Relativistic Quantum Mechanics
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Module - 1
Lecture - 4
Bohr-Sommerfeld semi classical solution of the Coulomb problem
The Dirac Equation and the Clifford algebra

Last time I mentioned that Sommerfeld described a more general version of Bohr's quantization formula, and that explained little more than what Bohr did. Bohr's formula for circular orbits around the nucleus gave the electron energy levels for the hydrogen atoms correctly. Sommerfeld when he included possibility for elliptic orbits as well added one more quantum number for the radial direction periodicity in the radial direction, and that explained the angular momentum degeneracy of the various hydrogen atom energy levels, and the condition as I wrote down last time is very similar to the action integral in the radial direction is quantized in the units of plank's constant.

Now, this integral can be evaluated explicitly and that is why we can obtain a relation between m prime and the energy levels, and it is very straight forward algebra to workout. For the Kepler problem, there are two constants of motion. One is the angular momentum and the second one is the energy, and the equations for the orbit can be explicitly written down in terms of two constants and I can explicitly now write them down.

The energy is the radial momentum square by 2 m plus the angular momentum square by 2 m r square minus z square r, which is the contribution of the potential energy. The angular momentum is already quantized as in the case of Bohr's formula, and the equation of the orbit explicitly is given by two parameters which is related to the semi major axis and epsilon, which is known as the eccentricity. In this particular case, the explicit form of these two constants is equal to m z e square divided by n square h cross bar square, and epsilon is square root of 1 plus. This now gives an explicit form for what p r a in terms of various constants and we can just evaluate the integral.

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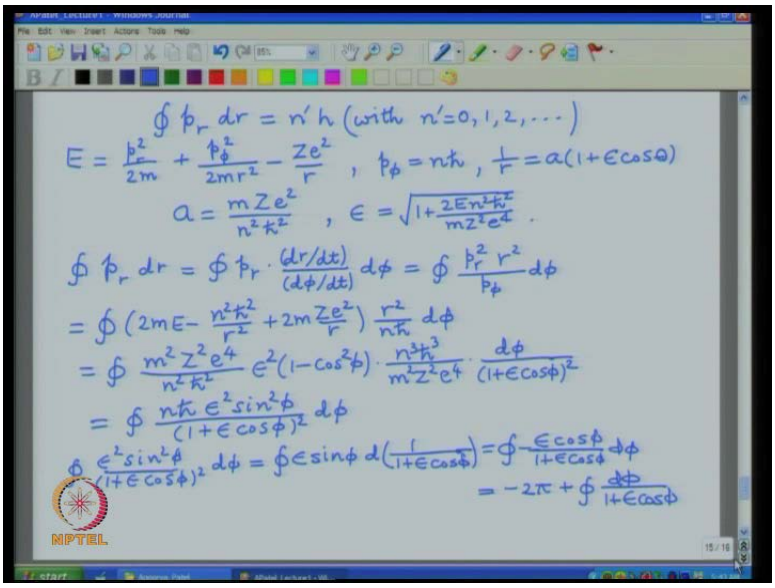

I will just write down the formula explicitly and you can go through it step at a time. The first step is essentially to rewrite the radial integral in terms of the angular variable which makes things little bit easier to evaluate, and now this can be written in terms of explicit functions.

These are straight forward manipulations and substitutions. After all simplification, we have a simple trigonometric integral and periodicity of this integral is just the angle phi going from 0 to 2 phi. Now, one can evaluate this integral by various tricks. One particular way is to do a contour integration around a unit circle and I can write it down.Where is the first step? This is integration by parts and then, you can separate a partial fraction which gives the form where there is an integer part and angular integral now is much smaller. Now, this last integral can be evaluated by contour integration around a unit circle.

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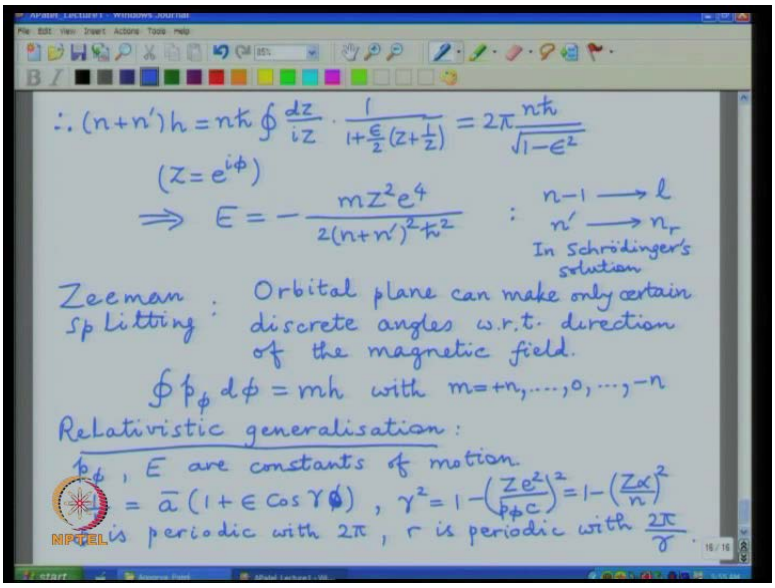

