Title Sampling the Hydrogen Atom

Author Norman Graves

Abstract

Since the emergence of quantum theory just over a century ago every model for the hydrogen atom that has been developed incorporates the same basic assumption. From Niels Bohr through de Broglie and Schrödinger up to and including the Standard Model all such theories are based on an assumption put forward by John Nicholson. Nicholson was the first to recognise that the units of Planck's constant were the same as those of angular momentum and so he reasoned that perhaps Planck's constant was a measure of the angular momentum of the orbiting electron. But Nicholson went one step further and argued that the angular momentum of the orbiting electron could take on values which were an integer multiple of Planck's constant. This allowed Bohr to develop a model in which the differences between the energy levels matched those of the empirically developed Rydberg formula. When the Bohr model was superseded Nicholson's assumption was simply carried forward unchallenged into these later models.

The main problem with Nicholson's assumption is that it lacks any mathematical rigour. It simply takes one variable, angular momentum, and asserts that if we allow it to have this characteristic quantisation then we get energy levels which appear to be correct. In so doing it fails to provide any sort of explanation as to why such a quantisation should take place.

In the 1940s a branch of mathematics appeared which straddles the boundary between continuous functions and discrete solutions. It was developed by engineers at Bell Labs to address problems with capacity in the telephone network. While at first site there appears to be little to connect problems of network capacity with electrons orbiting atomic nuclei it is the application of these mathematical ideas which holds the key to explaining quantisation inside the atom.

Sampling the Hydrogen Atom

In the 1930's and 40's telecommunications engineers were concerned to increase the capacity of the telephone network. One of the ideas that surfaced was called Time Division Multiplexing. In this each of a number of incoming telephone lines is sampled by means of a switch, the resulting samples are sent over a trunk line and are decoded by a similar switch at the receiving end before being sent on their way. This allowed the trunk line to carry more telephone traffic without the expense of increasing the number of cables or individual lines. The question facing the engineers at the time was to determine the minimum frequency at which the incoming lines needed to be sampled in order that the telephone signal can be correctly reconstructed at the receiving end.

The solution to this problem was arrived at independently by a number of investigators, but is now largely credited to two engineers. The so called Nyquist-Shannon sampling theorem is named after Harry Nyquist and Claude Shannon who were both working at Bell Labs at the time. The theorem states that in order to reproduce a signal with no loss of information, then the sampling frequency must be at least twice the highest frequency of interest in the signal itself. The theorem forms the basis of modern information theory and its range of applications extends well beyond transmission

of analog telephone calls , it underpins much of the digital revolution that has taken place in recent years.

What concerned Shannon and Nyquist was to sample a signal and then to be able to reproduce that signal at some remote location without any distortion, but a corollary to their work is to ask what happens if the frequency of interest extends beyond this Shannon limit? In this condition, sometimes called under sampling, there are frequency components in the sampled signal that extend beyond the Shannon limit and maybe even beyond the sampling frequency itself.

A simple example can be used to illustrate the phenomenon. Suppose there is a cannon on top of a hill, some distance away is an observer equipped with a stopwatch. The job of the observer is to calculate the distance from his current location to the cannon. Sound travels in air at roughly 340 m/s. So it is simply a matter of the observer looking for the flash as the cannon fires and timing the interval until he hears the bang. Multiplying the result by 340 will give the distance to the cannon in metres, let's call this distance D.

This is fine if the cannon just fires a single shot, but suppose the cannon is rigged to fire at regular intervals, say T seconds apart. For the sake of argument and to simplify things, let's make T equal to 1. If the observer knows he is less than 340 m from the cannon there is no problem. He just makes the measurement as before and calculates the distance D. If on the other hand he is free to move anywhere and there is no restriction placed on his distance to the cannon then there is a problem. There is no way that the observer knows which bang is associated with which flash, so he might be located at any one of a number of different distances from the cannon. Not just any old distance will do however. The observer must be at a distance of D or D + 340 or D + 680 and so on, in general D + 340n. The distance calculated as a result of measuring the time interval between bang and flash is ambiguous. In fact there are an infinite number of discrete distances which could be the result of any particular measured value. This phenomenon is known as aliasing. The term comes about because each actual distance is an alias for the measured distance.

