Select/Special Topics in Atomic Physics

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Lecture - 13

Relativistic Quantum Mechanics of the Hydrogen Atom

Greetings, I will begin unit 3, which is a very fascinating topic Relativistic Quantum Mechanics of the Hydrogen Atom. So, we obviously have to use relativistic formalism together with quantum mechanics. And I will be using predominantly these two books, both have the same title called Relativistic Quantum Mechanics, one is by Bjorken and Drell and the other is by Greiner. And these two are very good sources for much afford I will be discussing in this particular unit 3.

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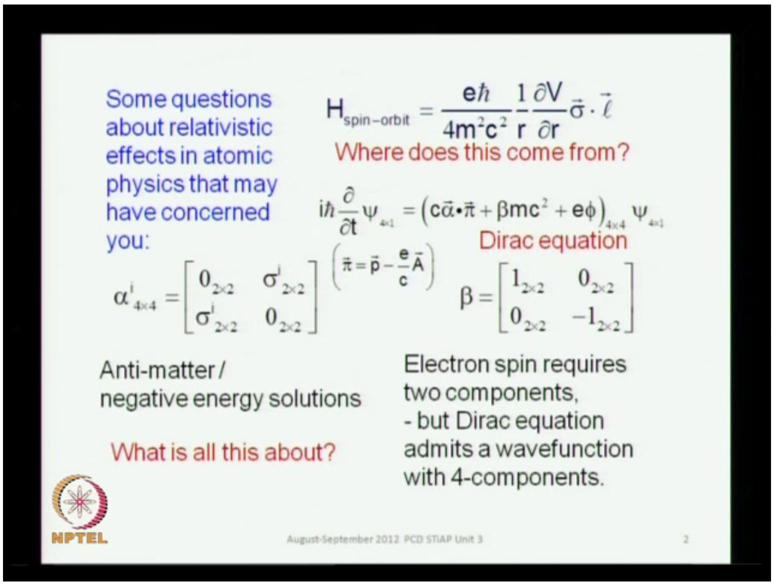

Now, again you would have had some exposure to some relativistic effects in atomic spectroscopy from your earlier courses in quantum mechanics or atomic spectroscopy or whatever the courses you have taken. Other various questions that may have been raised for example, you would have seen this term possibly, if you have seen it, that is what I am referring to, if you have not seen it, you are going to meet this term in this unit.

And a dominant relativistic effect in atomic spectra is the spin orbit interaction in the atomic structure and spectroscopy collision and although atomic processes, this is a spin orbit interaction. It has this form which you may or may not have seen earlier and if you did, the question that would asked itself is, where does this form really come from and we are going to figure out, how exactly you get this term. You also may have seen the Dirac equation, which we shall introduce and discuss in some detail from first principles.

And you will notice that, this equation has got a matrix structure alpha and beta are 4 by 4 matrices, the wave function has got a number of elements and then, you also know that, there are questions about negative energy solutions, antimatter and all that. Now, we do know that, electron spin requires two components, but you see in the Dirac equation that you have got four components. So, what is all this about, these are some questions that we shall tackle in this unit.

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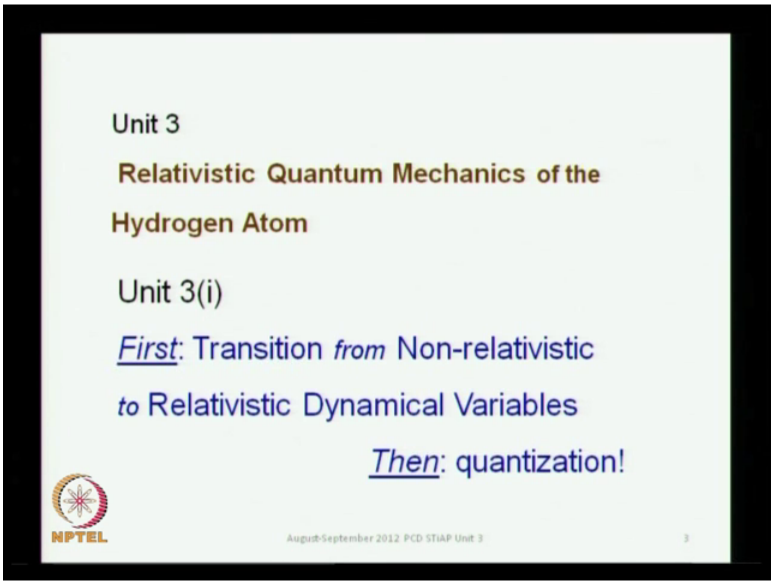