Let us do that and I will substitute this whole expression back into the original formula which gives the result. Here the complex variable z is e raise to I phi and evaluating this by residue theorem gives the final expression between all the quantum numbers, and the only variable which survives inside this expression is the eccentricity. If you now invert this whole expression back to obtain the energy levels, the result which is the Rydberg formula and one can now identify n plus n prime which appears in this formulation as the total quantum number, and explicitly if you want correspondence with solution to the Schrodinger equation, it can be mapped by a simple relation that n minus 1 goes to the value of l and n prime gets mapped into n r.

So, this actually is a correct answer for mapping onto the observed spectrum of hydrogen atom and it predicts the degeneracy's of various orbital angular momentum states, in particular for all the pairs of radial and orbital quantum number. When the sum of them is the same, they will have the same energy and since, n prime will have values starting from 0 up to some level, the values of n correspondingly restricted to its maximum value which is specified by the total sum. So, this was Somerfield's first result. Of course, this semi-classical derivation left several things unexplained. First, the interpretation of why only certain discrete orbits are allowed and some were not. What is the plane of the orbit in respect to the three-dimensional space?

These kind of question were left unanswered and it was only hope that some complete theory which in particular case turns out to be the quantum mechanics will come back and explain those results in some more complete algebraic structure, but as long as these things match with experiments, people went ahead and did various kind of calculations and they had a reasonable amount of success doing that. Somerfield himself explained the quantization of orbital angular momentum by going one step further, and that is to explain the Zeeman splitting of the energy levels that the orbital plane rather can make only certain discrete angles with respect to the direction of the magnetic field, and this for instance produced this modified version of the angular momentum rule because now the value of p phi is measured with respect to a specific axis and depending on the particular angle the value of m could go from plus n to minus n in steps of one all the way going from 0, this was for states where the angular momentum was integral, but of course the problem came when the spin of the electron was discovered and the orbital angular momentum was not enough to explain Zeeman splitting.

You have to add the degeneracy coming from spin and the value for angular momentum which it contributed was half. So, that was not possible to include in this particular formalism and that became another problem, but even before spin was discovered, Somerfield was encouraged by his explanation of the various degeneracy's corresponding to orbital angular momentum, and he immediately went ahead and included the relativistic corrections as well and it was amazing that calculation produced the correct structure required to explain the fine structure of the energy levels. So, we can quickly go through the relativistic generalization of the previous formula for the orbit. In a Kepler problem, several things essentially remain unchanged. One is that the angular momentum and energy are constants of motion.

So, the orbit is still in a particular plane and one can now solve its equation of motion describing the relation between radius vector and the angle, and this relation turns out to be similar to the non-relativistic case. It can be written in terms of two constants measuring the semi-major axis and the eccentricity, but there appears a new parameter which I have called gamma here and its value is which can be rewritten in terms of the fine structure constant a small correction to 1 when atomic charge is significantly smaller than 137. This is a equation which describes a not an elliptical orbit, but an orbit which precocious as it goes around the nucleus and the precision is due to the fact that this

constant gamma is not equal to 1. So, phi is periodic when it goes from 0 to 2 phi, but r will be periodic when phi grows from 0 to 2 phi divided by gamma. So, the two periodicities are not equal in applying the action angle principle. We have to apply each variable with its own periodicity and not a common periodicity for all individual components is necessary, and the formulation then continues just the same way. So, phi is periodic with 2 pi and r is periodic with 2 pi by gamma.

The fact that the orbit precocious is general feature of relativity even in special relativity, the orbit precede and of course, when it go to general relativity, there is an additional precession which gets added to this result which comes from gravitational field and Einstein's actually calculated the complete contribution for general relativity which was helpful in explaining the precession of the perihelion of mercury, but here we need only special relativity. In that case, there is an exact solution which describes the precession of the orbit and that is what I wrote down the parameters are slightly different compared to the non-relativistic case.