Restricting the observer to be within 340 m of the cannon is a way of imposing Shannon's sampling limit and by removing this restriction we open up the possibility of ambiguity in determining the position of the observer due to aliasing.

Let's turn the problem around a little. If instead of measuring the distance to the cannon the position of the observer is fixed. Once again to make things simpler, let's choose a distance of 340m. This time however we are able to adjust the rate of fire of the cannon until the observer hears the bang and sees the flash as occurring simultaneously. If the rate of fire is one shot per second then the time taken for the slower bang to reach the observer exactly matches the interval between shots and so the two events, the bang and the flash are seen as being synchronous. Notice that the bang relates, not to the current flash, but to the previous flash.

If the rate of fire is increased then at first, for a small increment, the bang and the flash are no longer in sync. They come back into sync however when the rate of fire is exactly two shots per second, and again when the rate is three shots per second. If we had a fast enough machine gun this sequence would extend to infinity for a rate of fire which is an integer number of shots per second. It is interesting to note that if the rate of fire is reduced from once per second then the observer will never hear and see the bang and the flash in sync with one another and so once per second represents the minimum rate of fire which will lead to a synchronous bang and flash. In fact what we have here is a system that has as its solutions a base frequency and an infinite set of harmonic frequencies. Suppose now that there is some mechanism which feeds back from the observer to the cannon to drive the rate of fire such that bang and flash are in sync, and suppose that this feedback mechanism is such as to always force the condition to apply to the nearest rate of fire which produces synchronisation.

We now have a mechanism which can cause a value, in this case the rate of fire of the gun, to take on a series of discrete values even though, in theory at least, the rate of fire can vary continuously. Equally important is that if the feedback mechanism is capable of syncing the system to the lowest such frequency then all the multiples of this frequency are also solutions, in other words if the base frequency is a solution then so are harmonics of the base frequency.

This idea of are multiple discrete solutions to a problem which are harmonics of a base frequency is an interesting one since it straddles the boundary between domains in which there are continuous variables, but only discrete solutions. What the example of the cannon shows us is that any system which produces results which are a harmonic sequence must involve some sort of sampling process. This becomes clear if we consider the Fourier representation of a harmonic sequence. A harmonic sequence of the type described consists of a number of discrete frequencies, spreading up the spectrum and spaced equally in the frequency domain with each discrete frequency represented by a so called Dirac function. Taken together they form what is described as a Dirac comb, in this case in the frequency domain. The inverse Fourier transform of such a Dirac comb is itself another Dirac comb, only this time in the time domain, and a Dirac comb in the time domain is a sampling signal.

This link between a Dirac comb in the frequency domain and a corresponding Dirac comb in the time domain means that if ever we observe a set of harmonics in some natural process there must inevitably be some form of sampling process taking place in the time domain.

One such example, in which this relationship has seemingly been overlooked, is found in the structure of the hydrogen atom.

By the beginning of the 20th century it was becoming evident that the universe was composed of elements which were not smooth and continuous but were somehow lumpy or granular in nature. Matter was made up of atoms, atoms themselves contained electrons and later it emerged that the atomic nucleus was itself composed of protons and neutrons.

Perhaps even more surprising was that atoms could only absorb or emit energy at certain discrete levels. These energy levels are characteristic of the atom species and form the basis of modern spectroscopy. The problem facing the scientists of the day was that this discrete behaviour was not associated with the discrete nature of the structure of the atom; that could readily be explained by asserting that any atom contained an integer number of constituent particles. Where energy levels were concerned however, the quantisation effects concerned some sort of process that was taking place inside the atom.

The atom with the simplest structure is that of hydrogen, comprising a single proton surrounded by an orbiting electron and work began to investigate its structure and to understand the mechanisms which gave it its characteristic properties.

The first such theoretical model was proposed by Niels Bohr. Bohr used simple classical mechanics to balance the centrifugal force of the orbiting electron against the electrostatic force pulling it towards the nucleus. He needed a second equation in order to solve for the radius and velocity of the orbiting electron and came upon an idea proposed by John Nicholson. Nicholson had noticed that the units of Planck's constant matched those of angular momentum and so he proposed that

angular momentum could only take on values which were integer multiples of a base value and that the base value was Planck's constant.

