## Select/Special Topics in Atoms Physics Prof. P.C. Deshmukh Department of Physics Indian Institute of Technology, Madras

# Lecture - 14 Relativistic Quantum Mechanics of the Hydrogen Atom

So, we saw the quantization relation last time, we have to quantize this momentum operator, momentum in classical mechanism is a dynamical variable, and then quantum mechanics it is an operator.

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$$\begin{split} p^{\mu}p_{\mu} - m^2c^2 &= 0 \\ E^2 &= \vec{p}\boldsymbol{\cdot}\vec{p}c^2 + m^2c^4 \end{split} \qquad \begin{aligned} p^{\mu}p_{\mu} &= m^2\gamma^2c^2 - m^2\gamma^2v^2 \\ &= \frac{E^2}{c^2} - \vec{p}.\vec{p} = m^2c^2 \end{aligned}$$
 $\vec{\mathbf{p}} \cdot \vec{\mathbf{p}} - \mathbf{m}^2 \mathbf{c}^2 = 0$   $\int \mathbf{p}^0 = \gamma \mathbf{m} \mathbf{c} = \frac{\mathsf{E}}{\mathsf{c}} \rightarrow \frac{1}{\mathsf{c}} i\hbar \frac{\partial}{\partial t} = i\hbar \frac{\partial}{\partial (\mathbf{c})}$ **QUANTIZATION!**  $(\mathbf{p}^1, \mathbf{p}^2, \mathbf{p}^3) = \mathbf{\vec{p}} \rightarrow \mathbf{\vec{p}}_{op} = -i\hbar \vec{\nabla}$  $\frac{1}{\mathbf{c}^2}\frac{\partial^2}{\partial t^2} + \left(\vec{\nabla} \cdot \vec{\nabla}\right) - \left(\frac{\mathbf{mc}}{\hbar}\right)^2 \left[\psi_{\mathbf{b}} = 0\right]$ 

So, we begin with the momentum scalar, which is this p mu p mu which we found equal to m square and c square, and now we know what mass we are talking about. And you will recognize them important of defining mass carefully, because you cannot define a relatively mass separately. Since, mass an energy equivalent the interpretation of mass it is uses in the relatively equation is of important, it is very hard of relativistic quantum mechanics. A within this in our previous class, and that is a mass which goes and over here, and we see this tailor p mu p mu is an invariant quantity, because it is equal to the square of m and the square of c.

And this m is as much in variant it is as much as a scalar as c is it has to be the same and every frame of reference, if it was the other mass it would not be. So, we have this relationship, this p mu p mu this is the i psi summation convention as it is sometimes call that few have an index which is repeated than you sum over it. So, this is a sum of four terms, and one term gives you this e square over c square and the remaining 3 terms give you the conventional three dimensional scale of product p dot p.

So, those are the 4 terms which are included in this summation, now we follow the same quantization prescription, because we have done this in done relativistic quantum mechanics, that this operator is replaced by the gradient operator. Likewise, this operator p 0 will also be replaced by the corresponding gradient like term, which is a derivative essentially gradient is a derivative with respect to space, but then we are not making any distinction between space and time.

And here we take, therefore, the derivative with respect to the fourth co-ordinate which is time, and therefore, the e or c which is p o when quantized becomes the derivative operator with respect to time. So, this is about quantization condition, and when you plug in this in this invariant relationship, and now that you have an operator for completeness the operator to get physics out of it. You would have the operator operate on an operant, which the wave function is, and then from this operation you would then develop the algebra further at dirac callus, and then extract physical properties about it.

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So, this is the equation that you get by having the operator operate on the wave function psi, which is the Klein-Gordon equation. Sometimes, you found it written in a different notation, because this whole this operator, which is the set of these operators gradient

like or Laplacian like operator. This is the second derivative with respect to time, and second derivative with respect to space both.

So, this is sometimes called as D'alembertian operator written as a box, it is also called as a box operator sometimes, and this is your Klein-Gordon equation the difficulty with that equation is that it leads to an indefinite probability density. And there are other issues fairly complex issues, some of which can be handled some of which cannot be handles. So, the Klein-Gordon equation has a own range of compatibility, it also has it is limitation, and it is not the appropriate equation for electrons our focus of interest is the atomic structure and we want to describe the electron dynamics in a native.

So, we are going look for a relativistic quantum equation for an electron, which the Klein-Gordon equation is not, and therefore, we will not discuss this any further. The only thing I have like to point out over here is that you should note that, this is a second derivative with respect to time whereas, the Schrodinger equation you have the first derivative. So, you would like to look for any equation, which was one of the motivation to look for an alternative equation that was the not only equation, but again I am not going to be able to trace the historical development of the dirac equation. That will take me off the target, and that is not my intention, with those of you who are you interested will find it very interesting to read some of the developments in relativistic quantum mechanics.

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1928: Dirac → Relativistic QM Proc. Roc. Soc. (Lond.) A117 610 (1928) Proc. Roc. Soc. (Lond.) A118 351 (1928) P.A.M.Dirac: Principles of Quantum Mechanics Dirac equation: - fundamental role in accounting for atomic properties and processes.  $p^{\mu}p_{\mu} - m^2c^2 = 0$  $p^{0} = \gamma mc = \frac{\mathsf{E}}{\mathsf{c}} \longrightarrow \frac{1}{\mathsf{c}} i\hbar \frac{\partial}{\partial t} = i\hbar \frac{\partial}{\partial (\mathsf{c}t)}$ How would one get 1<sup>st</sup> ORDER TIME  $(p^1, p^2, p^3) \equiv \vec{p} \rightarrow \vec{p}_{op} = -i\hbar\vec{\nabla}$ DERIVATIVE?

