM STATE PROPAGATION

FIG. 10: The propagation of a particle in quantum mechanics. In (a) we see the ‘sum over paths’, in which a particle follows all possible paths simultaneously between 2 points; in (b) this propagation is shown in as a wave propagation, and in (c) we see some of the paths through a multi-slit ‘multiple choice’ system. Finally (d) shows the propagation of 2 plane wave quantum states - the short wavelength one is moving faster than the long wavelength one. See text for more details.

Now all of this is looking very much like things we have already seen, in our discussion of EM waves. From this we know that any wave can be entirely described in terms of its wavelength (ie., the distance  $\lambda$  between successive wave crests), and its amplitude. The amplitude for a conventional water wave would just be the height of the wavecrests; for a sound wave it would be the amplitude of the oscillations in pressure of the medium (air, water, or some solid) through which the sound moves; and so on. So does this mean that Quantum states are just like classical waves? And if so, what is the fuss all about?

The answer to this question will not be fully described until we have covered all three of the documents in this series. However the bottom line is that for the quantum state, the amplitude at some point in space is not a *classical* amplitude, as it might be for a water wave. In fact the amplitude turns out to be connected to the *probability* of finding the particle at this point in space. This result is so strange that it needs a whole discussion on its own - in part III of this series.

**Dynamics of the Wave-function:** Since quantum states propagate in space like waves, it is important to understand how they do this.

We recall the key result that if a wave is moving past a point with some velocity  $v$ , then at this point we will see the wave amplitude oscillate at a frequency  $\omega$  per second, because  $\omega$  wavecrests go past each second; and that

$$\omega = \frac{v}{\lambda} \quad (0.13)$$

since the total distance traveled by the wave in one second is  $v$  metres, and each wave takes up a length of  $\lambda$  metres.

So the obvious question to ask now is - how fast do the quantum waves move, and what are their frequencies and wavelengths? We will look at this question for 2 kinds of particle, viz., photons and electrons.

(i) *Dynamics of Photons*: For photons we have actually already seen the answer, since it is the same as what we found for EM waves. Thus for photons we have a frequency of oscillation  $\omega = c_o/\lambda$ , where  $c_o$  is the velocity of light. You will recall that for visible light, the wavelength  $\lambda$  is pretty small - for example, for green light, the wavelength is about  $5000 \text{ \AA}$ , ie.,  $\lambda \sim 5 \times 10^{-7} \text{ m}$ . Since  $c_o$  is enormously high - in fact  $c_o \sim 3 \times 10^8 \text{ m/s}$ , ie., 300,000 km/s, this means that an enormous number of wavecrests pass by each second - the frequency of green light is  $\omega \sim (3 \times 10^8)/(5 \times 10^{-7}) = 6 \times 10^{14} \text{ Hz}$  (where the unit "Hz" means number of times per second). On the other hand for much longer wavelength EM waves, like radio waves, the frequency is much lower. Typical frequencies of radio waves you get on your car radio are around 100 MHz, ie., 100 million Hz or  $10^8 \text{ Hz}$  (the names of radio stations often tell you this frequency; eg., "Rock 101" has a frequency of 101 MHz). Now a wave of frequency 100 MHz is easily seen to have a wavelength of 3 metres, which is similar to a sound wave in the audio range of frequency 100 Hz. These wavelengths are important - because they are so long, both radio waves and sound waves are very easily diffracted, and can 'go around corners'. This is why you can hear a sound around a corner, and why radio signals can be picked up even when you are blocked from seeing the transmitter. On the other hand visible light is only very weakly diffracted - this is why we think of it as traveling in rays.