Bohr's equations worked, but they threw up a strange anomaly. In Bohr's model each energy level is represented by the orbiting electron having a specific orbit with its own particular orbital velocity and orbital radius. The really strange thing was that in order to fit with the conservation laws, transitions from one energy state to another had to take place instantly and in such a way that the electron moved from one orbit to another without ever occupying anywhere in between. This ability to jump instantaneously across space was quickly dubbed the Quantum Leap in the popular media, a phrase which still has resonance today.

The Bohr model			
$i = m \mathbf{v}_n \mathbf{r}_n = n \hbar$	Equation 1		
K_22			
$\frac{Kq^2}{r_n^2} = \frac{mv_n^2}{r_n}$	Equation 2		
$v_n = \frac{Kq^2}{n\hbar}$	Equation 3		
$r_n = \frac{n^2 \hbar^2}{m K q^2}$	Equation 4		
Where:			
<i>m</i> is the rest mass of the electron			
q is the charge on the electron			
<i>r_n</i> is the orbital radius for the n th energy level			
v_n is the orbital velocity for the n th energy level			
<i>I</i> is the angular momentum			
K is the Coulomb force constant			
ħ is Planck's constant			
Equation 1 represents Nicholson's assumption that angular momentum can on which are integer multiples of Planck's constant	ly take on values		
Equation 2 balances the centrifugal force against the electrostatic force			
Equation 3 shows that the orbital velocity decreases with increasing energy lev	el		
Equation 4 shows that the orbital radius increases as the square of the energy level and leads			
directly to the idea of the Quantum Leap.			

It was widely accepted that the Bohr model contained substantial flaws. Not only did it throw up the quirky quantum leap, but it took no account of special relativity, it failed to explain why the electron orbit did not decay due to synchrotron radiation but most important of all it failed to explain the nature of the quantisation of angular momentum¹. The fact is that Bohr's assumption that angular momentum was quantised lacks any mathematical rigour, the assumption is arbitrary and expedient and does not address the question as to why and how such quantisation occurs but merely asserts that if we make the assumption then the numbers seem to fit. Nevertheless and despite this, the Bohr assumption has continued to be accepted and forms an integral part of every theory which has come along since.

¹ It is also interesting to note that the computed energy of the orbiting electron in fact decreases with increasing energy level thus forcing the introduction of the idea that this was not the energy level of the electron itself but instead was some sort of energy potential or negative energy of the atom. The absorption and emission spectra of the atom are calculated by taking the difference between energy levels and so, with the exception of the odd minus sign, these differences match the values calculated empirically by Rydberg.

In a paper published in 1905 Einstein had shown that light, which had hitherto been considered a wave, was in fact a particle. In an effort to explain quantisation the French mathematician de Broglie turned this idea on its head and suggested that perhaps the electron was not a particle but should be considered as a wave instead. He calculated the wavelength of the electron, dividing Planck's constant by its linear momentum and found that when he did so the orbital path of base energy state contained one wavelength, that of the second energy state contained two wavelengths and so on, in what appeared at first site to be a series of harmonics².

On any other scale the wavelength, which can be associated with orbital path length, is derived as a result of dividing angular momentum by linear momentum. According to Nicholson Planck's constant is an integer fraction of angular momentum. In choosing to substitute Planck's constant in this way what de Broglie was doing was to inherently accepting Nicholson's assumption. Viewed in this light de Broglie's contribution can be seen as less of an insight and more of a contrivance.

Other later models, such as that of Schrödinger, are based directly on the work of de Broglie and therefore inherently follow the Nicholson/Bohr assumption, up to and including the currently proposed Standard Model.

The trouble with all of these models is that Nicholson's assumption was not based on finding any mechanism that leads to angular momentum being quantised in this way. Bohr's assumption was simply expedient – it just happened to give the right answers for the absorption and emission spectra of the hydrogen atom. Having been adopted by Bohr, later theorists simply continued with this working assumption and incorporated it into all subsequent models for the atom, without ever bothering to go back and justify it until now it has become an item of received wisdom.

The year 1905 was an eventful one for Albert Einstein. In that year, he not only published his paper on the discrete nature of the photon but he also published two further seminal works as well as submitting his PhD thesis. The most famous of his other papers concerned the dynamics of moving bodies. This is the paper whose later editions contained the equation $e=mc^2$. The paper was based on a thought experiment and concerned the perception of time, distance and mass as experienced by two observers, one a stationary observer and one moving relative to the stationary observer at speeds approaching that of light.