So, you going to look for an equation, which involves the first derivative with respect to time, and this has been achieved in dirac equation into excellent papers and proceedings of the royal society of London in 1928. And there are excellent sources for dirac work including his book, and this is the fundamental relation which is at the very foundation of atomic structure, and atomic processes in which we are really interested.

So, we know that p mu p mu, this scalar is Laurence invariant, this is a fundamental requirement of any relativistic theory, because we are branching out from Galilean relativity. So, we have to look for a relationship, which has the dynamical variables which can be quantize, so it has to have the momentum operator. So, this is; obviously, the correct relationship to begin with it has got the attractive features, that it has got the momentum built into it has got Laurence it various built into it.

And we are interested in quantizing, we are also interested in looking for an operator, which in was the first derivative with respect to time. Whereas, p mu p mu as we saw and the Klein-Gordon equation; obviously, has the second derivative with respect to time. So, can we play with this relationship a little bit, so that we can look for, how to extract the first derivative term rather than the second derivative which is manifesto over there. So, these are the quantization conditions, which we will continue to use, but we are going to look for a relationship, which will have the first derivative in time rather than the second derivative, which is manifest.

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 $(p^1, p^2, p^3) = \vec{p} \rightarrow \vec{p}_{op}$ How would one get 1st ORDER TIME DERIVATIVE?  $p^{0}p_{0} + p^{1}p_{1} + p^{2}p_{2} + p^{3}p_{3} \vec{p}.\vec{p} - m^2 c^2 = 0$ THEN (p°) factorize:  $(p^{0} + mc)(p^{0} - mc) = 0$ Either or Both

So, what you can see is if you look at this relation the p mu p mu, at this scalar expanded is p 0 square minus p dot p minus m square c square, so this is the what fundamental relation. And if you now taka a special case in which this term is 0, if the 3 momentum that tradition 3 momentum, that 3 dimensional momentum, that we normally use even in non-relativistic mechanics. If this momentum is 0, then you get only p 0 square minus m square c square equal to 0, and this is like a square minus b square equal to 0. So, you can factorize, it as a plus b and a minus b, so p 0 plus m c into p 0 minus m c equal to 0.

You can factorize it, and this relation is valid either when p 0 plus m c is equal to 0 or when p 0 minus m c equal to 0 or both, and now you have p 0 if you peel out one of these factors. And set p 0 plus m c equal to 0 or p 0 minus m c equal to 0, then you get p 0 alone and not the quadratic momentum, the 0 it component of momentum is now no longer contradict and you get the first derivative with respect to time.

So, your requirement of finding a first order time derivative equation is satisfied, you are consistency with low range in variant is also satisfied, because it has come out of that basically. And you can take either of this two relationship, and continue to develop the algebra further, you can take either p 0 plus m c equal to 0 or p 0 minus m c equal to 0, you can take either of these and it turns out that.

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 $-m^{2}c^{2}=0$  $(p^1, p^2, p^3) = \vec{p} \rightarrow \vec{p}_{op} = -i\hbar\vec{\nabla}$ WHEN:  $\vec{p} = \vec{0}$  $(p^{0})^{2} - m^{2}c^{2} = 0$  factorize:  $(p^{0} + mc)(p^{0} - mc) = 0$ How would one factorize  $p.p - m^2 c^2 = 0$  $\vec{p} \neq 0$ Explore  $p_{\mu} + mc)(\gamma^{\lambda} p_{\lambda} - mc)$ 

It really does not matter, which one you take because you are let the same physics no matter which you take, but that is a matter of detail and essentially what we find is that

this factorization is possible. And we then ask that is factorization possible when p is not equal to 0, because we know that we cannot be dealing with special cases. We if you do the algebra only with special cases, then you can apply at only to special cases, and that will limit about range.

So, we are looking for a relationship, in which you have a similar kind of factor, but now it cannot be based on assuming that this 3 vector scale a product p dot p is equal to 0. Now, that is a tough one, and that is where you need somebody with the intuition and intellect of dirac, so what dirac dealt is to explore of factorization of this kind. Explore, try it out, set this quantity on the left hand side, equal to a product of two factors, and you know that it cannot be easily factorized.

So, you insert some unknowns, and you insert a beta over here, and gamma over here and then you ask is such a factorization possible, because if it turns out to be possible. Then you can peel out one of this factors and set it equal to 0, and you will get that del by del theta. So, there is some motivation for it there is some hope, but then there is the query as to what will make such factorization possible, will some very peculiar properties of beta and gamma which are the unknown over here, will they make such factorization possible. May be, may be not and inspired by the hope that it will be possible, you then demand what properties of beta and gamma, will unable such a factorization and then you include that in your condition.

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 $p^{0} = \gamma mc = \frac{E}{c} \rightarrow \frac{1}{c} i\hbar \frac{\partial}{\partial t} = i\hbar \frac{\partial}{\partial t}$ **Explore**   $p^{\mu}p_{\mu} - m^{2}c^{2} = (\beta^{\kappa})p_{\kappa} + mc)(\gamma^{\lambda})p_{\lambda}$  $\beta^{\kappa} \equiv \left\{\beta^{0},\beta^{1},\beta^{2},\beta^{3}\right\}$ 8 coefficients to be  $\gamma^{\lambda} \equiv \left\{\gamma^{0}, \gamma^{1}, \gamma^{2}, \gamma^{3}\right\}$ determined  $p^{\mu}p_{\mu} - m^{2}c^{2} = \left(\beta^{\kappa} p_{\kappa} + mc\right)\left(\gamma^{\lambda} p_{\lambda} - mc\right)$  $=\beta^{\kappa}\gamma^{\lambda}p_{\mu}p_{\lambda} - mc\beta^{\kappa}p_{\mu} + mc\gamma^{\lambda}p_{\lambda} - m^{2}c^{2}$ 

So, this is what you going to look for which is to explore the possibility of factorization of this term, and ask the question what properties of beta and gamma will unable this notice that is the beta kappa p kappa is actually is summation over kappa. So, there four term over there, kappa goes from 0 1 2 3 that is a Einstein summation convention, likewise you have four terms over here, this is gamma lambda p lambda. So, lambda takes four value 0 1 2 and 3, and between these 4 term, there are 8 unknown which are to be determined, that is a part of your exploration process.