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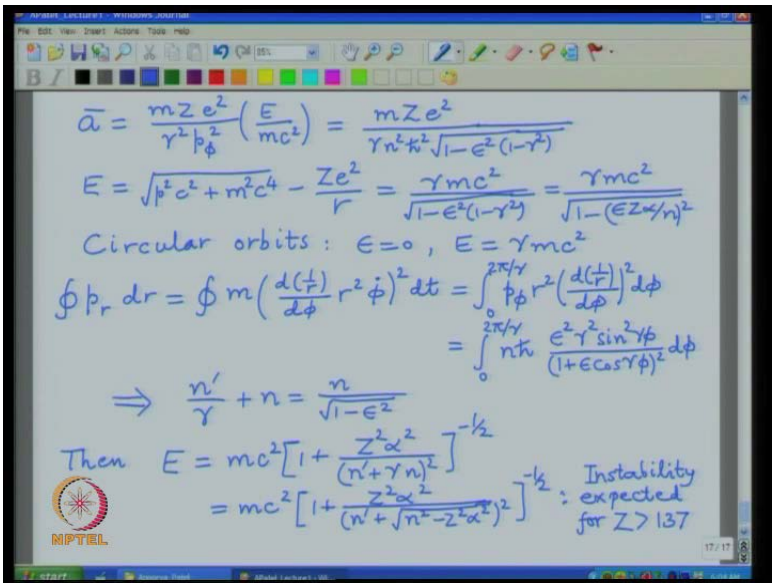

I will write them down as well. This is what the relations of a bar and epsilon to the energy looks like. The energy itself can be re-expressed in terms of these constants after certain manipulations.

In particular for the circular orbits, when the eccentricity vanishes and e is equal to gamma m c square and that is the reason for using the particular notation of gamma,

though in general gamma differs from the Lorentz contraction factor. So, now, let us plug in all these things back into the formula which defines the radial integral and again, the trick is to convert this formula into an angular integral where calculations are easier. Now, in this particular form, one can substitute the orbit equation and simplify the whole calculation. The expression is essentially the same as in the non-relativistic case except for the factor of gamma which appears inside the argument of the trigonometric functions.

Hence, this can be rewritten as this particular trigonometric integral. One can see that the form is identical to what we did in case of non-relativistic case. When you substitute this gamma phi by a new variable which is just phi prime and then, the angular integral will also go from 0 to 2 pi from the new variable phi prime or you can just substitute the values we had earlier, and the final result relating all the quantum numbers essentially is the same except for the simple factor of gamma and has the form expressed here. Then, once can now re-express this eccentricity and gamma in terms of the energy and that leads to the result which is…

The particular form agrees with experiments and in general, it works when the nuclear charges sufficiently small compared to the inverse of the fine structured constant when z becomes bigger than 137. Of course, these things breakdown, but no particular contradiction arises with experiments because there are no nuclei with charge bigger than 137 occurring in nature and this formula can be compared with what we got for Klein Gordon equation. The whole expression is more or less the same except that there is a little difference in the various quantum numbers. One of them is instead of z square alpha square; we had four z alpha square. In case of Klein Gordon equation, the instability occurred much earlier when z was bigger than 137 by 2, and that certainly had conflict compared with experimental data because there are lots of nuclei with z greater than 137 by 2.

The other difference is a shift in the quantum number by a simple change that instead of integer, we had an extra half integral coming in. I mentioned earlier that half integral formula does not work very well, but the integer one does and that corresponds to a rather curious cancellations between two changes by half. One of the source of the half is the value of the spin which is a genuine thing which must be included if you want to treat

an electron, and other shift of half is the correction to this semi-classical quantization rule which comes from inclusion of topological effect.