What Einstein showed was that time elapsed more slowly for the moving observer, that distances measured by the moving observer were foreshortened relative to those same distances measured by the stationary observer and that the stationary observer's perception of the mass of the moving object was that it had increased. All three effects occur to the same extent and are governed by a factor γ (Gamma). The time between two events observed by the stationary observer as time t is seen by the moving observer as time $T=t/\gamma$. Similarly the distance between two point measured by the stationary observer as distance d is seen by the moving observer as distance $D=d/\gamma$. And as far as the stationary observer is concerned the mass of the moving object is seen to increase by this same factor γ .

Gamma is referred to as the Lorenz factor and is given by the formula:

 $^{^{2}}$ In fact they are not harmonics of a single fundamental frequency, but instead each harmonic relates to a different base frequency and these two effects combine in such a way that they form a sub harmonic or inverse harmonic sequence.

Equation 5

$$\gamma = \frac{c}{\sqrt{c^2 - v^2}} = \frac{1}{\sqrt{1 - \frac{v^2}{c^2}}}$$

Both observers agree on their relative velocity, but go about calculating it in different ways. For the stationary observer the velocity of the moving observer is the distance travelled divided by the time taken as measured in his stationary domain. For the stationary observer the velocity is:-

$$v = \frac{d}{t}$$
 Equation 6

For the moving observer the distance as measured in his own domain is foreshortened by the factor Gamma, but the time taken to cover that distance reduced by the same factor Gamma.

$$v = \frac{D}{T} = \frac{d'\gamma}{t'\gamma} = \frac{d}{t}$$
 Equation 7

There is a great deal of experimental evidence to support Einstein's Special Theory. One of the more convincing experiments was carried out at CERN in 1977 and involved measuring the lifetimes of particles called muons in an apparatus called the muon storage ring. The muon is an atomic particle which carries a charge, much like an electron, only more massive. It has a short lifetime of around 2.2 microseconds before it decays into an electron and two neutrinos.

In the experiment muons are injected into a 14m diameter ring at a speed close to that of light, in fact at 99.94% of the speed of light. At this speed the value of Gamma is around 29.33. The muons, which should normally live for 2.2 microseconds, were seen to have an average lifetime of 64.5 microseconds; that is the lifetime of the muon was increased by a factor Gamma. This comes about because the processes which take place inside the muon and which eventually lead to its decay are taking place in an environment which is moving relative to us at 99.94% of the speed of light and where the time, relative to us is running 29.33 times slower. Hence the muon, in its own domain still has a lifetime of 2.2 microseconds, it's just that to us, who are not moving, this appears as 64.5 microseconds.

Traveling at almost the speed of light a muon would normally be expected to cover a distance of 660 metres or roughly 7.5 times around the CERN ring during its 2.2 microsecond lifetime, but in fact the muons travelled almost 20,000 metres or 220 times around the ring. This is because distance in the domain of the muon is compressed so what we stationary observers see as being 20,000 metres, the muon sees as being just 660 metres.

During its lifetime the muon completes some 220 turns around the ring and both parties are agreed on that. We stationary observers see this as having taken place in some 64.5 microseconds, while the muon sees these 220 turns as having been completed in just 2.2 microseconds. Hence for the muon and indeed all objects moving at close to light speed frequency is multiplied by a factor Gamma relative to that of a stationary observer. We have seen that speed is invariant with respect to relativity. Both the moving object and the stationary observer agree on their relative speed. This invariance of speed is central to the derivation of special relativity and so is deemed to be axiomatic. There is however one circumstance where this may not be the case. For a stationary observer we normally require the use of two clocks in order to measure velocity; one at the point of departure and one at the point of arrival (at least conceptually). An object which is in orbit however returns once per cycle to its point of departure and so we can measure the orbital period of such an object with a single clock.