So, you ask is such a factorization is possible, and then you just expand this product, so beta kappa p kappa times gamma lambda p lambda gives you the first term. And the two terms in the first bracket, another two terms in the second bracket, so you get a set up 4 terms, and you make sure that you write them in a consistent order, because you have to be careful about commutation properties if any are involved. And if they happen to commute you would not have to worry about it, but that is a question that is a matter of detail, so you get these 4 terms.

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So, these are the 4 terms, 1 2 3 and 4, and you find that this m square c square minus m square c square is common to both left side and the right side. So, you can cancel it, that is make life easy, and you are left with fewer terms, and since lambda is some doer it is an dummy index, and instead of lambda you could kappa as well it is dummy index. So,

instead of gamma lambda p lambda, I use gamma kappa p kappa, because now I find that I can actually combine these terms, in which I have a summation over kappa.

And then I get the left hand side equal to this quadratic term in momentum, and them minus m t m c times the linear terms in momentum. Now, this is an interesting relationship, because you find that the left hand side is quadratic in momentum, you find that the first term is quadratic in momentum, but this one is not. And that suggests that to get freedom the linear term you can choose beta to equal to the gamma, if each beta kappa is equal to the corresponding gamma kappa, beta 0 is equal to gamma 0 beta 1 is equal to gamma 1. Then you can get rid of linear term.

And then on both sides of the equation you have quadratic term and you can really balance the equation. So, that is a good strategy that you can use, so our query was what properties of beta and gamma would allow such a factorization, we get partial answer to it that whatever beta and gamma you discover or you hope to discover will need to be equal to each other. So, that is something, we make some progress, so beta must be equal to gamma, now that we know that beta must be equal to gamma, we can put that beta equal to gamma over here.

So, let us do that, so the left hand side which is p mu p mu scalar, which e equal to beta kappa, which is the same as gamma kappa, because that is something that we have already learned. And now you have got a summation over kappa, and also a summation over lambda each taking 4 values, so you get 16 terms of the right, which should give you the four term on the left.

And that will put some additional requirement on the right hand side, which will lead us to what gamma must be like, we have already learned that beta must be equal to gamma. And now we are going to find what this unknown gamma will turn out to be, so this is the condition that must be satisfied, so let us look at these 16 terms of the right and the 4 terms of the left carefully this is the relationship that has to be satisfied. (Refer Slide Time: 17:50)

 $\mathbf{p}^{\mu}\mathbf{p}_{\mu} = \gamma^{\kappa}\gamma^{\lambda}\mathbf{p}_{\kappa}\mathbf{p}_{\lambda}$  $p^{\mu}p_{\mu}=\gamma^{0}\gamma^{\lambda}p_{0}p_{\lambda}+\gamma^{1}\gamma^{\lambda}p_{1}p_{\lambda}+\gamma^{2}\gamma^{\lambda}p_{2}p_{\lambda}+\gamma^{3}\gamma^{\lambda}p_{3}p_{\lambda}$  $p^{\mu}p_{\mu}=\gamma^{0}\gamma^{0}p_{_{0}}p_{_{0}}+\gamma^{1}\gamma^{0}p_{_{1}}p_{_{0}}+\gamma^{2}\gamma^{0}p_{_{2}}p_{_{0}}+\gamma^{3}\gamma^{0}p_{_{3}}p_{_{0}} \quad \boxed{\lambda=0}$  $+ \gamma^0 \gamma^1 p_0 p_1 + \gamma^1 \gamma^1 p_1 p_1 + \gamma^2 \gamma^1 p_2 p_1 + \gamma^3 \gamma^1 p_3 p_1$  $\lambda = 1$ +  $\gamma^0 \gamma^2 \mathbf{p}_0 \mathbf{p}_2 + \gamma^1 \gamma^2 \mathbf{p}_1 \mathbf{p}_2 + \gamma^2 \gamma^2 \mathbf{p}_2 \mathbf{p}_2 + \gamma^3 \gamma^2 \mathbf{p}_3 \mathbf{p}_2$   $\lambda = 2$  $+\gamma^{0}\gamma^{3}p_{0}p_{3}+\gamma^{1}\gamma^{3}p_{1}p_{3}+\gamma^{2}\gamma^{3}p_{2}p_{3}+\gamma^{3}\gamma^{3}p_{3}p_{3}$  $\lambda = 3$ 

So, let us write this explicitly, so I have summed over kappa for kappa equal to 0, I get gamma 0 and this kappa is also equal to 0, so this is p 0, and then there is this gamma lambda p lambda. So, this is the double summation, so there are actually 4 terms sitting in this single term. Likewise, there are 4 terms sitting in the second, another 4 over here, and another 4 over here, these are the 16 terms that we have referred to. So, now, you sum over lambda by explicitly, so these four terms you sum over lambda, so lambda equal to 0 is the first term, so this is gamma 0 and this lambda is 0.

So, this is gamma 0, and this p 0, and then you take next value of lambda and whatever done or this would be p 0 p 1. This would be p 0 p 1, now it is alright this is actually typographical error, but in our situation it really does not matter, which is y did not heat me, because the components of momentum we know that they actually do commute with each other. X does not commute with p x, but p x commute with p y, p y commute with p z, so it really does not matter.