In quantum mechanics there is only one extra ingredient here for light. It is that each photon, whose amplitude in space looks like a wave, is also associated with a packet or 'quantum' of energy. This energy  $E$  is uniquely related to its wavelength, by the fundamental relation  $E = \hbar\omega$ , where  $\omega$  is the frequency as before, and  $\hbar = h/2\pi$ , where  $h$  is Planck's constant (thus  $\hbar$  is very small - in fact  $\hbar \sim 10^{-34} \text{ Js}$ ). We are thus led, for photons, to the result that their energy is given by

$$E = \hbar\omega = \frac{\hbar c_o}{\lambda} \quad (\textit{photons}) \quad (0.14)$$

We have actually used this result already above, in discussing spectral lines. We saw that a photon with a wavelength of  $\lambda \sim 4000 \text{ \AA}$  had an energy  $E \sim 3 \text{ eV}$ ; and now we see that a very long wavelength photon, such as that in a radio wave, will have a much lower energy.

There is actually another way to look at this. In physics we say that photons have no 'rest mass', meaning that they cannot exist as particles with some mass, moving at some arbitrary velocity  $v$ . Thus the usual Newtonian relation that  $E = \frac{1}{2}mv^2 = \frac{p^2}{2m}$ , where  $m$  is the photon mass and  $v$  its velocity, is meaningless for photons. Photons can only move at a velocity  $c_o$ , and they have no rest mass. However they DO have a momentum (if a photon hits something, it actually gives it a push). And this momentum, for a photon, is given by  $p = \hbar/\lambda$  (which has nothing to do with either the photon velocity or any fictitious mass for the photon). In other words, we also have the relationship

$$E = \frac{\hbar c_o}{\lambda} = pc_o \quad (\textit{photons}) \quad (0.15)$$

for photons - their energy and mass are just proportional to each other! This is very different from what happens for a slow-moving massive particle of mass  $m$ , which we discuss below. The difference is actually understandable in relativity theory - photons are 'relativistic particles', whereas an ordinary massive particle cannot move at the velocity of light.

This completes our discussion here of photons - we see that a photon has basically 2 properties, viz., its wavelength  $\lambda$ , referring to its motion in space, and its polarization, which we can think of roughly as its 'spin'. The classical 'amplitude' of a light beam (ie., its intensity) turns out to be just proportional to the number of photons. Thus a very high intensity laser pulse is just a set of very many photons, all concentrated in a very small volume.

(ii) *Dynamics of Massive Particles*: Let us turn now to the propagation of a particle like an electron. The key difference with a photon is that a photon has no mass. In this case we can also consider a plane wave quantum state, just as we did for the photon (as in Fig. 10(d)). However now the relationship between the energy and the wavelength is actually quite different. We still have the relationship  $E = \hbar\omega$  between the energy and the frequency. But, unlike the photon, which is a relativistic particle with no 'rest mass', we are now dealing with a slow-moving object which has a mass  $m$ , and is described by a momentum  $p = mv$  and an energy given by  $E = \frac{1}{2}mv^2 = \frac{1}{2m}p^2$ . The question that was answered by de Broglie, even before the discovery by Schrodinger of the wave formulation of quantum mechanics, was: what is the relationship between the velocity and the momentum for a massive particle? His answer was given by the key relationship

$$p = mv = 2\pi \frac{\hbar}{\lambda} = \frac{h}{\lambda} \quad (\textit{slow massive particle}) \quad (0.16)$$



(remember that  $\hbar = h/2\pi$ , so that  $h = 2\pi\hbar$ ). This equation is valid if the particle is moving at a velocity much less than that of light. Thus we see that the wavelength now for a particle is not inversely proportional to the energy, although it is still inversely proportional to the momentum. In fact, since  $E = \frac{1}{2m}p^2$  for a massive particle, we have instead that

$$E = \hbar\omega = (2\pi)^2 \frac{\hbar^2}{2m\lambda^2} = \frac{h^2}{2m\lambda^2} \quad (\text{slow massive particle}) \quad (0.17)$$

so that if we increase the wavelength of the particle, instead of the energy decreasing in proportion to this, it goes down like the inverse SQUARE of the wavelength. Or, to put it another way, if we try to make short wavelength quantum states for a massive particle, we get a rapid increase in their energy - for example, halving the wavelength increases the energy by a factor of 4.

