Select/Special Topics in Atomic Physics
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Lecture - 16
Relativistic Quantum Mechanics of the Hydrogen Atom

Greetings, so we will discuss the Foldy Wouthuysen transformations today, and the whole reason to do, so is to recognize that.

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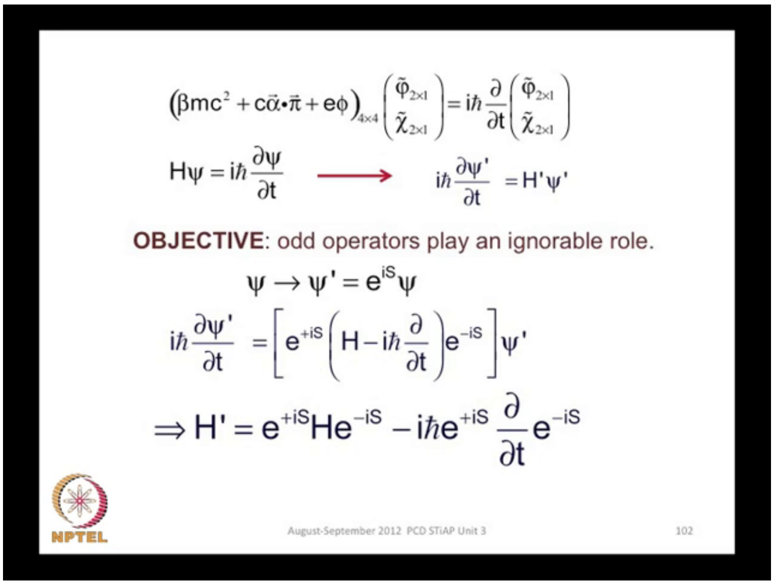

Now, this is the dirac equation, the operators of 4 by 4 matrix vector operators, quantum operators the wave function is a 4 by 1 wave function it has got 4 components. And the unit operator or the beta operator has got 0 elements in the off diagonal blocks, but the alpha operator has got the poly matrices on the off diagonal block. So, the alphas are odd operators, the betas and the unit operators they are called as even operator.

So, the odd operators are the one which makes the, so called large component and the small component, they are the one which makes the particle states and an antiparticle states. You can really decoupled, because of the presence of these odd operators, so what one hopes to do is to transform the dirac equation, at this h psi equal to i h cross h psi by del t is the dirac equation that I am now looking at this is a dirac equation.

You subjected to a transformation to the primed representation, which is the Foldy Wouthuysen transform representation, and in this representation. It is our hope that the operators in the transform representation will also have the odd operators, but hopefully they will be less important than, what they were in the original unprimed representation. For example, this could happened, if they get scaled by a factor 1 over m, so that is a kind of strategy that we are going to apply following the technique that was introduced by Foldy Wouthuysen.

So, this would involved transformation of the wave function psi to psi prime through a transformation operator e to the i s. And if we did that the corresponding Hamiltonian would transform to the sum of these two terms, which is e to i S h e to the minus s. And there would be this additional term, because it cannot be assumed that the operators S is independent of time, it may be in some cases, but it does not have to be. So, this is the general form of the transformed Hamiltonian under the Foldy Wouthuysen transformation, this we discussed in our previous class.

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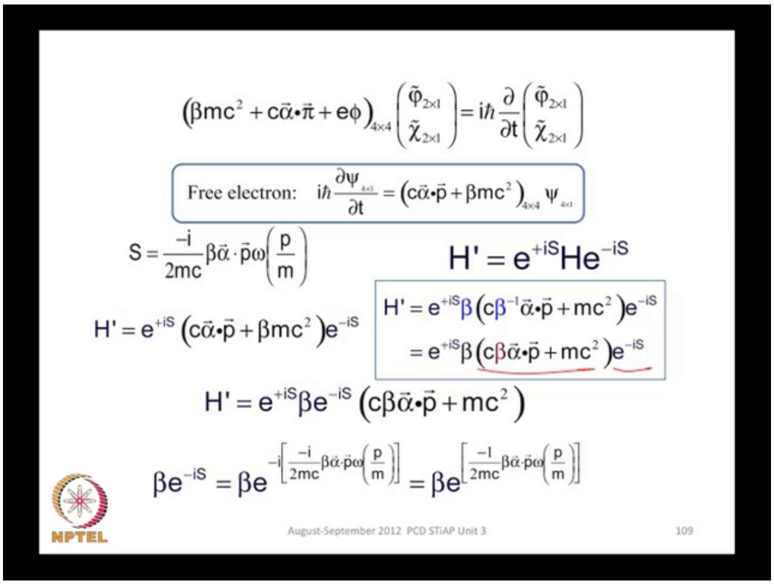

So, let us begin with this c alpha dot pi plus e phi, and to illustrate the method we first take a very simple case which is the case of a free electron, so the vector potential and the scalar potential phi do not appear in our equation of motion. So, the Hamiltonian is just c alpha dot pi plus beta m c square, instead of pi you get p pi is a generalized momentum, which includes the magnetic vector potential. So, you get only the alpha p term instead of alpha dot pi, because there is no vector potential, likewise this term e phi is also missing, and we have a much simpler relation to work with.

And you can already see that even for this equation even for the free electron, you have got the odd operator alpha and the even operator beta. And if you wanted to get freed of the odd operator, you could give a Lorentz boost to the electron frame, if you go over to the electron frame, then the mechanical momentum p of the electron in that frame would be 0, and you would get rid of the alpha dot p term.

So, there is some hope that he has this can actually be achieved, and the residual equation that you will have will then have a relationship which will not involve the odd operators. So, that can be done, but the general transformation operator, which is e to the i S followed by that reasoning Foldy Wouthuysen consider this particular operator, which is minus over i twice m c beta alpha dot p scaled by some unknown function omega of p over m.

This is a hitherto unknown function, but it is some arbitrary function of p over m and at in an appropriate juncture, we could choose yet to be whatever we will find it to be the most convenient one for us, for our purposes. We have not the objective very well defined, we want get rid of the odd operators our motives are you know very clear. So, this is this does not involve any times independence, so h prime is e to the i S h e to the minus i S, and that is what I have written here h prime is this.

This is the free electron Hamiltonian c alpha dot p plus beta m c square, this is the free electron Hamiltonian, and if you moved this beta outside the bracket move it to the left. And take it outside the bracket, then you would need to pre-multiply this by beta inverse right the first term. So, that is what to do over here, beta and beta inverse of beta m c square gives you the appropriate second term, and to make the first term appropriate you must include the beta inverse, but beta inverse is same as the beta.

So, you get e to the i S beta and then you get c beta alpha dot p plus m c square e to the minus i S, so that is the term that you get. And then since the transformation operator S is already made up of beta alpha dot p, which is what you have over here which is beta alpha dot p, this is just plus m c square multiplied by the unit operator. So, that is going to commute with e to the minus i S without any difficulty, but even this one mode and this e to the minus i S can be written before this bracket.