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$$\mathbf{p}^{\mu}\mathbf{p}_{\mu} = \gamma^{0}\gamma^{0}\mathbf{p}_{0}\mathbf{p}_{0} + \gamma^{1}\gamma^{0}\mathbf{p}_{1}\mathbf{p}_{0} + \gamma^{2}\gamma^{0}\mathbf{p}_{2}\mathbf{p}_{0} + \gamma^{3}\gamma^{0}\mathbf{p}_{3}\mathbf{p}_{0}$$

$$+ \gamma^{0}\gamma^{1}\mathbf{p}_{0}\mathbf{p}_{1} + \gamma^{1}\gamma^{1}\mathbf{p}_{1}\mathbf{p}_{1} + \gamma^{2}\gamma^{1}\mathbf{p}_{2}\mathbf{p}_{1} + \gamma^{3}\gamma^{1}\mathbf{p}_{3}\mathbf{p}_{1}$$

$$+ \gamma^{0}\gamma^{2}\mathbf{p}_{0}\mathbf{p}_{2} + \gamma^{1}\gamma^{2}\mathbf{p}_{1}\mathbf{p}_{2} + \gamma^{2}\gamma^{2}\mathbf{p}_{2}\mathbf{p}_{2} + \gamma^{3}\gamma^{2}\mathbf{p}_{3}\mathbf{p}_{2}$$

$$+ \gamma^{0}\gamma^{3}\mathbf{p}_{0}\mathbf{p}_{3} + \gamma^{1}\gamma^{2}\mathbf{p}_{1}\mathbf{p}_{3} + \gamma^{2}\gamma^{2}\mathbf{p}_{2}\mathbf{p}_{3} + \gamma^{3}\gamma^{3}\mathbf{p}_{3}\mathbf{p}_{3}$$

$$\mathbf{p}_{1}\mathbf{p}_{1} = \mathbf{p}_{1}\mathbf{p}_{1} \quad \text{we can combine the terms having common, equal, factors}$$

And to look at these terms I have the same 16 terms on this slide, but I have inserted some gaps, so that I can show you what is going on with the terms. What you will big use of is this commutation, which I mentioned that p i p j is equal to p j p i, which essentially means that these two terms p 1 p 0 and p 0 p 1, these are actually equal to each other. And you can combine this two term, so this two terms can be combined then you do the same with the remaining one, so you have got p 2 p 0 over here, and p 0 p 2 over here.

So, essentially what you are going to find is terms, I have written these 16 terms in such a manner, then those terms which are equal distant from the diagonal can actually, become combined that is actually, how I have written them. So, terms which are equal distant from diagonal can be combined, so you have this term which is p 3 p 0 which e equal to p 0 p 3.

So, these two terms can be combined, then these two terms can be compiled which is p 2 p 1 and p 1 p 2, then these two term p 3 p 1 with this p 1 p 3 and finally, these two terms p 3 p 2 and p 2 p 3. So, all of these terms which are equal distant from the diagonal can actually be combined, and that leads to sum simplification that we are looking for.

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So, this is how we have combined them, these four are the diagonal terms with the indices 0 1 2 and 3, so these are the terms in the i through and i with column, i going from 0 1 2 3. And then the off diagonal terms which we decided can be combined had these coefficients gamma 0, gamma 1 and gamma 1 gamma 0, so no approximation made is yet no postulate made is yet.

We have written them exactly, and we know that this must correspond to the left hand side, which has got only these terms only 4 terms, so now, , what is it that we can demand on gamma. So, that the 16 terms on the right hand will give you 4 terms on the left, can you make some demand on gamma, you see that if the gamma 0 square is equal to 1. You get the first term happily, you see that if gamma one square is equal to minus one you get the second term.

So, you start making these demands, and then you have to get rid of this term. So, our question is if we could achieve that, then the factorization the dirac equation not in the raw equation that we began with from the invariant momentum scalar, but by inserting unknown beta's and gamma's and by making demand on beta's and gamma's.

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We find that such a factorization is possible and these are what the gammas must be, because they have the right properties, that we are looking for. Notice, that these are 4 by 4 matrices, these are not just numbers, this are matrices, they have a block diagonal form as you can see. They have got a structure which is immediately manifest, they have got block diagonal structure, and you can see that this is 2 by 2 unit metrics.

This is a 2 by 2 negative unit metrics, and what you find in the remaining positions are the poly matrices, the poly 2 by 2 matrices, which we have used earlier. So, you have a sigma 1 over here and a minus sigma 1, and then you have to sigma 2 and sigma 3, so these matrices which have made up of the poly matrices, but the poly matrices are 2 by 2 matrices.

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These are 4 by 4 matrices, they appear in a block diagonal form, and these are the poly 2 by 2 matrices, which we are going to be using. And with the use of the matrices we can actually factorize the dirac, which we can factorize the invariant momentum scalar p mu p mu which is what leads to the dirac equation. So, together with the poly matrices the 4 by 4 matrices are called as dirac matrices, and this is the 0 at component, which is written here 2 by 2 metrics, but each element is 2 by 2 metrics. So, these are the 4 by 4 matrices, so this is the structure of these 4 by 4 matrices, these are called as the dirac matrices and there are three poly matrices gamma i, i equal 1 2 3. And these are made up of the 3 sigma's, which are the poly matrices, I going from 1 2 3.