It is useful to see some examples here with numbers. Suppose, for example, that we have an electron, which has a very small mass - the electron mass is  $m_e \sim 10^{-30}$  kg. Suppose the electron is moving at a velocity of 1 m/s, so that its momentum  $p$  is then  $p = mv = 10^{-30}$  kg m/s. But then it follows that the wavelength  $\lambda$ , given by the de Broglie relation (0.16), is just  $\lambda = \hbar/p$ , ie., we have  $\lambda \sim 10^{-34}/10^{-30} = 10^{-4}$  m, which is 0.1 mm (just visible to the naked eye). This is a long wavelength - much longer than that of light, for example, and far bigger than the size of an atom. Consider instead an electron with wavelength roughly the size of an atom (suppose, eg., it is confined to the atom, in a bound state). Then we have a wavelength  $\lambda \sim 1\text{\AA} = 10^{-10}$  m. So what then is the velocity of the electron? We have that  $p = mv = \hbar/\lambda$ , so that  $v = \hbar/m\lambda$ . Now we find that, since the wavelength has decreased by a factor  $10^6$ , and the velocity is inversely proportional to the wavelength, the velocity must have increased by  $10^6$ , to become  $10^6$  m/s (or  $10^3$  km/s. This is pretty fast - it would take you from Vancouver to Toronto in just over 3 seconds (however it is still 300 times less than the velocity of light!). Thus, if we think of an electron inside an atom 'bouncing around' inside the Coulomb binding potential, we see that its typical velocity is very high indeed.

As far as the energy is concerned, the relationship (0.17) between energy and wavelength can be employed in another way. Suppose we consider a bound state as a kind of 'standing wave', produced by a traveling wave bouncing back and forth inside a potential well. But then, for the ground state, where the wavelength  $\lambda \sim L$ , the size of the potential well, we immediately get back the relation that we used above, in equation (0.12). In this way we can justify, at least in a rough and ready way, our explanation of how chemical bonds work.

**Quantum Tunneling:** Finally, let us look at a very counterintuitive property of waves and of quantum states. Suppose we have a quantum state that is trapped inside some potential well, but that outside the potential well, the potential energy falls again - sort of like a crater with a high outside wall, so that the region outside the crater is also at low energy. Alternatively we can also imagine a situation where a free unbound quantum state is traveling happily along until it meets a potential barrier, ie., a region of high potential energy, such that the barrier energy is actually higher than the energy of the incoming particle - but also such that the barrier is limited in spatial extent, so that on the other side of the barrier, the potential energy is again low. What will it then do?

In Figs. 11(a)-(c) we actually show such a situation. In Fig. 11(a) we see a particle approaching a potential barrier - the particle is of course described by a quantum wave state, and its energy  $E$  is lower than the barrier height. Now *classically* we know what would happen - the particle would simply be reflected back off the barrier. However a wave will not do this - part of it will be reflected for sure, but part of it will also 'leak through' to the other side. If you have ever looked through a thin sheet of Gold you will have seen this (one sometimes finds such thin sheets on windows, eg., windows of banks); part of the light is reflected and part of it goes through. Normally Gold does not allow the transmission of light - a piece of Gold is opaque, because the photons would have to have really high energy to get into it (light has a very high potential energy in gold). But light can leak through a very thin sheet of Gold. We call this phenomenon "*quantum tunneling*", and it can happen to any quantum state.

In Figs. 11(b) and (c) we see one example of this; they depict the potential well for nucleons (ie., protons and neutrons) inside the nucleus of an atom. Fig. 11(b) shows the potential well at 'large scales', ie., extending a long way from the nucleus, and Fig. 11(c) shows the situation close into the nucleus. Now the force between nucleons has two components. First, there is the Coulomb repulsion between the protons (since they all have positive charges). As we have seen before, this falls off like  $\sim 1/r$  at long distances - so it is still there at very long range, even though a lot smaller. The second component is called the 'strong force'; it is attractive, and it acts between protons and neutrons alike (ie., it causes protons to be attracted to each other and to neutrons, and it causes neutrons to be attracted to each other). This force is much stronger than the Coulomb force, but it is short-ranged - by the time the nucleons are separated by a distance only a little more than their size, it has practically disappeared.