So, before I get into the main subject of discussion, I will spend some time in today's class, which is the first class first lecture on this unit on brushing up the transition to relativistic dynamics. So, before we get into relativistic quantum mechanics, I will remind you of, what is involved in the transition to relativistic dynamics as opposed to non relativistic classical mechanics. So, I will spend just some time recapitulating those ideas, I am sure that you are aware of that, but this will be just a quick brush up.

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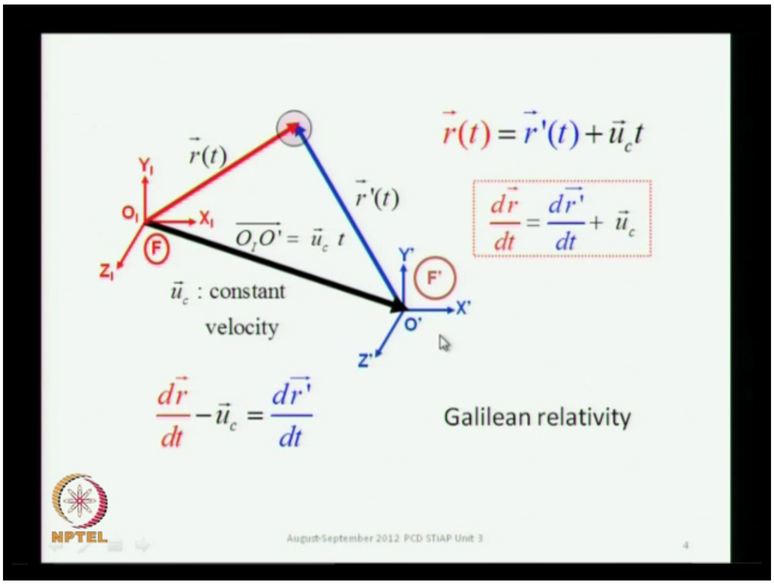

So, let us look at phenomena seen by two observers, one in an inertial frame of reference, which is this red frame and the other also inertial frame of reference. We have second observer in this blue frame is also an inertial frame and inertial frame is one, which moves the constant velocity with respect to another one. So, the second observer is moving at a constant velocity, which is this u with respect to the first observer.

And let us say that, these two observers whose observations we are comparing and the first observer looks at an object, whose position vector in his frame of reference is this r, this is the instantaneous position vector at time t. The position vector of the same object for the second observer is r prime t, this is a primed frame of reference, this is the unprimed frame of reference. And from the triangle law of addition, you know the relationship between these two vectors, the differences this displacement of the second frame of reference.

We assume that the X Y Z axis of both the frames lied on top of each other at t equal to 0. So, the displacement in time t would be this velocity times t and this is the relationship between the two position vectors. Now, if you took the time derivative of this relation d r by d t, you get the velocity of this object in the first frame and d r prime by d t gives you the velocity in the second frame and these two velocities are obviously not the same, because you must add u c to this to get the velocity in the first frame.

Now, essentially this is the relationship between the velocities of an object in two inertial frame of references. Now, this is Galilean relativity, this makes a certain assumption that, the speed of light is finite and all of these conclusions are consistent with this assumption. And as long as you do not question this assumption, you are ok, so the relative velocity between as seen by two observers, it depends on their relative motion, that is the essential point in this.

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And I like to show this little radial of this kid, let me see it comes up, yes it does and I really like this video. And what you see is, if you ask the question as to what is it is velocity, is it positive, is it negative, is he going forward, is he coming backward, does his velocity even have the same direction and it really depends on, what the frame of reference is, that is something that you must ask, is it nice fellow, he makes it. This I downloaded by the way from the YouTube and I have given the reference here, so this is the full reference, you can also view it if you like.