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 $0 = p^{\mu}p_{\mu} - m^{2}c^{2} = (\gamma^{\kappa} p_{\kappa} + mc)(\gamma^{\lambda} p_{\lambda} - mc)$ Factorization employing the  $\gamma_{4\times 4}$ matrices is possible!  $(\gamma^{\kappa} \mathbf{p}_{\kappa} - \mathbf{mc}) = 0$  $(\gamma^{\kappa} \mathbf{p}_{\mu} + \mathbf{mc}) = 0$  $\mathbf{p}_{\kappa} = \mathbf{i}\hbar\partial_{\kappa} = \mathbf{i}\hbar\frac{\partial}{\partial \mathbf{x}^{\kappa}} = \mathbf{i}\hbar\left(\frac{\partial}{\partial \mathbf{ct}}, \vec{\nabla}\right)$  $-\mathbf{mc}) = 0$  $-\mathrm{mc})\psi = 0$  (  $i\hbar \gamma^{\kappa} \partial_{\kappa} - \mathrm{mc}$ The Dirac Equation can be solved for the Coulomb potential exactly

So, we have, in fact found that factorization of the 4 momentum scalar product is possible, and it is possible by demanding that the gammas are 4 by 4 matrices. This is wonderful, because now you can peel out one of these factor, and again it does not matter which factor you peel out. You can take either this or that, the two of these factor and either one of them must be 0 or both of them could be 0, but you can take any one and this is the one that one normally take.

And it does not matter, which one you take, this is the one that you take gamma kappa, p kappa minus m c, this is the factor equal to 0, and this is the summation over kappa going from 0 1 2 3. So, there are 4 terms in the summation, the momentum is quantized the 4 momentum operators, the 0 is component gives you the time derivative the remaining 3 components give you the space derivative. And you quantize this and keep track of the indices, which is a super scribe, which is subscribe, which is contra variant, which is covariant, you can lower the indices make sure that the operator written in the consistent fashion.

And then you have got an operator relation, because this momentum is now replace by the operator, which is the derivative operator and this derivative operator this is just a matter of notation the kappa is derivative with respect to x super scribe comma. So, use the covariant and contra variant indices carefully, and this operator as we know from the non-relativistic quantum mechanics, as well could operate on an operant which is what over wave function would be. And the result in equation would be the quantum relativistic equation of motion, the operator here; however, is now a 4 by 4 operator, it has got an operator structure.

And that also has a metrics structure and that demands then the wave function over here must have 4 components. Now, this equation can be solved for a few problems exactly, for other problems you have to make a certain approximation, our interest will be in the hydro genitive for the column field for, which exact solution is possible. And we will discuss that this is sometime refers to as a fundament notation, this gamma kappa p kappa is written as a p slash this is sometime called as a slash notation fundament notation. And this is just a matter of notation, basically this is what it is wherever you see a p slash, you should recognize that it is gamma kappa p kappa and it is a set of four terms, which are sum to 1.

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So, this your dirac equation, now you can recognize these gammas to be the 4 by 4 matrices, so this is gamma 0 p 0, this is gamma 1 p 1 look at the metric structure. So, you can simplify some of these things by just doing metrics algebra.

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And that will find that this p 0 will come here, here, here and here, so you can write this relationship in a metric form as well, so this is just matter of you know, writing it in different forms and you might find it in different books.

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But, essentially what we have got is, a relativistic quantum equation in which we have got first order time derivative operator, which is nice, because it has got something similar to the Schrodinger equation. But, then you also have the first derivative operator with respect to space, but that is let us see what it is just, but we should certainly make a note of it.

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So, this is what we have got you can now, you are dealing with very simple matrices, you can use the poly matrices, their properties well known you have done some algebra and you know manipulation with these matrices. So, you can easily figure out that alpha is beta inverse gamma, and you know you can write this in a representation, which is called as a poly representation. And in which you use two operator beta and alpha, alpha is defined as beta inverse gamma, where gamma is made up of these poly matrices, and this is your alpha metrics.

So, alpha is equal to 0 sigma, sigma 0 this is the 4 by 4 metrics, each element is made up of a poly matrices, which are 2 by 2. So, in the poly representation instead of the gamma, you use 1 beta and 3 alphas, but this is just a matter of renaming them this known you physics. This known you mathematics it is just a new normal clincher, and that is one which is commonly seen in a lot of literature, but 2 by 2 matrices the poly operators operate in the poly space. The 4 by 4 dirac operator and what is sometime refer to as the dirac space, and you can see the poly space is a subspace of the dirac space.

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You can do a lot of very interesting mathematics with the dirac matrices, and this is a good exercise, although I will not spend much time discussing the mathematics of the dirac matrices, but these property can be very easily verified. And I will not spend any time other, because we will not be using some of these relationship directly in our development of the subject. But, I will certainly like to mention that you can actually build additional matrices, like from the gammas you built the gamma square, you can built the sigma like define as i gamma mu gamma mu.

You can build these additional matrices not all of the linearly independent, but 16 linearly independent matrices can be built, and you can classify them in different, you know structures. So, you have got only one element of this kind you got 4 matrices of this kind with mu going from 0 1 2 3, you get 6 matrices of this kind, you get one metric of this kind and another four of this kind. So, you can you know place them in different sets, and place them in 5 sets which are the conventional sets, and which these are structured.

And the reason to do it, because if you consider the transformation properties and the Lorentz transformation, then they have similar properties this one in the first set, you know it transforms as a scalar, these transform as a vector, these transform as a tensor, this one has a pseudo scalar, and this one has a initial bracket. So, there are these are the reasons that they are put in different sets, and I will not spend too much time on this.

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I will proceed with the dirac equation, but now we are going to invoke the electromagnetic potential, that is a big important was because we know our interest is in hydrogen atom. And the electron is in the presence of electromagnetic potential, it mix the column potential with the nucleus that is the electronic potential. We have to look not just for a relativistic quantum equation, but for a relativistic quantum equation which also has the electromagnetic potential.

So, this is the electromagnetic potential, now this is it has got the 4 components, this is the electrics scalar potential, this is what you very often called as a magnetic vector potential. And we make an insert for the Lagrangian for the system or the electron in the electromagnetic potential, they make this insert that the Lagrangian will be given by this. And this is a point, which I am sure has been emphasized a number of times in your interaction mechanics class, that whenever you set up the hamiltonian. You never write it as t plus v or anything like that, the first thing to do is to set up the Lagrangian for the system, then obtain the Lagrangian is always in terms of position and will last set.