So, what you have is h prime operator is e to the i S beta e to the minus i S, and then you have c beta alpha do p plus m c square. Now, let us look at this term over here, beta e to the minus i S, I am looking at this part alone, which is beta e to the minus i S. I write S explicitly there is a minus i here, and a minus i here, so I get minus 1 over twice m c the rest of the operator.

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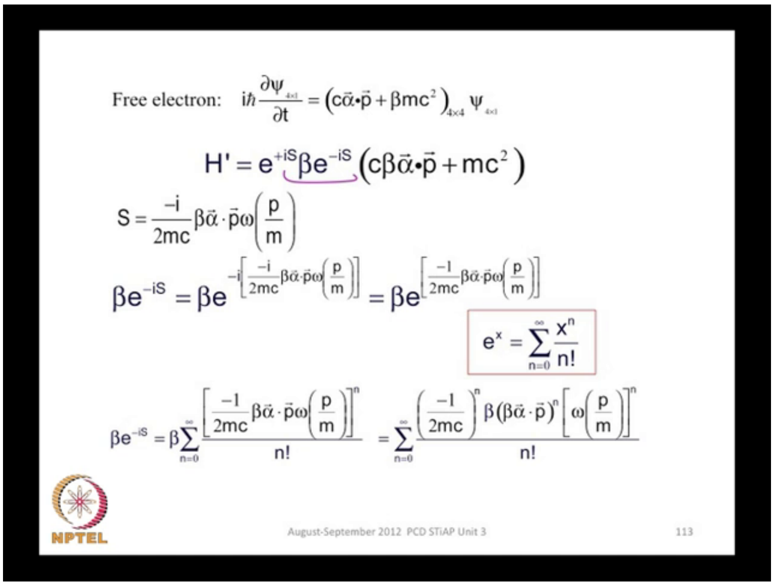

Now, let us analyze this expression further, because essentially beta e to the minus i S is this operator here, and you can use a power series expansion as you have for e to the x. So, that is a well known series, it is an infinite series, expect that x for us is an operator, and you must take it appropriate power of that operator. So, we plug in this infinite series, and it has got minus 1 over 2 m c to the power n, and then you have got beta alpha dot p times. This omega function which is yet to be determined to the power n, so this is to the power n and then you have a omega to the power n.

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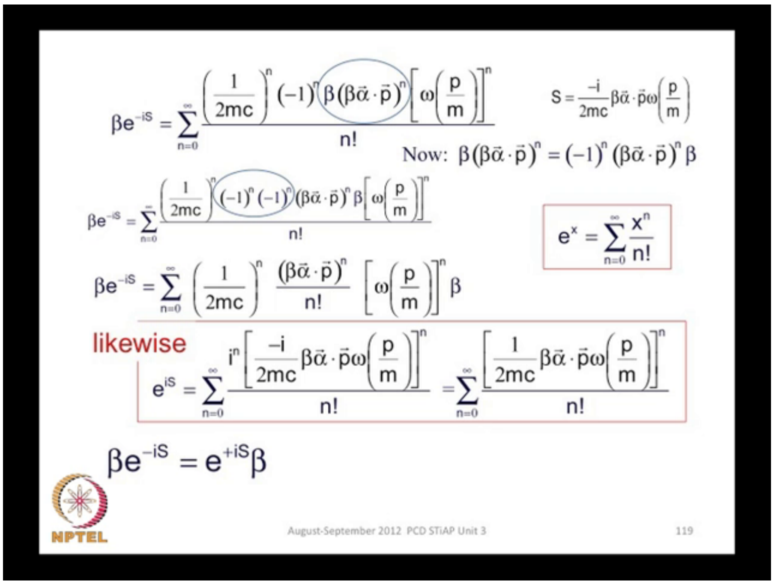

So, let us have a look at this expression, so you have minus when to the n here, this is your transformation operator S, now this is the identity that one can use. You can easily establish this by simply using the explicit form of the beta and alpha matrices, so very simple block diagonal structure. So, you can you know carry out the matrix multiplication law, and you will find that this operator to the power n is a same as the minus 1 to the n, beta alpha dot p to the n, and then there is a beta with 6 out.

So, you can substitute this operator by this term, you get minus 1 to the n which is already here another minus went to the n over here. So, that will give you minus 1 to the two n which is always be plus one no matter what n is odd or even, and then the remaining terms take a rather simple form. So, this is your expression for beta e to the minus i S, and using the same kind of analysis, you can show that e to the plus i S has this form, and you need both of them.

So, you have e to the i S which has this form you using exactly the same reasoning, and if you look at these two forms you find that if you multiply this expression on the right by beta, then you find that beta e to the minus i S is equal to e to the plus i S beta. This is not a commutation relation remind you, there is a minus sign here, and a plus sign here, and you have this operator identity.

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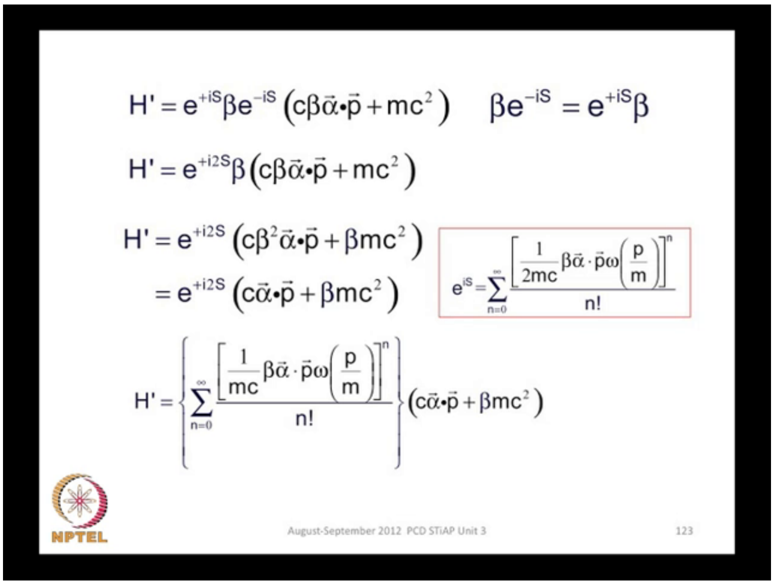

So, this is the one we can make use of over here, and this beta e to the minus i S, then becomes e to the i S beta, and together with this you get e to the i 2 S beta, and that you have got the c beta alpha delta p plus m c square. So, now you have got e to the i 2 s, but you know how to expand e to the i S, so e to the i 2 S will just have this coefficient multiplied by 2. So, instead of 1 over 2 m c you will get the 1 over m c, in the rest of the term rest of the expansion would be essentially the same. So, you have got 1 over m c instead of 1 over 2 m c, and then the rest of the expansion, and then followed by c alpha dot p plus beta m c square, now this is your transformed Hamiltonian.