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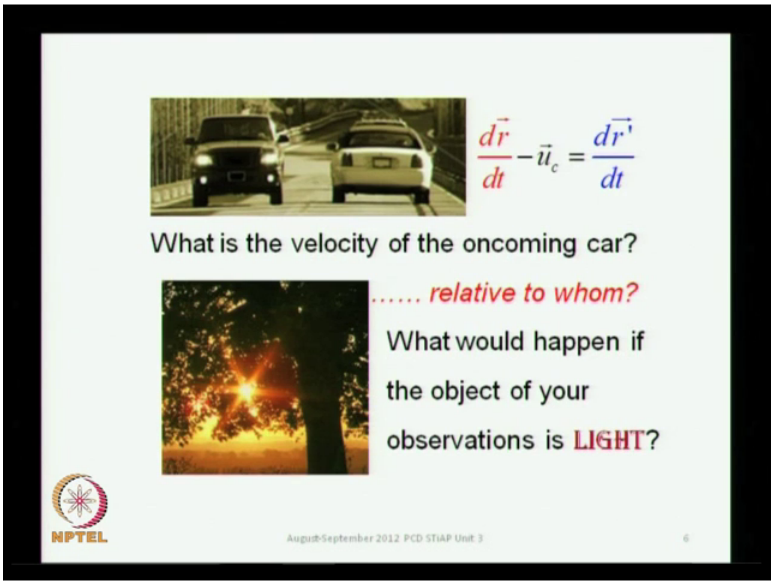

And then, our conclusion is that, whenever you are looking at the velocity of an object, you must ask, velocity with respect to whom. Now, is it this car or the other car and with respect to whom, is it with respect to somebody on the road or is it somebody who sitting in one car or the others. So, these are the questions of immediate relevance, whenever you are looking at any object and ask, how fast is that object moving.

Now, it turns out that, if the object of your interest is light, you are not looking at a car or you are not looking at this little kid on the treadmill, if you are looking at light, a pulse of light is fire then, what kind of considerations are involved. So, let us actually see, what we are talking about.

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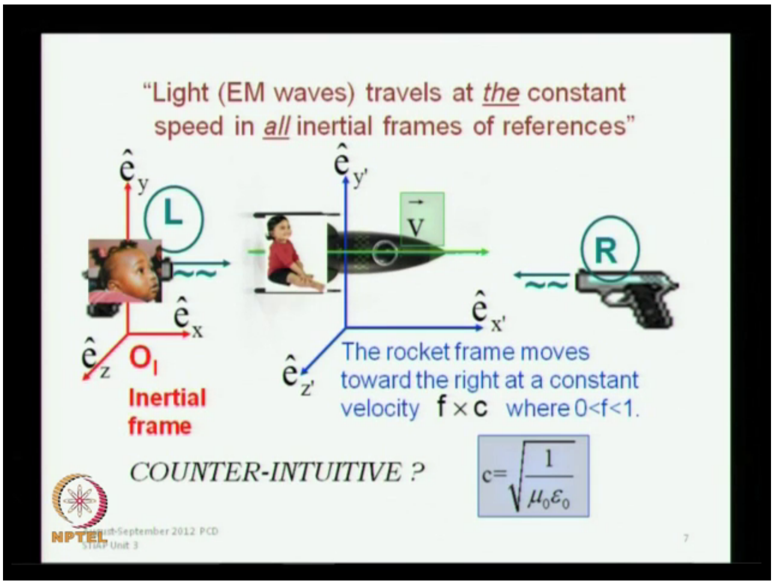

So, here you have got a light source or laser gun if you like and you fire, a pulse of light and this light goes from left to the right in this frame of reference and you have got an observer in this red frame of reference and this is our observer. Everybody is getting smart these days, younger and younger people do more and more challenging things. So, you have your observer over here, who is looking at this pulse of light and this observer would measure the speed of this light in power frame of reference.