And then from the Lagrangian you find the momentum the generalize momentum, and once you have it then you proceed to build the hamiltonian, and then you quantize it. So, we begin with the Lagrangian, for the system we make an insert, that this would be the Lagrangian, we need to verify it is a right Lagrangian, it is not something we are going to take for granted. So, we propose this Lagrangian, and we ask if it satisfies the Lagrangian equation, if it does what kind of relationship will come out of it, because the Lagrangian equation must give you the equation of the motion for the electron in the electromagnetic field, and we already know that do not.

Equation of motion for an electron and the electromagnetic field must exact acceleration is equal to the force, and we know that that force is that the Lorentz force, which is f is equal to charge time what is it v which is or pi which is the scalar potential. Plus the v cross beta the electric intensity e plus v cross v times a charged will give you the Lorentz force. So, does this Lagrangian give us the equation of motion is a question that we ask, so we look at it set it up for each component, so q or the three degrees of freedom for this Lagrangian.

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 $L = \frac{1}{2}mv^2 - q\phi(\vec{r},t) + \frac{q}{c}\vec{v}\cdot\vec{A}(\vec{r},t)$  $L = \frac{1}{2}m\left(v_{x}^{2} + v_{y}^{2} + v_{z}^{2}\right) - q\varphi(\vec{r},t) + \frac{q}{c}\left(v_{x}A_{x}(\vec{r},t) + v_{y}A_{y}(\vec{r},t) + v_{z}A_{z}(\vec{r},t)\right)$  $\frac{\partial L}{\partial \dot{x}} = mv_x + \frac{q}{c} A_x(\vec{r}, t) \qquad \qquad \frac{d}{dt} \frac{\partial L}{\partial v_x} - \frac{\partial L}{\partial x} = 0$   $\frac{d}{dt} \frac{\partial L}{\partial \dot{x}} = m\dot{v}_x + \frac{q}{c} \frac{dA_x(\vec{r}, t)}{dt} \qquad \qquad \frac{d}{dt} \frac{\partial L}{\partial v_x} - \frac{\partial L}{\partial x} = 0$  $\frac{d}{dt}\frac{\partial L}{\partial x} = m\dot{v}_x + \frac{q}{c}\left\{\frac{\partial A_x(\vec{r},t)}{\partial x}\frac{dx}{dt} + \frac{\partial A_x(\vec{r},t)}{\partial y}\frac{dy}{dt} + \frac{\partial A_x(\vec{r},t)}{\partial z}\frac{dz}{dt} + \frac{\partial A_x(\vec{r},t)}{\partial t}\right\}$  $\frac{\partial L}{\partial x} = -q \frac{\partial \varphi(\vec{r},t)}{\partial x} + \frac{q}{c} v_x \frac{\partial A_x(\vec{r},t)}{\partial x} + \frac{q}{c} v_y \frac{\partial A_y(\vec{r},t)}{\partial x} + \frac{q}{c} v_z \frac{\partial A_z(\vec{r},t)}{\partial x}$ 

And we set up the v square is a sum of these three components square, I am using a simple Cartesian coordinate system, it is very easy to use and it is all about the propose in this case. So, your m v square the kinetic energy is part in the Lagrangian is given by this, your Lagrangian, which is t minus v gives you this minus q times pi and then you have got this velocity term, and the vector potential and the equation of motion that you expect is this.

So, the what you do is to find out what the momentum is and the momentum, of course, is the derivative of the Lagrangian with respect to the velocity momentum is not must time it is velocity. It is much more than that the primary definition of momentum is the partial derivative of the Lagrangian with respect to the velocity. So, you take the derivative of the Lagrangian with this respect to the velocity, and you find from this term you get m into v x, but them this term also has got the velocity, so the derivative of this term with respect to the velocity, will give you this q by c a x.

So, your momentum now, which is the generalize momentum not just the traditional mechanical momentum, so this traditional mechanical momentum we can quantize using the variant operator, but momentum itself will include this vector potential as well. So, the next you do in the Lagrangian equation is to take time derivative, of the partial derivative of Lagrangian with respect to the velocity. So, that is what it is you take the time derivative of the right hand side, so muss is a consent you get the derivative of velocity which is v dot which would be the classical acceleration.

So, there is a dot on this v, it is a tiny dot, but do not ignore it that is the time derivative of the velocity, and you can get the time derivative of the vector potential, which could be 0 if the vector potential is not independent of time, but it would not be 0 in general. So, now, you take the partial derivative of this vector potential with respect to time, but the dependence of the vector potential on time is through an explicit dependence of the component on time.

And in implicit dependence through the dependence of this a on the coordinate, which in turn depend on time, this is the convective derivative like idea that we have used employed dynamics or in electromagnetic theory earlier. So, the same kind of you know the reasoning is involved all you have to do to recognize that the dependence on time is not just, because of how a x depends explicitly on time, but also on how it depends implicitly on time, why are it is dependence on the position are which in turn depends on time.

So, you have a derivative with respect to x which in turn depends on time, so this is the x y d t. Likewise you have got terms and y and z, and then you have got the final term which comes from the explicit dependence of a x on time. So, you handle this derivative carefully, and that is give you to the derivative of the momentum, which is a keen to mass exact acceleration, but not just the traditional plutonian must exact acceleration, but it has got this term coming from the vector potential.

Then, this must be equal to del l by del x and del l by del x is something that you can obtain from here, because you find out which are the terms in this relationship is depended on x, so here is one the pi the scalar potential depends on x. So, that you get the derivative of pi with respect to x, and you have got the vector potential e x, which also depends on x because it depends on r, likewise a y also depends on r. So, there is an x dependence of a x there is also an x dependence of a y, so you get a term and del a x y del x times d x by d t, and a term in del a x by del y times d y by d t and there is a term in z.