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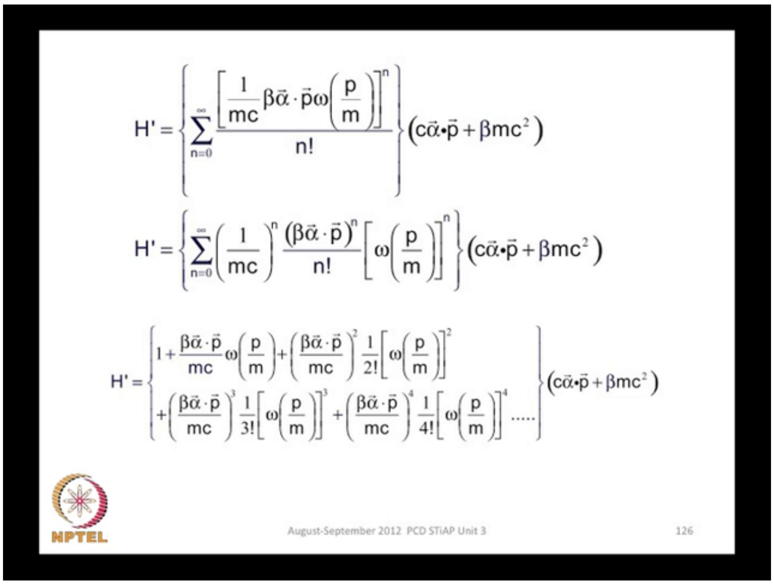

Now, let us look at this expansion in some further details, you recognize that this beta alpha dot p this 4 bracket is rest to the power n, so each factor 1 over m c is be is rest to the power n. The beta alpha dot p operator is rest to the power n, and omega function is rest to the power n, so you have this power series expansion now of these operators. So, for n equal to 0, you get the unit operator, then this is the term corresponding to n equal to 1, which is beta alpha dot p over this m c. And then you have got this omega to the power 1, then you get the second term which will have a 1 over factorial 2, which is sitting over here. Then you have the beta alpha dot p over this m c to m power 2 and then omega to the power 2, so you write each term explicitly.

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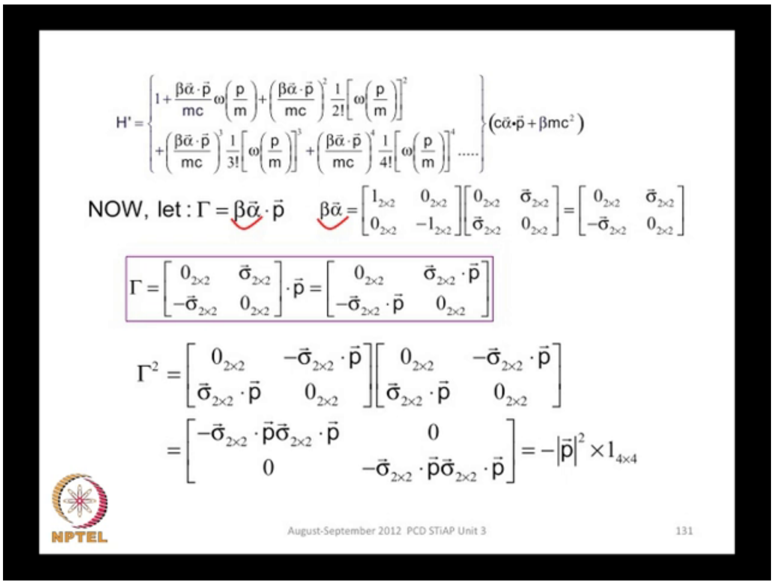

That is what we have, we bring this term to the top of this slide, and now to analyze this it is useful to introduce beta alpha dot p to be equal to gamma, and then look at the form of this gamma. So, beta alpha we can find out exactly what it is, beta is this matrix, alpha is this matrix, so beta alpha is this matrix operator, all that we have done is to use the matrix multiplication property.

And gamma is beta alpha dot p, so this is beta alpha, this you should take the scalar product with this p, for some reason this dot appear nicely as a dot or not as a box, as I did earlier, so it has decided to be kind to wash now. And you have this sigma dot p, and minus sigma dot p in these two locations, 0 in the diagonal locations, and now take the square of this, to get the gamma square.

So, let us take the square of this, and you can go head and work this out and find that this is nothing but minus p square times the 4 by 4 unit matrix. You know how to handle sigma dot p times sigma dot p, so it will give you the p dot p, and then you will get a cross product of p with itself which we will throw, so you get essentially minus p square.

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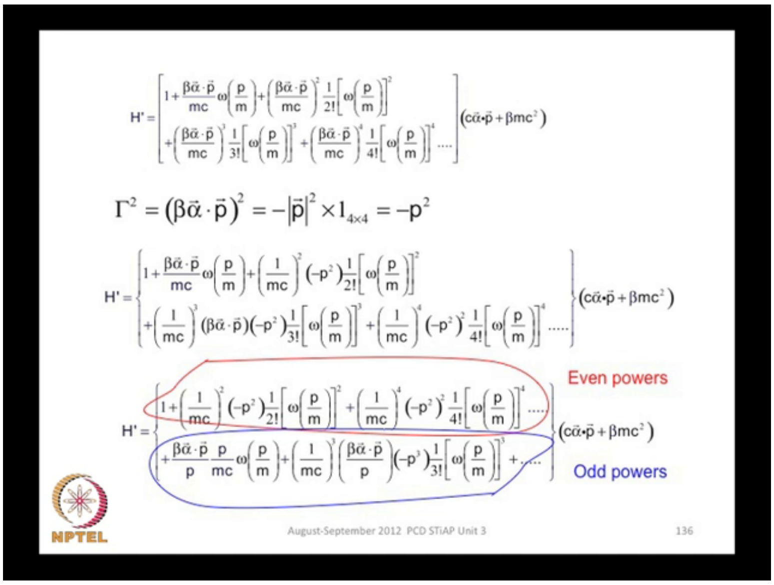

So, now you have gamma square and this really allows us to write this expression in a form which is very familiar to all of us, because now you write these terms explicitly. And you had the n to the power 0 term, then n to the power 1, n to the power 2, n to the power 3, and so on. Those are the terms which are written out explicitly, but whenever I have beta alpha dot p square, I have replaced that by minus p square, so I have a minus p square over here.

Here, I will have square of minus p square, this is the 4th power, so in all the even powers I will get raising exponent of p square by 2. So, that is an advantage that you get, and here you have got all the even powers in a first row, and all the odd powers in the second row, but notice that in the all the odd powers. Since, you get powers of you know p and then p square and p to the 4 and so on, so if you take one of those powers factored out this beta alpha dot p by p. If you factored out, then you will get odd powers over here, now I will show you how it is done, because you can take this beta alpha dot p as a common factor in each of these terms.