You have another observer who is moving in another frame of reference, which is also inertial frame of reference and he is going at a constant velocity with respect to the first observer and he also measures the speed of light. You can think of another experiment, in which light is fired from a different gun in the opposite direction and now, you have these two observers, who are measuring the speed of light. Now, what is the interesting is that, no matter which observer is measuring it and no matter which light you are talking about.

If it is a light which is going to from left to right or the other one from right to left, all the observers get essentially the same answer, which is root of 1 over mu 0 epsilon 0, which is a permeability of light, permeability of vacuum and electric permittivity of vacuum. So, the speed of light is determined by properties of vacuum and it makes no reference at all to which observer you are talking about. Now, this is very strange thing, because this was not a very experience when we talked about the velocity of the child that we were looking at.

If you are the child, it would be fun, but the speed would always be 0, whereas if you are standing behind him or on the treadmill, it would be different for all the different observers. Same thing with, if you are looking at a car which is moving, but the speed of light does not make any reference to the observer, it is always the same, no matter which observer you are referring to, it is always the same value in every inertial frame of reference and physics has to reconcile with this.

This is a result which physics was not really prepare for and this is a result, which Einstein was a first one to see and not just from the Michelson Morley experiment, but from many other consideration that I will not going to the history of the special theory of relativity, which is very fascinating. Because, in this course, I just want to refer to some other main conclusions to lay the foundation for our discussion.

Now, this is what I would called as counter intuitive, because if our intuition was built on our experience with regard to our conclusions on our observation about the child's walk on the treadmill or looking at a car from one frame of or another then, we would think that, it is counter intuitive, but intuition is a function of education. And then, if you get educated and built your intuition based on further knowledge of the laws of nature then, you might find that, this particular conclusion would completely meet the expectation of your intuition. It is a result which once you understand the implications of the special theory of relativity, you would find that this is precisely what you would expect.

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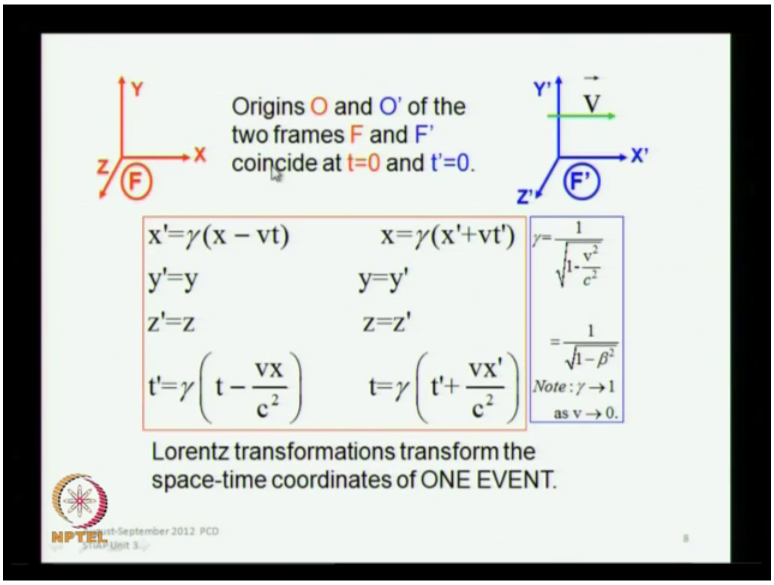

So now, the reconciliation comes from the fact that, the laws of transformation between the coordinates in one frame of reference and another frame of reference, are no longer Galilean, they must be modified and they are what are known as Lorentz transformations and these transformations transform not just the space coordinates, but also the time. So, time is no more to be treated as absolute, this is one of the upshot of the special theory of relativity, where we always think that, time is absolute and we do not connected to the state of motion of the observer himself.

But, that is something that, we have to reconcile with and these are the Lorentz transformations, you go from X Y Z and t to X prime, Y prime, Z prime and t prime. Through these transformations, gamma is this ratio and V is a constant velocity of the second observer with respect to the first observer along the X axis, so that is the coordinate system that I am chosen over here.