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 $d \partial L = \partial L$ dt dv x 2X  $=m\dot{v_x}+\frac{q}{c} \Biggl\{ \frac{\partial A_x(\vec{r},t)}{\partial x} \frac{dx}{dt} + \frac{\partial A_x(\vec{r},t)}{\partial y} \frac{dy}{dt} + \frac{\partial A_x(\vec{r},t)}{\partial z} \frac{dz}{dt}$ d aL dt ai ðt  $\frac{\partial L}{\partial x} = -q \frac{\partial \phi(\vec{r},t)}{\partial x} + \frac{q}{c} v_x \frac{\partial A_x(\vec{r},t)}{\partial x} + \frac{q}{c} v_y \frac{\partial A_y(\vec{r},t)}{\partial x} + \frac{q}{c} v_z$  $\partial A_z(\vec{r},t)$ ax  $m\dot{v}_{x} + \frac{q}{c} \left\{ \frac{\partial A_{x}(\vec{r},t)}{\partial x} \frac{\partial x}{\partial t} + \frac{\partial A_{x}(\vec{r},t)}{\partial y} \frac{dy}{dt} + \frac{\partial A_{x}(\vec{r},t)}{\partial z} \frac{dz}{dt} + \frac{\partial A_{x}(\vec{r},t)}{\partial t} \right\}$  $=-q\frac{\partial \phi(\vec{r},t)}{\partial x}+\frac{q}{c} V_x \frac{\partial A_x(\vec{r},t)}{\partial x}+\frac{q}{c} V_y \frac{\partial A_y(\vec{r},t)}{\partial x}+\frac{q}{c} V_z \frac{\partial A_z(\vec{r},t)}{\partial x}$  $\dot{mv_x} = -q \Biggl\{ \frac{\partial \varphi(\vec{r},t)}{\partial x} + \frac{1}{c} \frac{\partial A_x(\vec{r},t)}{\partial t} \Biggr\}$  $\frac{q}{c}v_{y}\left\{\frac{\partial A_{x}(\vec{r},t)}{\partial y}-\frac{\partial A_{y}(\vec{r},t)}{\partial x}\right\}+\frac{q}{c}v_{z}\left\{\frac{\partial A_{z}(\vec{r},t)}{\partial x}-\frac{\partial A_{x}(\vec{r},t)}{\partial z}\right\}$ 

So, you write all of these terms carefully make sure you bring them to the next slide carefully, and then you can insert them in the Lagrangian equation, because now you have got both the left hand side of the Lagrangian equation and the right hand side. And the left hand side is given by this, and the right hand side, which is del l by del x is given by this, here just put the two to be equal to each other done. You find simplify this little bit notice, that you got the velocity terms over here, likewise you have got d y by d t here and v y over here d z by d t here and v z over here.

So, you can combine corresponding terms, and you are left with a relationship for mass time acceleration, which is the traditional neutronion mass time acceleration which is what would go into the lorentz force law. And on the right hand side I have moved these terms to the right with appropriate signs, combine them and I find combine the terms and the velocity, because I can combine the term d y by the d t here, which is on the left with this v y which on the right, and this will move to the right on the minus sign. So, I will have both of them with the minus sign, now one of them with a minus sign this is a with minus sign and this is with plus sign, so I get these terms in which the v y and v z terms are combined.

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Now, let us bring it up and we will make use of something else, which we also know that the magnetic field is given by the curl of the vector potential, and if you just write look for the x component of the velocity crossed the b term. You find that you have identical terms, which we have seen on the previous slide see exactly the same slide, so you can insert the x component of v cross v over, there and this very easy to see.

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So, I will not work out this determine for you, and you can see that with the recognition of b being the curl of a, you find that the x component of v cross the v is what gives you these terms, which you have found, in the equation of motion coming from the Lagrangian equation. You insert the corresponding terms, so this term in the Lagrangian equation is replaced by q over c time v cross v, you have seen, it for the x component you have got corresponding terms for the y and z component.

And you get exactly what you are looking for what you are hoping to find, because now you find the x component of the traditional mass time acceleration, which is the neutron ion force is equal to q into e plus v cross v. And, we are using the Gaussian system of units, so which is why I have got the one over c is taking a long vector potential, and I you would not have the one over c, but in atomic physics it is more convenient to use Gaussian system. So, everything hangs together and you get the Lorentz force relationship as 1 over c time v cross b, which gives this the confidence that the insert we made for the Lagrangian is a correct, and we can use the Lagrangian further.

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 $L = \frac{1}{2}mv^2 - q\phi(\vec{r},t) + \frac{q}{c}\vec{v}\cdot\vec{A}(\vec{r},t)$  $L = \frac{1}{2}m(v_{x}^{2} + v_{y}^{2} + v_{z}^{2}) - q\phi(\vec{r},t) + \frac{q}{c}(v_{x}A_{x}(\vec{r},t) + v_{y}A_{y}(\vec{r},t) + v_{z}A_{z}(\vec{r},t))$  $\begin{array}{ll} \mbox{Generalized} & p_x \rightarrow \frac{\partial L}{\partial \dot{x}} = m v_x + \frac{q}{c} A_x(\vec{r},t) \end{array}$  $\vec{p} \rightarrow m\vec{v} + \frac{q}{c}\vec{A}(\vec{r},t)$   $\vec{p} \rightarrow m\vec{v} - \frac{e}{c}\vec{A}(\vec{r},t)$  $p^{\mu} \rightarrow \left(\pi^{\mu} = p^{\mu} - \frac{e}{c} A^{\mu}\right) \rightarrow \underbrace{i\hbar\partial^{\mu}}_{c} - \frac{e}{c} A^{\mu}$  $\pi^{\mu} = \left\{ \left( \pi^{0} = p^{0} = \gamma mc \right), \left( \vec{\pi} = \vec{p} - \frac{e}{c} \vec{A} \right) \right\}$ Quantization generalized energy momentum 4-vector

So, let us to use it Lagrangian, now we know that it is no longer s postulate it has led to the correct equation of motion, for the electron in the electromagnetic field. So, we will use this Lagrangian, we opting the momentum which we have done already, and now we are ready to put the charged, which is the electron charge which is minus e. So, this m v plus q over c a becomes m v minus e or c a, and now you quantize. This which is to replace all the momentum operators by the corresponding derivative operators, along with the i h cross and so on.