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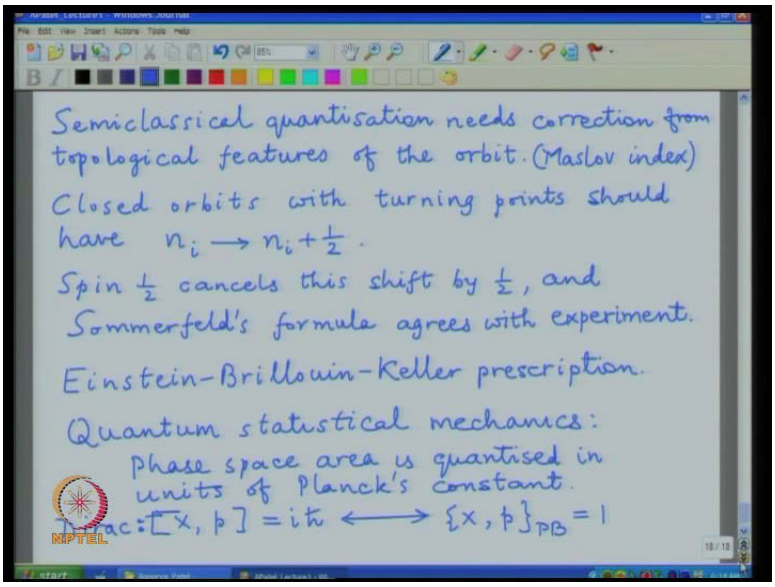

This in modern terminology is referred to as a Maslov index, but it was immediately noticed by Einstein and he already specified that how the numbers should be shifted and in case of orbits which are open, and the angular orbit p phi d phi actually is open. It goes from 0 to 2 pi and keeps on going around and around. The quantization number is an integer, but orbit which has turning points. So, the quantization numbers should be replaced by an I plus half and this is the case for the radial coordinate. When the radial coordinate reaches the maximum value, turns around reaches a minimum value, turns around again and there are actually two turning points.

If you want counts of full orbit, the same thing occurs in a more familiar situation of a quantum problem which is one-dimensional harmonic oscillator where the coordinate x goes in the plus direction to a maximum and comes down, and then it goes in the negative direction to a minimum and then, again turns around and there we know that the correct quantum number for energy has n plus half and not an integer number.

This is the same correction which has to be applied to the radial quantum number formula which was derived by Somerfield, and once this correction of half from topology and another correction from half from spin, both are included. They mutually just shift the quantum numbers, integers to another integer and we can just redefine the

various numbers, so that the result look finally as is a correctly described by the experimental spectrum. So, Somerfield actually derived the correct answer without knowing anything about the spin by this curious shifts of half by two different contributions. So, spin half actually cancels this shift by half and Somerfield's formula agrees with experiment.

Of course, this was done in the old days and several things were noticed, but once more concrete formulation of quantum mechanics came along, this whole thing was kind of forgotten or swept aside, but one can still go back and look at this in some detail to understand the connection between classical and quantum theory through this process of quantization of adiabatic invariants, and this whole prescription including the topological corrections works rather well and now a days, it is referred to as Einstein Brillouin Keller prescription. This is one important part of the semi-classical connection. There is of course another and much more famous part of the semi-classical connection and that is referred to as connection between the commutator in quantum mechanics, and the Poisson bracket of classical mechanics and this connection was pointed out by Dirac, and that was actually the basis of formulating many of the results in the quantum statistical mechanics.

So, the phase space area is quantized in units of Planck's constant. It is a reflection of the same principle which we use for quantization of the orbits because the orbit integral actually measures nothing, but the phase space area between those two canonically conjugate variables and the connection which was stressed a lot by Dirac is that between the commutator in quantum mechanics and the Poisson bracket in classical mechanics. He developed a set of rules converting the classical prescription, particularly in case of constrained dynamical system and how to quantize them consistently in terms of appropriate variables, but we leave these things aside. Now, most of it is only of historical interest and we will go back to a standard description of relativistic quantum mechanics.

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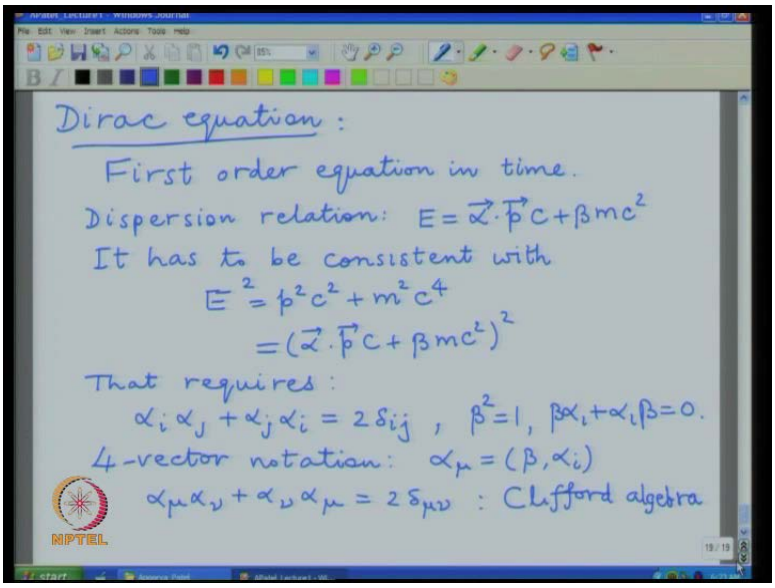