Thus for an object in orbit it is possible to define two velocity terms³. The first of these I have called the Actual Velocity and is simply the distance around the orbit divided by the orbital period as measured by the stationary observer. The second velocity term is the distance around the orbit as measured by the moving observer divided by the time as measured by the stationary observer. Such a velocity term straddles or couples the two domains and so could sensibly be called the "Coupling Velocity" or possibly the Relativistic Velocity. A simple calculation shows that the Coupling Velocity is related to the Actual Velocity by the same factor Gamma an hence

$$v_c = \frac{d}{T} = \frac{d}{t\gamma} = \frac{v}{\gamma}$$
 Equation 8

Thus far Coupling Velocity is only a definition and if it has ever been considered before it has been assumed to have no physical significance. However there is one set of circumstances where such a velocity term may indeed be justifiable and that is when dealing the orbital velocity. It is considered meaningful to use this Coupling Velocity term when dealing with orbital velocities such as occur when calculating angular momentum centripetal and centrifugal force.

If Nicholson was right about Planck's constant being a measure of the angular momentum of the orbiting electron, but wrong in suggesting that it could take on values which are an integer multiple, then, using Relativistic Velocity, Planck's constant is seen as a limiting value for angular momentum. The effect would not be significant at low velocities, but if the electron orbiting the hydrogen atom were to do so at close to light speed then -

 $I = \hbar = (m\gamma) r\left(\frac{c}{\gamma}\right)$ Both the mass term and the velocity term are affected by relativity. The mass term because mass increases by factor Gamma as the object's velocity approaches the speed of light and in this case the

velocity term is affected because we are dealing with an object in orbit and it is therefore appropriate to use Coupling Velocity which is the Actual Velocity divided by Gamma.

The two Gamma terms will cancel. The terms for rest mass, Planck's constant and the speed of light are all constants, which must therefore mean that the orbital radius is also a constant.

Equation 10

Equation 9

$$R = \frac{\hbar}{mc}$$

³ In fact it is possible to define a further two velocity terms, the relativistic distance divided by the relativistic time and the actual distance divided by the relativistic time. The first of these is the invariant velocity discussed earlier. As a stationary observer we do not have any direct access to the moving clock and so these velocities can only be described mathematically and appear to have no physical significance.

This not unfamiliar term is known as the Reduced Compton Wavelength although here it takes on a new and special significance as the characteristic radius at which an electron will orbit at or near light speed. This explains why the orbiting electron does not emit synchrotron radiation. It does not do so because it is not driven to orbit the atomic nucleus by virtue of being accelerated by forces towards the orbital centre in the normal way, instead it is constrained to orbit at this radius by the limiting effect of Planck's constant. It is as if the electron is orbiting on a very hard surface from which it cannot depart and which it cannot penetrate. Equation 10 also means that there is no need to introduce the idea of a quantum leap. If the electron is constrained to always orbit at a fixed radius, then changes in energy level have to take place as a result of changes in velocity, with no accompanying change of radius.

Substituting Coupling Velocity into the force balance equation that Bohr himself used yields another interesting result

$$\frac{\kappa q^2}{r^2} = \frac{(m\gamma)}{r} \left(\frac{c}{\gamma}\right)^2$$
 Equation 11

Which combines with Equation 10 and simplifies to give

$$\frac{\kappa q^2}{\hbar c} = \frac{1}{\gamma}$$
 Equation 12

Readers may be familiar with the term on the left of this equation which is known as the Fine Structure Constant often written as α (Alpha). And so

$$\gamma = \frac{1}{\alpha}$$
 Equation 13

From this and Equation 5 we can easily calculate the corresponding orbital velocity and frequency.

$$\frac{v}{c} = \sqrt{1 - \alpha^2} = 999973371$$
 Equation 14

And the frequency (in the domain of the stationary observer)