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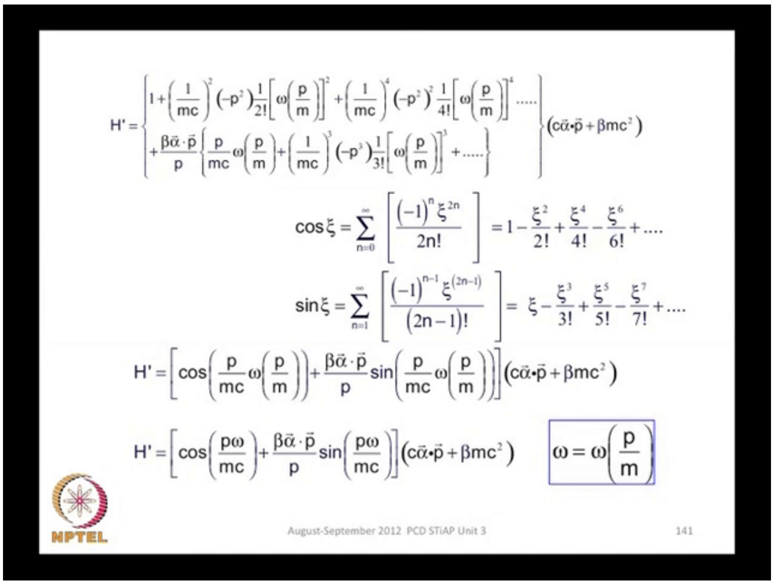

So, let us do that this beta alpha dot p, I have factored out then you get this term to the power 1, you have got a term in cube, but this one comes with a minus sign then next one is come with a plus sign. And you recognize that power series or you recognize the both the power series, so these are the cosine and the sine power series. So, we have succeeded in writing this power series in a very familiar form, so this is a cosine term, this is a sine term, but the sine term must be operated upon by beta alpha dot p by p which we factored out.

So, that we can get these odd powers, and the remaining powers came in p square p to the 4 p to the 6 and so on, so that is what we have got. And now you have got a rather simple form, these you instead of those infinite power series and so on, you have got cosine and sine functions, which are of course, power series and infinite terms in that. But, then these are familiar well known easy functions to work with, we know we used them all time in geometry trigonometry, so we can do some very simple mathematics for that.

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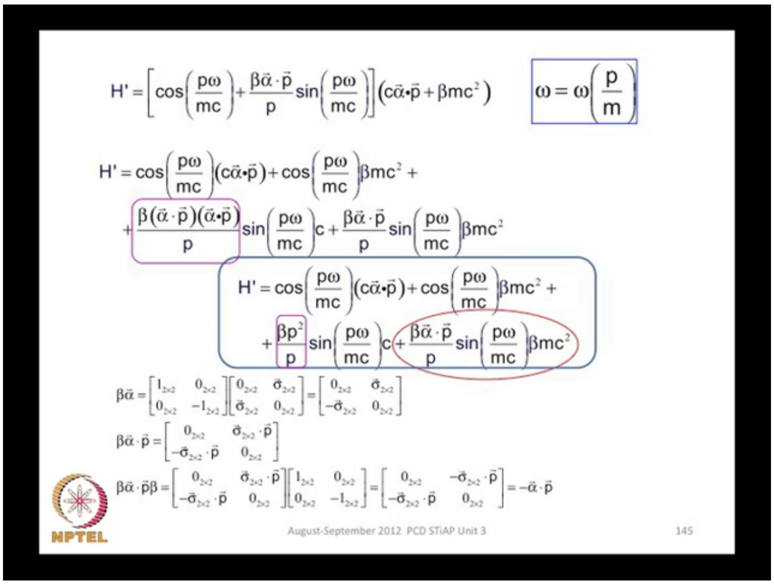

So, this is our there are two terms over here which operate further, which pre-multiply these two terms, so you have a total of 4 terms. This times this, then this times this, and then this times this, and then the second term times, the second term over here, so these are the 4 terms. Now, here you get alpha dot p and alpha dot p again, and this one is a dot this one is also a dot, but we know what it is.

So, we have this beta p square by p coming from this using the same kind of analysis as we did earlier, and now if you look at this 4th term, it has got the operator beta alpha dot p, and then there is another beta on this side. So, the essential operator structure, which is sitting in the last term involves beta alpha dot p beta in that order, which is what you have in the bottom here, beta alpha dot p beta.

That is what we are looking for, and to get that we first get beta alpha, then get beta alpha dot p, and then get beta alpha dot p beta and all you have to do is used the dirac matrices. And carry out the multiplication systematically, it is a very simple thing to do, and you find that this beta alpha dot p or alpha dot p, when it is bracketed by beta on either side is nothing but minus of alpha dot p.

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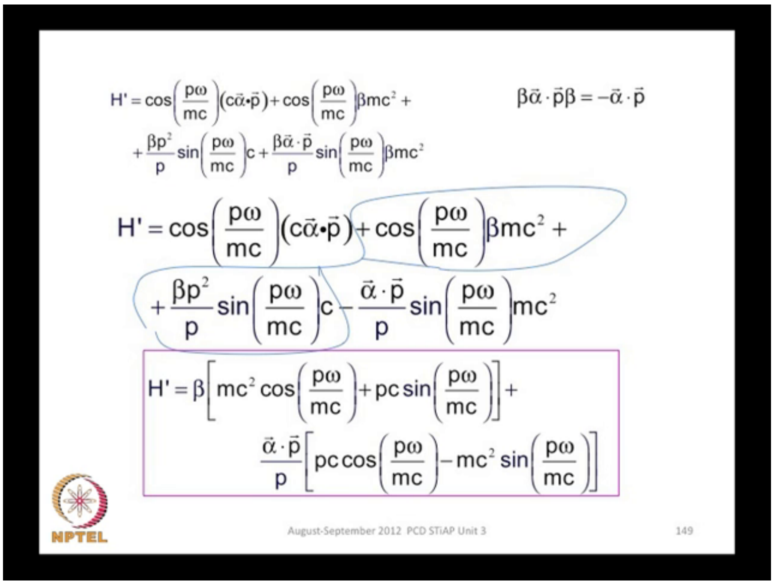

So, you can simplify this operator over here in the last term, so that is what we have done here, you have got the beta alpha dot p beta equal to minus alpha dot p, and that is what comes over here in the 4th term. Have good enough, now let us combine these two terms and these two terms, so this has got beta, this term has a beta, this term also has a beta, so these two terms are combined.

So, beta and the remaining part of this term is m c square cosine of this function, and the remaining part of this term after having extracted beta is p c here is a p square by p and here is a c here. And then you have got a sine function, so these two terms come as a first two terms, and the first and the 4th term come as the next two terms.