So, that is something that you know how to do go ahead, and quantize it, and what you have is you have the fourth component you got the 3 traditional components of momentum. And the fourth component  $p \ 0$  of the generalize momentum of four momentum is nothing but the gamma times m c.

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As, you can see and this is what leads you to the dirac equation, for the chasse particle in the electromagnetic field. Now, you no longer have to ignore the electromagnetic field, in fact that is what you are really interested in. So, let us collect all the terms and this is the 4 by 4 dirac equation that you get, along with the operators, it has got the derivative operators.

It has got the magnetic vector potential, which has come from the generalize momentum, and you have all of these terms stack together in a metrics equation, but the wave function is got 4 components. That is a new feature, we did not have written the schrodinger equation now you have a wave function, which has got 4 components.

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So, this is a 4 by 4 metric operator, and of the right side is a 4 by 1, 4 rows and 1 column null metrics, these are the 4 dirac matrices, and make sure that you use the indices carefully, because of your signature of the g. You have got this a 0, a 1, a 2, a 3, which translate to a 0 minus a 1 minus a 2 minus a 3 keep track of sign carefully, use this signature correctly. And you can write these terms expand them in term of the betas and the alphas beta have introduced, write out the components of the vector potential explicitly.

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And you get a relationship, which you can also write in terms of the Cartesian component and this is your dirac equation, as it is refer to in the standard form. This is beta times alpha dot p this i h cross gradient gives you the momentum operator, this plus sign goes over to the minus sign, and this is what refer to as the dirac equation. In the, so called standard representation, you can transform it and put it in different equivalent presentation, but this is the representation that I shall make you use of it.

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Now, we have used the momentum operator p, but now we have the fourth component, so it is called as generalize energy momentum 4 vector, it includes the magnetic vector potential. And you can write the 4 vector function, if you want to write it in a block diagonal form because you know that the 4 by 4 dirac matrices can be written in the block diagonal form. You can write wave function also in 2 blocks, a top block made up 2 elements and the lower block made of 2 elements, and you can write it as Fital the Kaital the, and alpha and beta matrices are the gamma matrices that we have defined earlier.

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Now, for a free electronic rest, you can simplify it and it has got these solutions, so before we consider more general solutions, let us look at the free electron solutions. So, you set the electromagnetic field equal to 0, that traditional mechanical momentum equal to 0, that is what gives you the particle addressed. And this is a very simple first derivative equation involving only the beta operator, and it has got 4 solution not one psi 1 satisfies it psi 2 also satisfies it, psi 3 and psi 4 also satisfy it, but here you have got minus m c square by h cross as you expect.

Whereas, over here you have plus m c square over h cross as you do not expect, or you did not expect, these are the positive energy solution, these do not surprise us. The negative energy solution too, and one has to see, where these are coming from and what do they have to what is their place in physics.

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So, you first of all you get a multi component wave function, and whenever you have multi component function that is a signature of a spin, that the particle must have a spin. And all elements in particles which obey Fermi statistics have 2 components, these are spin half particles this is result that you get from the quantum field theory. Electron is a fermion, so it is a two components of particle, but the dirac equation has given us 4 components, 2 more than what we want and we cannot avoid, because it came out of whatever we did to get a relativistic quantum equation.

And then these negative energy solutions, which cannot be avoided, in fact have a real place in physics, and the history of the interpretation of the negative energy particle is very fascinating one, but that goes beyond our domain of atomic physics. You need to study this in particle physics, but this is what led dirac to predict the positron the anti particle, in fact is a earlier prediction was that these were proton rather than positron, because anti particle were not known dirac had to postulate them, invent them.

And then Carl D Anderson actually found them, the origin actually lies in this relationship that we began with, because you have a quadratic energy term, which will have two roles one with plus sign and the other with minus sign. So, the origin can be traced to that, and these are what gave you the anti particles or anti matter. Now, where is all these anti matter we see matter as a anti matter does not matter, but it does it comes

out of the dirac equation, and where is all this anti matter, when I read this question when I was preparing for this slide.

I first saw that I will ask this question to cosmic horizon asking, where the anti matter, because he knows the cosmos, he rules a cosmos, but he rules only the cosmos and not the anti cosmos. So, he is going to tell us to go to the anti cosmic range, but that is a matter of particle physics, and I will not discuss this.

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These are interesting questions, now these are a conclusion is that you have 4 component function, two components is what we need for the electron. The remaining two component have made the negative energy solution, they correspond to the anti particles to the positron and present case, but we need only two components. And we need to find a mechanism to reduce over 4 component theory, to a 2 component theory, it is not clear that it is possible, but we are going to attempt to do.

So, there two ways of doing it one is the poly reduction, which I will discuss and other, which is the more correct one more appropriate one which is also what I will discuss and the Foldy Wouthuysen transformation are very important this context. And that will take a good bit of our time, in the next few classes, so today I will conclude the class over here I will be happy to take some questions.

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So, there these two techniques of reducing the 4 component theory to 2 component theory, and I will discuss this in next few classes next couple of classes, but for now if there are any questions I will be happy to take otherwise goodbye for now.