We see the net result at short ranges in Fig. 11(c), where the potential felt by a neutron in the nuclear region is shown in red/pink, and the potential felt by a proton is shown in black. The potential felt by a neutron is just coming from the strong force - it is neutral, and so does not feel the electrostatic Coulomb force. We see that the neutron finds itself in a deep potential well inside the nucleus, held in by the attraction to all the other nucleons. The proton

is also in a well, but it is not so deep, because it is also feeling the repulsion from the other protons. Notice now what happens when we emerge from the nucleus. The potential for the neutron is now flat - it feels no force at all. But the potential for the proton starts to fall slowly as we recede from the nucleus - this is the effect of the Coulomb repulsion.

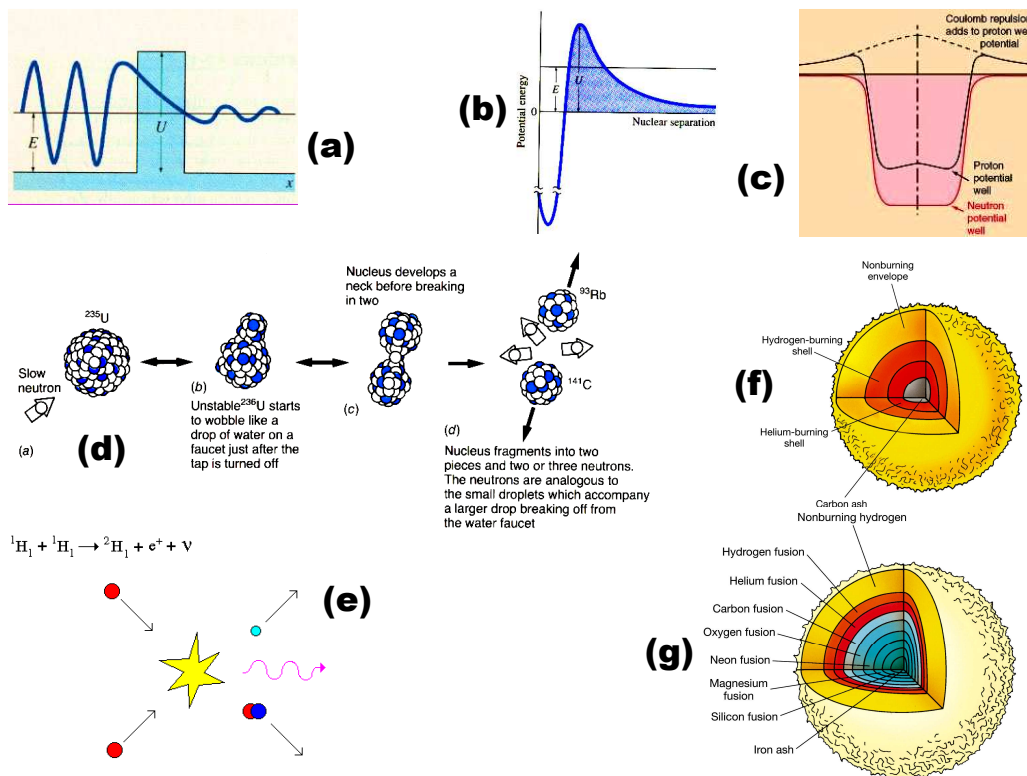


FIG. 11: Quantum Tunneling. In (a) we see tunneling through a potential barrier, with a wave incident from the left and emerging on the right. In (b) we see the potential energy for a nucleon in the region of a nucleus, and (c) is a close-up of this, with both the neutron and proton potential shown. In (d) we see the fission decay of a heavy  $^{235}\text{U}$  nucleus, after it has absorbed a neutron, and in (e) we see the fusion of 2 protons, which then form a deuteron (proton plus neutron) by emitting an electron and a high-energy gamma ray. In (f) we see the typical core structure of a light star like the sun, in which H nuclei fuse to make He nuclei, which then fuse to make C nuclei. In (g) we see the structure of a supergiant star, in which the fusion continues all the way to Fe.