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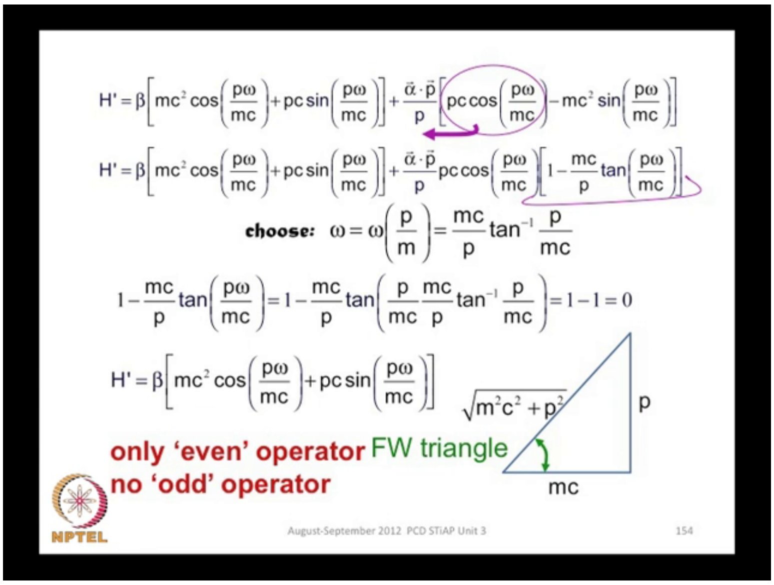

Now, we can really make a choice that we will find to be extremely convenient for us, let us take this cosine function multiplied by p c outside, because then you will get m c over p over here times the tangent of this function. So, let us get this cosine function now, and now if you choose your omega, because that is a choice, which we have left free for us, and we exercise that. Now, it is almost like you know manthra exercising her ride whenever she wanted, so we have our freedom now, but this is going to be for a good cause.

So, what is the choice, you choose omega to be m c over p tan inverse p over m c, because what it does to this term is throw it off, with this choice of omega, this 1 minus m c over p tangent term goes to 0. What you are left with, h prime equal to first two terms, where is the odd operator is gone, so the choice allows us and this is sometime called as a Foldy Wouthuysen triangle, because you will see that this is almost like root of m square c square plus p square. So, you are left with only the even operator, where you find the Hamiltonian and the odd operator is eliminated, now this is exactly what we wanted to achieve.

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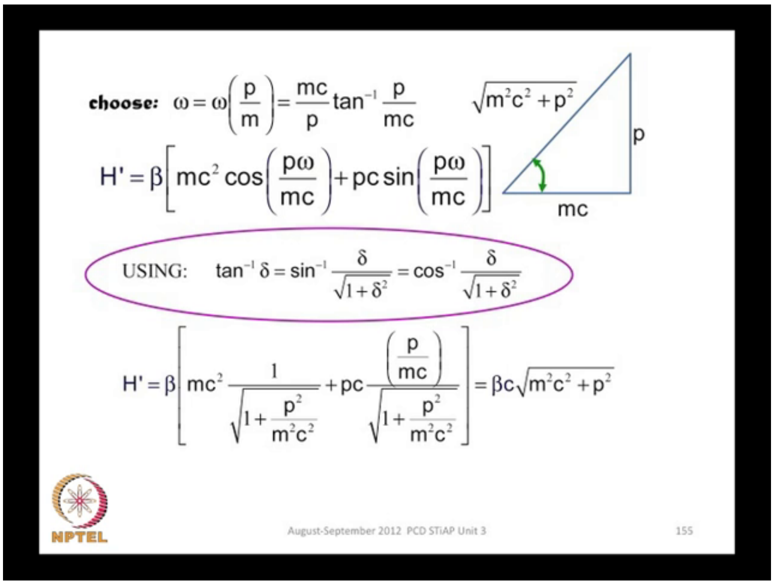

And using this identity for tan inverse function, you can write this as beta c times root of m square c square plus p square, there is beta of course, but beta has got 0es in the off diagonal locations. So, by choosing this particular angle, we have succeeded in throwing of the odd operators, that was the motive of carrying out this transformation.

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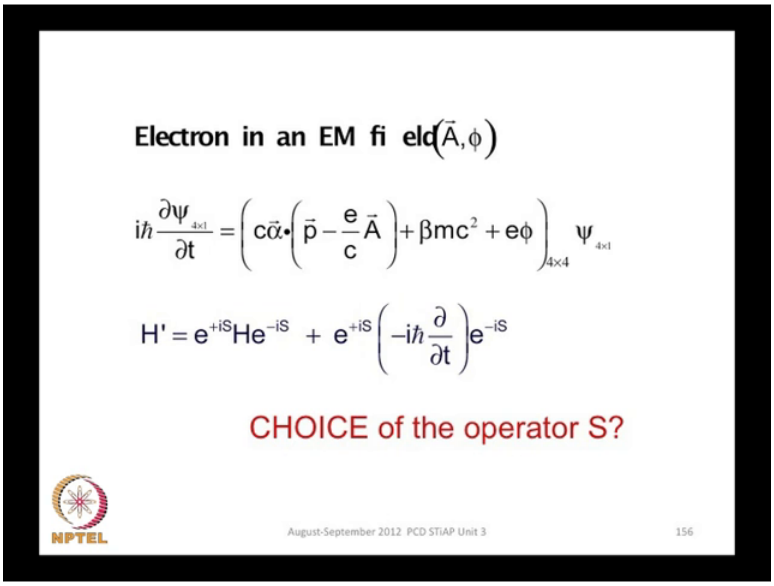

So, we know that is possible to do that, we had restricted ourselves to a free electron which is not the general case, so we have to now figure out, how to do it, when you have an electron in an electromagnetic field. And now, you cannot expect S to be independent of time, you will have to take this term into account, because you have got a vector potential which easily could be time dependent. So, now the operator S which will be involve in the Foldy Wouthuysen transformation will be will need to have the provision to be a times dependent operator, so how do we choose it.

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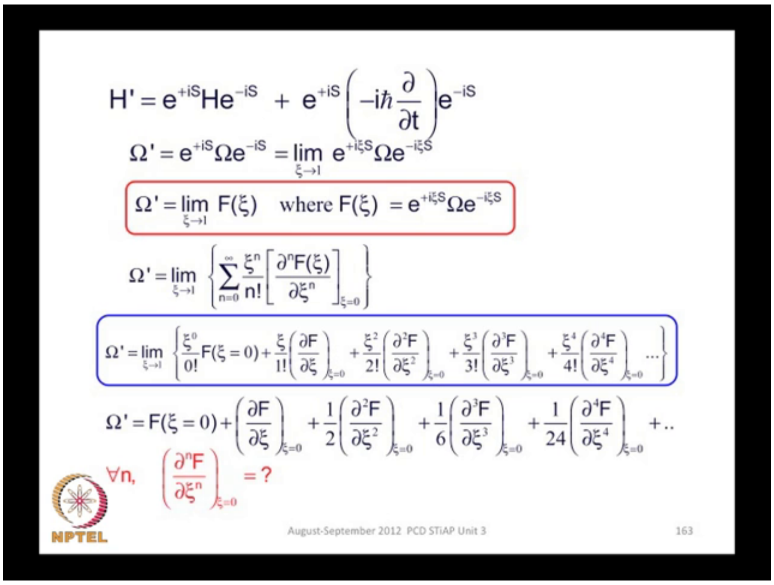

So, first of all we have to see how these operators are determined, because we definitely have times look at these operators, where h is whatever be the form of the Hamiltonian, and now it will include the vector potential and the scalar potential as well. So, here are well known techniques and this is another reason, why I think it is nice to learn the Foldy Wouthuysen transformations, because you learn some techniques, which you can find useful in many other applications in physics. And these are very powerful techniques simple techniques, but powerful techniques.