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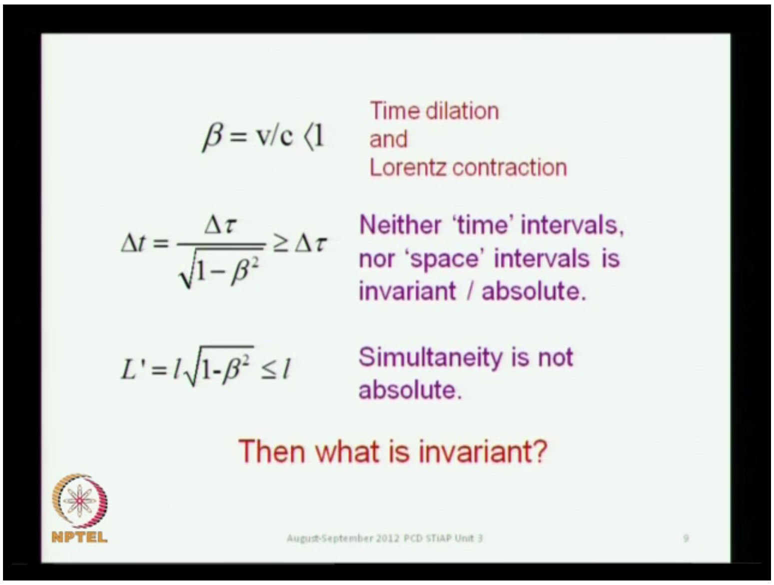

Now, what are the consequences then and then, again I am not going to spend any time discussing these consequences, because that will take us into specific discussion on the special theory of relativity, which is not my intention, because we want to get into relativistic quantum mechanics. But, I will just remind you that, time is not absolute nor a space, so what we think of space interval, the interval between two points in space or the interval between two events that we talk about between the time it took for you to come from your hostel to the classroom or whatever.

These intervals neither the time interval is absolute nor is the space interval absolute and they depend on the state of the observer and it leads to, what is referred to as time dilation and Lorentz contraction. So, both time and space intervals, we have to modify our perception of time and space intervals, this is guided by a reconciliation with our notion of simultaneity. What is simultaneous for one observer is not necessarily simultaneous for the other and then, one needs to ask that, if neither space nor time intervals are invariant under Lorentz transformations, what is it that is invariant and that is quantity of interest.

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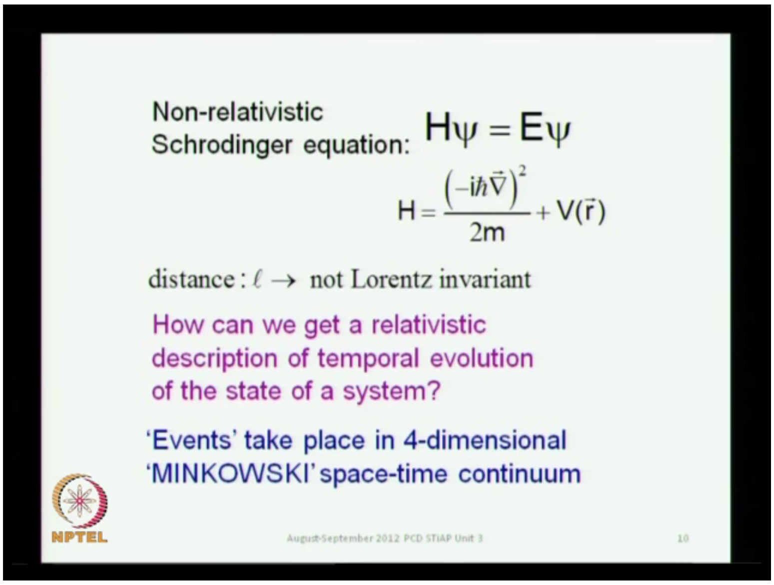

So, this quantity is of interest was, because our interested quantum mechanics is the following, we deal it with the Schrodinger equation in quantum mechanics, the non relativistic Schrodinger equation. You have got the dynamical variables position on momentum, you have the time derivative involved, when you take the time evolution of state function of the state vector and the space interval that would go into the potential function.