That is now the topic of the relativistic wave equation. Due to Dirac, this is a different equation compared to the Klein Gordon equation and one can wonder what motivated Dirac to cook up this equation because it came out of the blue without any experimental motivation. The surprise was that it fitted the experimental data and also made lot of predictions which were later verified. So, it is a tremendous success in term of the development of quantum mechanics, and it was not really motivated by the failure to explain the hydrogen atom when treated using the Klein Gordon equation. That failure made Schrodinger put away his equation, but Dirac was not much bothered by it.

He was much more bothered by the fact that when one uses that Klein Gordon equation, one obtains the current conservation equation where the density could have negative values and that is the stuff which he did not like. One should not have negative values for something which is ultimately going to describe the density, and he believed that there should be a description of density in the standard way where it will describe probability of some observation and then, if it is a probability, it must be positive. So, he wanted to construct a equation where the densities automatically came out positive and he did not have to worry about the sign which as I described earlier got associated with particle and anti-particle solutions in case of Klein Gordon equation.

Now, he succeeded in this effort to some extent, but on the other hand, the anti-particles did not really go back. They came back into the solution in a different manner and that is

the place where Dirac have to give up that I cannot avoid these anti-particle and he was actually responsible for providing a proper understanding of what these anti-particles meant in terms of physical observations and also, in terms of interpretations of variables which appear in his equation. Dirac attempted to get rid of the negative sign by looking at the quadratic dispersion relation and deciding that all the trouble came out for the fact that there was a relation which give e square is equal to p square plus m square and e square produced a second order time derivative, and when you wanted to get just the value of e, there was a square root with a plus or minus ambiguity.

So, he wanted to develop an equation where there was only an e and not an e square. So, he set out to develop an equation which was only first order in time and then, he believed that all the ambiguity of that square root will go away, and one does not have to play around with this plus and minus signs which followed into the later steps including the charge density and so on and so forth. So, the starting point was an assumption that one can write dispersion relation which was first order in energy instead of e square is equal to p square plus m square, and his hypothesis can be written as two different terms. One of them is m c square which is the energy of the system when momentum, the three momentum is 0 and another term was involved that three momentum, but because of relativistic symmetry if energy was going to be linear, the three momentum might as well be linear because they are the components of the same 4 vector in relativity, and they cannot appear in different forms if the equations was consistent with the special relativity.

So, he started out this, but this is not really consistent when alpha and beta are just some numbers and one must get back to the quadratic dispersion relation which is known to be true from this particular equation, and for that Dirac had to go beyond this, you know ordinary number systems and he sorted the generalisation in terms of alpha and beta being matrices. That was not an unfamiliar territory for him because he was actually trained as an electrical engineer and was very familiar dealing with matrices and linear algebra, and he just applied that knowledge to these particular structures.

So, once we take this equation and plug it back inside here, which means e square is also equal to the square of this whole quantity. One can now match term by term, each component of momentum as well as the component which is independent of the momentum on both sides of the equation and that requires a certain set of conditions or

constraints, and they can be easily written down in terms of alpha I alpha j plus alpha j alpha I is equal to 2 times delta I j and beta square has to be 1 and beta and alpha I have to anti-commute.

So, he explicitly required a set of objects which mutually anti-commuted and each one of them squared to identity and the simplest realisation of such objects was well known at that time. They are the Pauli matrices, but depending on how many objects of this type are required, the Pauli matrices can be generalized to higher dimension matrices and Dirac went on due to that and these matrices which came out are today known as Dirac matrices which obey all this particular algebra. The algebra can also be expressed in a 4 vector notation where let us refer to this alpha mu as the set of objects consisting of beta and alpha I and then, the relation can be rewritten as alpha mu alpha nu plus alpha nu alpha mu is equal to 2 delta mu nu and this is a object familiar and mathematics and it is known as Clifford algebra.