So, omega prime is this, and it is good to look this expression as the limiting value of e to the i psi S omega e to the minus i psi S in the limit psi going to 1, and then you are taking the limit of a function of psi. You are taking the limit of a function of psi this function is this operator, we know what it is and you can expand this function of psi in a power series.

This is a well known power series expansion of a arbitrary function of psi, here notice that the derivatives are to be taken as psi equal to 0, and after you take the derivatives, you complete the process of taking the derivative and then take the going to 1. So, there is no contradiction in the derivative begin taken as psi equal to 0, and then taking the limiting value of this function psi going to 1. It is absolutely no contradiction, you do it step by step one step at the time, so it is mathematically absolutely correct.

So, let us do this, so let us have this power series expansion now, take the derivatives as psi equal to 0, and then after taking the derivatives take the limit psi going to 1. So, let us do it term by term, these are the derivatives as psi equal to 0, and then you take the limit psi going to 1. So, all these psi square over factorial 1, becomes 1 over 2, psi cube over factorial 3 becomes 1 over 6, psi to the 4 over factorial 4 becomes 1 over 24, and so on, so that is a kind of you know set of terms that we get. So, this is your expression for omega, and in general you will need the nth partial derivative of f with respect to psi, at psi equal to 0.

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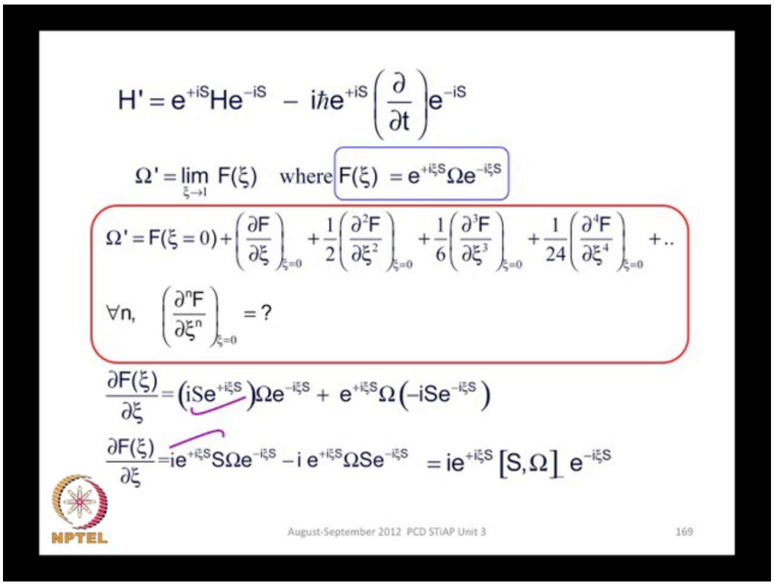

So, that is what you need in general, so this is the nth derivative that you are going to look for, and now let us take a look at this f of psi, this is your f of psi. Now, S may or may not commute with omega, we will not make any assumption on that, and you take the first derivative with respect to psi, then take the second and find a general expression for the nth derivative, because that is what you need.

So, the first derivative is e to the i S e to the i psi S, because e to the i psi S and S commute with each other, S may not commute with omega, but it does commute with e to the i S, because it is just a power series n S. And over here from the second term you get minus i S, because this is e to the minus i psi S, now these two terms commute. So, you interchange their positions, and now you can combine these two terms by sandwiching this commutator S omega minus omega S in between these two exponential operators.

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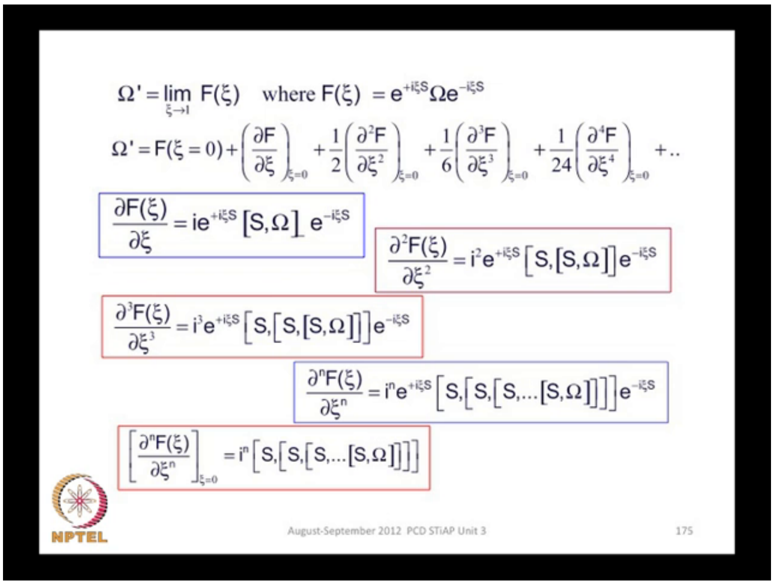

So, this is your first derivative with respect to psi, which involves this commutator, so this is your first derivative. Now, if you do the same thing and get the second derivative, you will get more commutators, and this is a very nice series that you get, it is a beautiful series. So, you get the commutator of S comma omega with S, then you get another commutator, when you go to the third partial derivative, you are extending the same technique, you can develop an expression for the nth partial derivative.

So, this is the expression for the nth partial derivative, you will have to raise this i to the power n, and then you will have so many you know commutators to work with. Now, this is a very good result, and then you take the value as psi equal to 0, so e to the i psi S becomes 1, e to the minus i psi S also becomes 1, and you can forget about it, because you have take the derivative at psi equal to 0. So, this is the term for n equal to 0, then for n equal to 1, you get i times S comma omega, then you get i square and then this commutator. And that is how you get subsequence terms you will have an infinite series actually.

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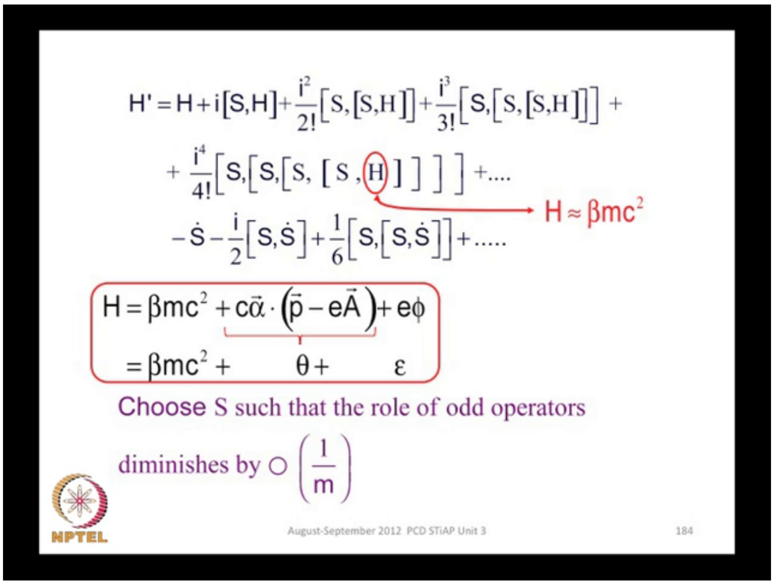

Now, we have figure out how to handle the first term and this is the infinite series that we had, but we also have to work with this time derivative term. So, you have got an infinite set of series coming from, how we handle this term and then we still have to figure out what to do with this. And over here we are not going to assume that the time derivative operator commutes with S, it may or it may not in general it will not.