In Fig. 11(b) we now see the net effect of this at longer distances from the nucleus. If the proton is initially at a high energy inside the nucleus, it can actually be at an energy higher than the potential energy from from the nucleus. This means it can tunnel through the barrier to escape from the nucleus. In other words, unlike a similar classical state, it is not bound at all. We say the nucleus is metastable - a proton or other charged particle will hang around inside the nucleus for a while, but eventually it will escape.

It is this tunneling that is responsible for radioactivity - which is the name we give to the emission of high-energy particles from the atomic nucleus. Typically these particles can be objects like a He nucleus (ie., a composite of 2 neutrons and 2 protons), or a deuteron (a composite of one proton and one neutron), plus perhaps a gamma ray (ie., a high-energy photon). And the way they escape is by tunneling - the particles pass through the barrier, and then when they reach the repulsive part of the potential for outside the nucleus, they are accelerated away from it at high velocities (approaching the speed of light). This is a simple kind of "nuclear fission". A much more dramatic kind of fission arises if a heavy nucleus absorbs a neutron - by forcing the protons a little farther apart inside the nucleus, it makes it less stable (the Coulomb repulsion now becomes a little more important relative to the strong force). Now one process that is possible is the fission of the entire nucleus - which look roughly like what is seen in the Figure.

One can also have the reverse process to fission, called "fusion". This can happen with nuclei when the energy of the particles outside the barrier (ie., outside the nucleus) is high enough so that they can tunnel in. For this to happen, they must be moving very fast. This is what happens in the centre of stars - the temperature is so high that charged particles can ram their way, by tunneling, through the potential energy barrier surrounding the nucleus. This

process is what powers the stars, whose initial composition is almost entirely H and He. At the centre of a light star like the sun (see Fig. 11(f)), the H nuclei fuse to form He (by first forming deuterons, which then fuse to form He); we can then fuse 3 different He nuclei to form a C nucleus. Very large energies are released in the form of gamma ray photons by this process - these photons eventually get out of the sun, and produce the radiation of the sun. The process in light stars stops with C; the temperature is simply not high enough for the C nuclei to be fused (the central temperature of the sun is 14.7 million degrees). However in supergiant stars, with masses greater than roughly 15 suns, the star can contract slightly, thereby heating its centre, and the temperature can rise eventually to billions of degrees; this allows the C nuclei to fuse, and a complex sequence of fusion reactions continues to produce ever heavier nuclei, until one gets to Iron (Fe); see Fig. 11(g). However, fusing Fe with anything does not produce energy - it actually *requires* it. So suddenly the star has run out of fuel, and it reacts by collapsing. When it reaches nuclear densities, the 'rebound' caused by the very strong really short-range repulsion between nucleons causes the star to explode, which is what we see as a supernova. The central remnants will then either collapse to form a neutron star, or, if they are massive enough, to a black hole.

Tunneling is important everywhere in physics - most chemical reactions involve tunneling of electrons between different molecules or inside a molecule, and in most modern electronic devices, tunneling plays a key role.

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This concludes part I of our discussion of quantum states. In it we have learned how states in quantum mechanics are described, and how they can be superposed to make other states. We have also seen how these states propagate like waves, and how they can lower their energy by 'spreading out', or increasing their wavelength. What we still have to do is see what happens when we have 'entanglement' between different states, and how the states actually lead to a description of *probabilities* rather than some unique objective reality. This is what we do in parts II and III.