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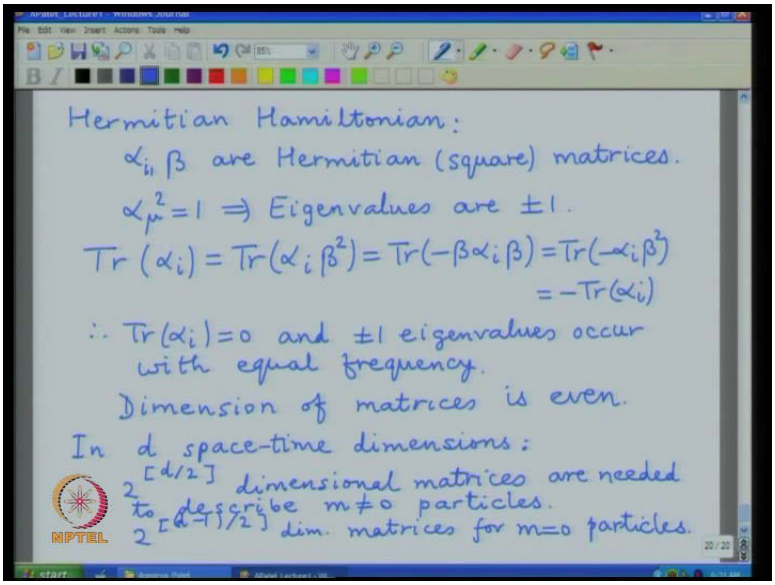

So, what Dirac ended up is writing a dispersion relation where the coefficients are particular set of elements satisfying Clifford algebra. If that happens to be true, then one can have a linear dispersion relation and now, with the usual prescription of converting the energy and momentum to the derivative operator with respect to time and space, one can get a quantum mechanics formulation from this equation and that is what is the

famous Dirac equation, but instead of this difference equations, we will discuss some simple properties of this matrices which obey Clifford algebra today.

One of them represent a term of a Hermitian Hamiltonian and that puts several constraints, in particular alpha and beta are Hermitian that automatically means that they are have to be square matrices. Not only that, the square of the matrix is equal to identity which means that the Eigen values are either plus 1 or minus 1. Hermitian matrix just means the Eigen values are real, but this thing explicitly fixes the magnitude because the algebra involves anti-commuting objects.

So, one can easily take advantage of that, say one can calculate the trace of say alpha I. It could be any of the anti-commuting object in particular, but rather simple manipulation using cyclicity of the trace as well as the anti-commuting nature leaves leads to the fact that trace of alpha I is equal to also minus trace of alpha I and therefore, it has to be equal to 0. Because the matrices are Hermitian, they can be diagonalized with the diagonal element just being the Eigen values, and the trace equal to 0 means that the plus and minus Eigen values occur with equal frequency.

In other words, half of the Eigen values are plus 1 and half of the Eigen values are minus 1. It also immediately follows that the dimensions of the matrices has to be even because otherwise one cannot have half Eigen values which are also integer in number, and all these properties are kind of independent of what actually the explicit choice for these matrices is and since, they are Hermitian matrices, we can actually rotate them from one basis to another and there are various problems in which different basis systems are convenient. We will come to them a little later about what kind of basis should be chosen for which particular problem.

Here, these properties are independent of the choice of the basis, and one can now workout based on this Clifford algebra property is what the minimum number of dimension for when you need a given set of matrices. As I said that the smallest system of such matrices known are the Pauli matrices, they are three in number and so as long as the equations require only three anti-commuting object, you can use Pauli matrices and that is the case when the dimension of the problem is small enough in our world in which Dirac wanted to apply these equations. There are three space dimensions and one time dimension.

So, Dirac needed a set of four matrices. That was not possible with just the Pauli matrices because there were only three of them. So, he had to go beyond, but there are general results for Clifford algebra which gives a number of anti-commuting objects. Once the dimension of the matrix is decided and the dimension of the matrix is always even, how many objects are required is related to number of space dimension of the problem. So, in d space time dimensions, the general result is 2 raise to d by 2 and the square brackets here means the integer part of it to describe mass non-zero particles. In particular in our three space and one time dimension, d is equal to 4. So, we will need 4 by 4 matrices to describe an electron. If the particle happens to be mass less, then this number is little smaller because we need only alpha and beta is not necessary.

So, 1 less matrix is completely and that number again can be written as subtracting 1 from d in the exponents. So, in our three space and one time dimensional bound, this one is the 2 raise to 3 by 2. The integer part is just 1, and 2 by 2 matrices will be enough and these are the three Pauli matrices. We can use Pauli matrices in place of alpha and beta is not required because the mass of the particle happens to be 0. So, these are the general results of the matrix dimensionality needed with respect to the number of matrices.