So, when you take that into the account very carefully, you get commutators of S with S dot whereas, dot is the time derivative of S, so I will not show you the intermediate steps, but you know how to work it out. And you will get commutators of S with S dot, and then each commutator with S, and subsequently you can have another infinite series. So, now, you have got two infinite series, which are summed over, they are added to each other in your transformed Hamiltonian.

Your original Hamiltonian has got this odd operator, and your whole intention is the expect the right hand side to have some form, in which the odd operator would become if not eliminated at least less important. And our first goal is to look for such transformation, which will reduce the odd operators at least by a factor of m, by 1 over m m is a huge mass, it is half a million electron volts. So, that is that is the motivation, that is how we look for this transformation operator.

Notice, that over here I am strike the full Hamiltonian inclusive of these terms, the first term, the second term and the third term, but in the 4th term, if I approximate h only by beta m c square, and choose S 2 have to be an operator of order 1 over m. Then I have 4 of these operators in this term, so I get 1 over m to the power 4, scaling coming from that. And then if I left the Hamiltonian to be written only by beta m c square, the whole importance of this term will be reduce by 1 over m cube.

And I can develop an approximation scheme in which we propose that retain only those terms which are of the order 1 over m cube, if it is 1 over m to the 4 or smaller throw it, that does not look like a bad approximate at all. And to retain to develop an approximation, which will have the leading term, which and then all the subsequent terms will become diminishingly small, because they have higher power a S, because there are more number of S operators, which appearing in these commutators. So, if S is of order 1 over m, the more number of S'es you have the weaker the commutators.

So, you can make this approximation beta m c square, for h in this term, but you cannot do it over here, because this will be 1 over m cube, this is of order m, and then you will have only 1 over m square approximation. So, that is not what we doing, we are doing 1 over m cube, we want to retain terms at least up to 1 over m cube. So, you can make an approximation to the Hamiltonian in this commutator, which have got 4 of these S operators as you see.

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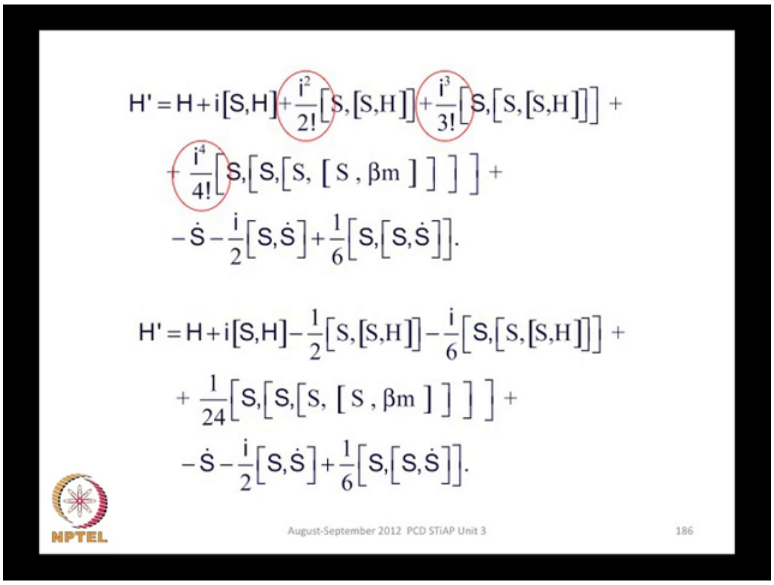

And correspondingly you make this term here also you have 3 of these S operators, in the times derivative terms which is again of order 1 over m cube. So, you make an approximation which is consistent, and put a period over here you are truncating the infinite series, that is an approximate, which is why in trigs book on the quantum mechanics he very categorically states. This the Foldy Wouthuysen transformations go as far as they do it is not that is exact, and this is the reason it is not exact, but it is good.

So, you truncate the series, which is various approximations involve put a full stop over here, forget about throughout the rest of the terms. Now, this is your transformed Hamiltonian h prime, now let us analyze this, bunch of commutators you are not choosing S'es yet.

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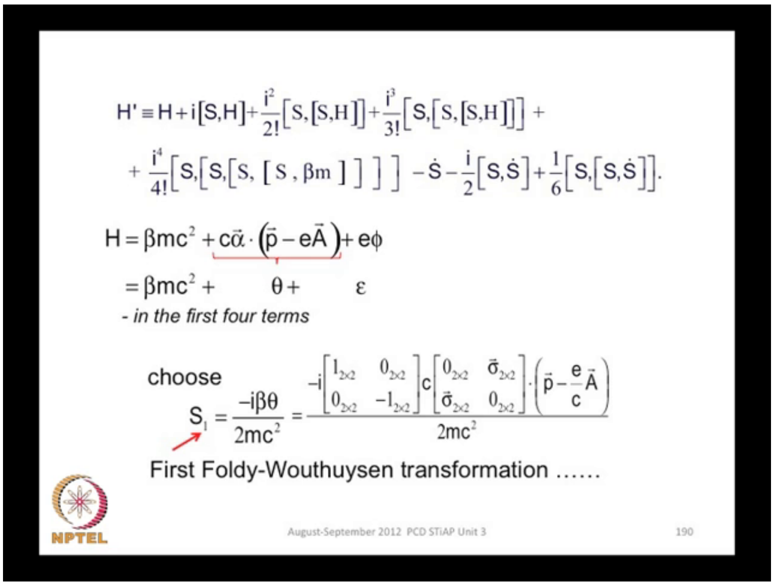

And you choose your Foldy Wouthuysen transformation operator to be given by minus i beta theta, theta is this coupling, it includes the generalized momentum, it includes the dirac operator alpha. So, let us write it explicitly this is your Foldy Wouthuysen transformation operator, it has got the similar form as you found was used for the free particle transformation operators.

So, there is some clue available from free particle transformation, and you can actually carry out the Foldy Wouthuysen transformation further more by carrying out these transformations further, you can reduce the importance of the odd operators further. So, this is the first Foldy Wouthuysen transformation as a matter of fact, it turns out that is most promising is subjecting the whole system of equations to 3 transformations.

Namely the first, second, and the third Foldy Wouthuysen transformations, so we will see how they look.