For example, even in the simple problem like a one dimensional potential barrier problem if you like, the distances that you are talking about, these are no longer to be consider as a invariant and you must take into account, the state of the motion of the observer to analyze these dynamical variables. So, the distance l is not Lorentz invariant and then, we should therefore ask that, the Schrodinger equation since it cannot be Lorentz invariant, how do we get a relativistic equation, which is consistent with the Lorentz equation with the Lorentz transformations, which reconciles with the fact then, the speed of light is finite.

So, this is a question that we must ask and again this comes from non relativistic classical mechanics that, you need to extend your idea of space to four dimensions. And this is an extension into a four dimensional space, which includes time, this is sometimes referred to as a MINKOWSKI space time continuum.

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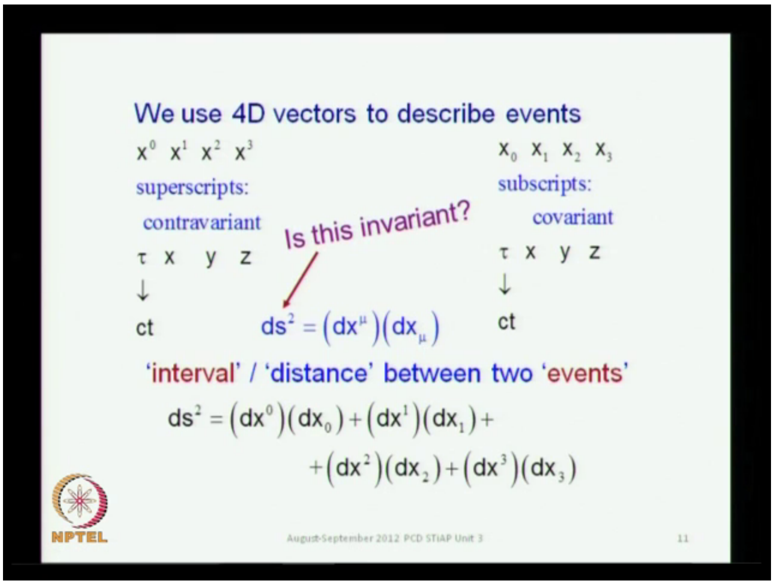

And then, an event in this space is characterized by four variables, these are the x 0 x 1 x 2 x 3. So, I will quickly remind you of the notation, I will not spend too much time working this way up, I just to quickly remind you. And then, introduce the invariant quantity, which is this scalar d x mu d x mu and this is the quantity, which is invariant under Lorentz transformations.

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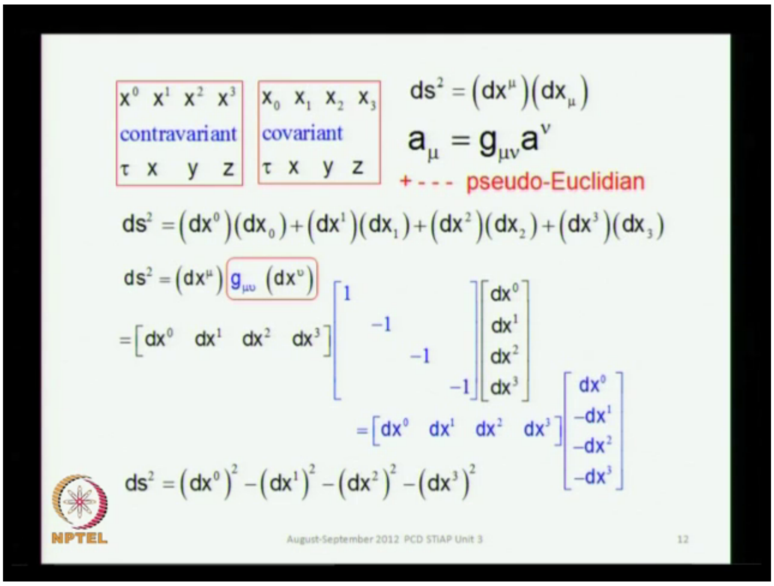

Now, how do we know that, this is invariant, now first of all the way that you get it is through this lowering of indexes, it called through the g matrix and this g has got a certain signature. This is a 4 by 4 matrix, which has got these diagonal elements, which are given by 1 minus 1 minus 1 minus 1, all the remaining elements in this 4 by 4 matrix are 0, so I have not written them out. And there is a specific difference between the interval in a four dimensional Minkowski space, which is referred to as a pseudo Euclidean space, as opposed to a Euclidian space at the difference is in the signature.