$$\omega_1 = \frac{v}{R} = 7.76324511^{20}$$
 Equation 15

The physicist Richard Feynman once said of Alpha that

"It has been a mystery ever since it was discovered more than fifty years ago, and all good theoretical physicists put this number up on their wall and worry about it. Immediately you would like to know where this number for a coupling comes from: is it related to pi or perhaps to the base of natural logarithms? Nobody knows. It's one of the greatest damn mysteries of physics: a magic number that comes to us with no understanding by man. You might say the "hand of God" wrote that number, and "we don't know how He pushed his pencil." We know what kind of a dance to do experimentally to measure this number very accurately, but we don't know what kind of dance to do on the computer to make this number come out, without putting it in secretly!" Equation 13 effectively solves the mystery, providing an explanation for the physical significance of the Fine Structure Constant. It is seen simply as the ratio of two velocities, the Coupling Velocity and the Actual Velocity of the orbiting electron. Since these two velocities share the same orbital period, it can also be seen as the ratio of two orbital path lengths, the one traversed at non relativistic speeds to that traversed by the orbiting electron at near light speed. The Fine Structure Constant is seen to be dynamic in nature. Its value relies on the fact that the electron is in motion, orbiting at near light speed; it does so at a speed that is necessary to maintain structural equilibrium within the hydrogen atom, since it is only by travelling at this speed that the structural integrity of the atom can be maintained. In the world of the atom, where there is no friction and in the absence of any sort of external input, the atom remains stable and, unless disturbed in some way, the electron will continue in this state indefinitely. In this sense it defines the speed at which the electron has to travel in order to achieve a stable orbit.

We have seen that one of the effects of relativity is to multiply frequency in the domain of a moving object by Gamma. The frequency in the domain of the electron which corresponds to this stable state is simply calculated by multiplying by Gamma – equivalent to dividing by Alpha - to give.

$$\Omega_1 = \frac{\omega_1}{\alpha} = 1.06378925^{23}$$
 Equation 16

But just as was the case with the observer and the cannon if there is a frequency Ω at which the atom is stable then frequencies of n Ω must also be stable for all n = integer which in turn means that there are stable states for all

$$\gamma_n = \frac{n}{\alpha}$$
 Equation 17

And so

$$r_n = R = \frac{\hbar}{mc}$$
 Equation 13

And

$$\frac{v_n}{c} = \sqrt{\frac{n^2 - \alpha^2}{n^2}}$$
 Equation 19

Table 1 below shows the resulting orbital velocities for the first 13 energy states and the theoretically infinite state of the hydrogen atom and as you might expect they match the absorption and emission spectra of the hydrogen atom perfectly.

8

n	v _n /c	$1/\gamma_n$	ω_n	Energy eV	∆Energy eV	
1	0.999973371	0.007297559	7.76324511E+20	255485.925	13.607	
2	0.999993343	0.003648853	7.76340016E+20	255496.130	3.402	
3	0.999997041	0.002432577	7.76342887E+20	255498.020	1.512	
4	0.999998336	0.001824435	7.76343892E+20	255498.682	0.850	
5	0.999998935	0.001459549	7.76344357E+20	255498.988	0.544	
6	0.999999260	0.001216291	7.76344610E+20	255499.154	0.378	
7	0.999999457	0.001042536	7.76344762E+20	255499.255	0.278	
8	0.999999584	0.000912219	7.76344861E+20	255499.320	0.213	
9	0.999999671	0.000810861	7.76344929E+20	255499.364	0.168	
10	0.999999734	0.000729775	7.76344977E+20	255499.396	0.136	
11	0.999999780	0.000663432	7.76345013E+20	255499.420	0.112	
12	0.999999815	0.000608146	7.76345040E+20	255499.438	0.094	
13	0.999999842	0.000561366	7.76345061E+20	255499.452	0.081	
x	1.000000000	0.000000000	7.763451838E+20	255499.532	0.000	
Table 1						

The introduction of the idea of a Coupling Velocity, a velocity term which is affected by relativity, solves all of the problems that faced Niels Bohr and produces a model for the hydrogen atom which matches the emission and absorption spectra of the atom. It also introduces the idea of a mechanism to explain the presence of quantisation in the energy levels of the atom, rather than an arbitrary assumption.

It explains all of the shortcomings of the Bohr model, the absence of orbital decay due to synchrotron radiation, the need for a quantum leap and the introduction of negative energy. Bohr had ignored the effects of special relativity on the energy levels of the atom, even though they should have been small but significant at the velocities predicted by his model. Here they are fully integrated into the model.

It also sheds a new light on the nature of the wave particle duality. The electron is seen as a point particle in the classical sense. Electrons are thus objectively real. The waves are seen as the result of the circular orbit of the objectively real electron around the atomic nucleus the size and frequency of this orbit being a characteristic of the particle. There is no need to invent the ether or what has more recently passed for the ether, the so called fabric of space time, as a medium in which these waves exist. In the final analysis where vacuum contains absolutely nothing, there is nothing to wave except the particle and that is what the model provides.

And finally it provides a simple mechanical explanation for the existence and the value of the hitherto mysterious Fine Structure Constant.