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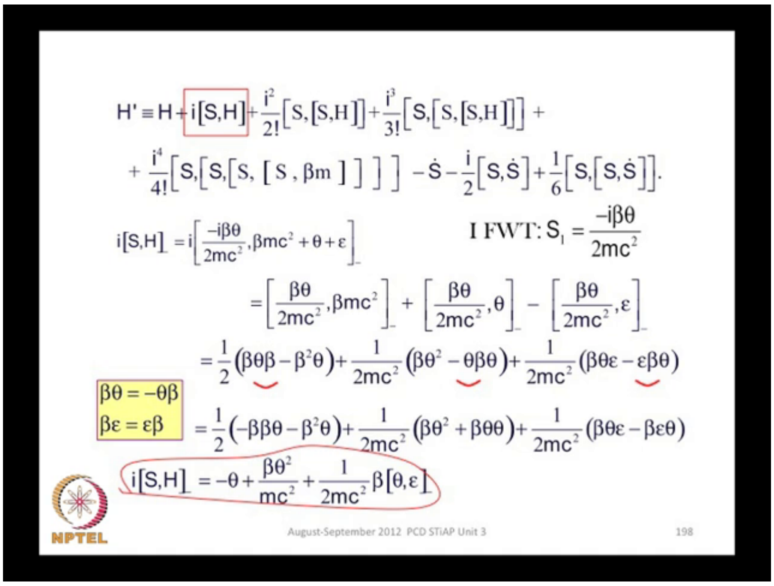

So, this is the first Foldy Wouthuysen transformation, through an operator which is minus i beta theta over twice m c square, and now you can plug in this explicit form of the dirac operators beta and theta. And you know the commute, how to find the commutation of beta theta with h, and using that you would know how to find the commutator of S comma h with S, so it is simply, but laborious. And that is where your youth will coming handy, because you can do such things without getting tired, you have boundless energy, although it is said that youth is vested in the young people, so this is the operator i S comma h.

So, this is the Foldy Wouthuysen transformation operator S, then you have got the dirac Hamiltonian and find the commutator of the Foldy Wouthuysen transformation operator with a first term, with the second term, and with the third term. Do it term by term simplify, use the properties of dirac operators, the dirac matrices, you see how it is developing. Find out how these dirac operators multiply each other, theta beta is minus of beta theta.

Beta epsilon is same as epsilon beta, but these this is different, so you used a correct signs over here, you also know that beta square is equal to 1. And when you combine all of those terms this is what you get for i S comma h, but that is only the this box over here. And these things some time to do, especially after removing the careless mistakes it takes a little while.

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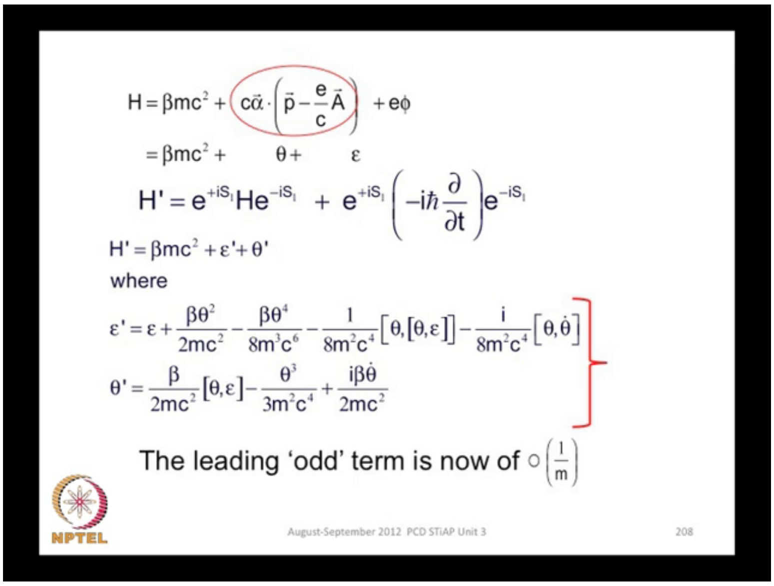

And then you do it, you know what this i S comma h is, this is what turns out to be, then using, this you find the second term, and then using this you get the next term, by now you have missed your dinner. Lost a little bit of sleep, and then when you handle all of these terms very carefully, you get this S comma S comma h. Then you can get the next one, similarly and I am not going to show you all the terms, but now you know how to do it.

This is very simple, same thing with the times dependent, also that is the other infinite series, which you have truncated happily to 1 over m cube, but at least those terms those commutators, you have to determine there is no escape from that. So, you get the commutator of S with S dot, and what you get is the transformed Hamiltonian h prime, which can be written as beta m c square plus 2 new operators epsilon prime and theta prime, whose leading term is of the order of 1 over m.

So, all the odd operators are now reduced by factor of m, that is a significant achievement in getting this transformed Hamiltonian, which is to reduce the importance of the odd operator. So, that you avoid the mixing of the particle, and the antiparticle states, so that is the leading term that you get in the odd operator.

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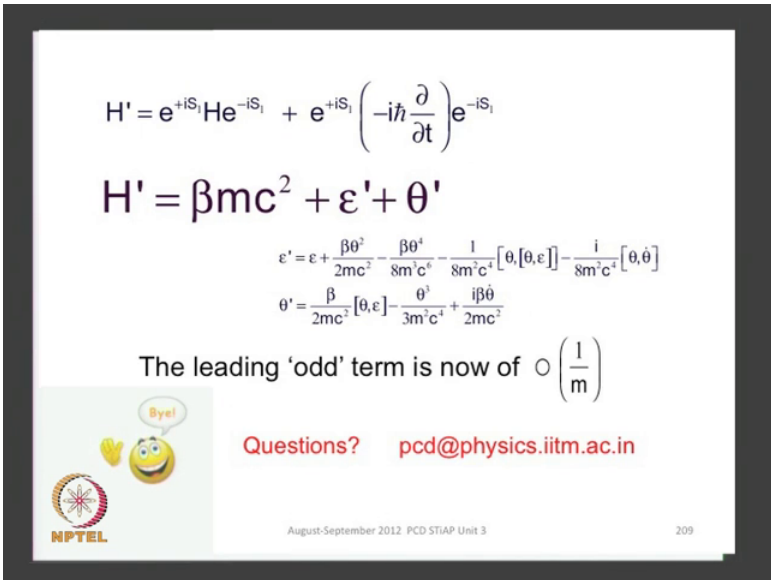

And that is where I will stop for today, I will be happy to take some questions, but essentially you have seen, how the first Foldy Wouthuysen transformation works. And then we will have a second Foldy Wouthuysen transformation, and then we will have a third Foldy Wouthuysen transformation. And when you do that, you will see very happily where the spin orbit interaction term really comes from, you really need to subject the dirac Hamiltonian to 3 conjugative Foldy Wouthuysen transformations. For that term to become manifest in the 2 component form, but for now if there are any questions, I will be happy to take otherwise goodbye for now.