Because, d s square is defined as this particular summation of these quadratic terms, but the signature 1 minus 1 minus 1 minus 1 of the g matrix assigns the specific signs. Whereas, if the four dimensional space was Euclidian, if it was an ordinary extension of how we go from a two dimensional flux space into a three dimensional Euclidian space, that is a straightforward extension, this is different, this is why it is called as a pseudo Euclidean space.

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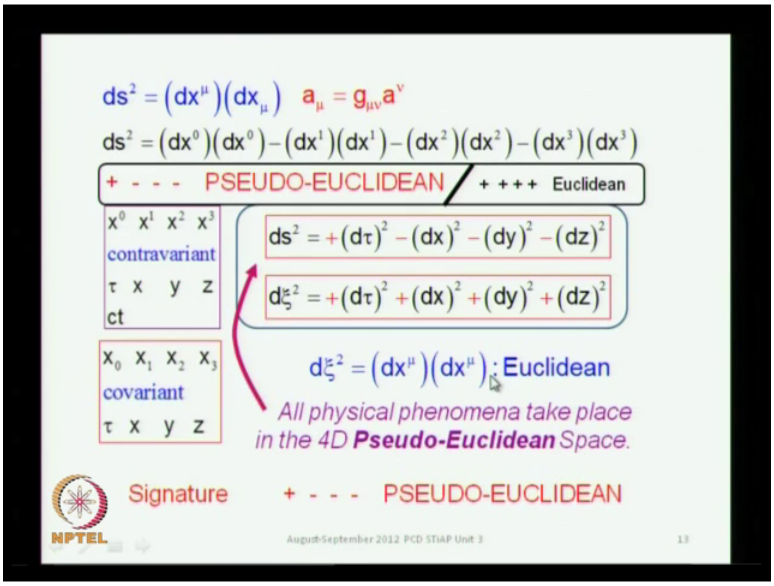

And in this pseudo Euclidian space, the signature of g is particularly important and special theory of relativity is built on this pseudo Euclidian space, in which all physical events are described to take place in this particular pseudo Euclidian space. Now, this is the signature of the pseudo Euclidean space.

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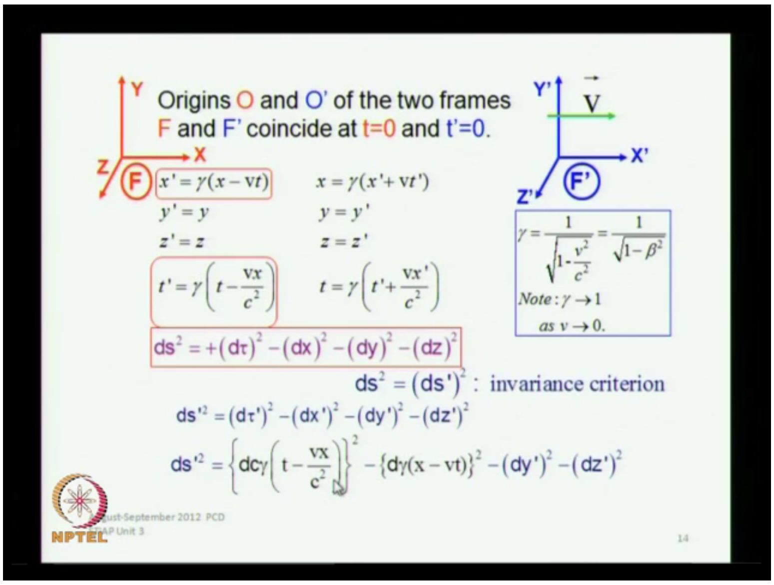

And what you can do is, look at this invariance criterion, because we expect if our contention is correct that, d s square must be exactly equal to the square of d s prime. And we can very easily verify this by subjecting all of these t prime X prime Y prime Z prime through the Lorentz transformations, plug in the corresponding substitutes.

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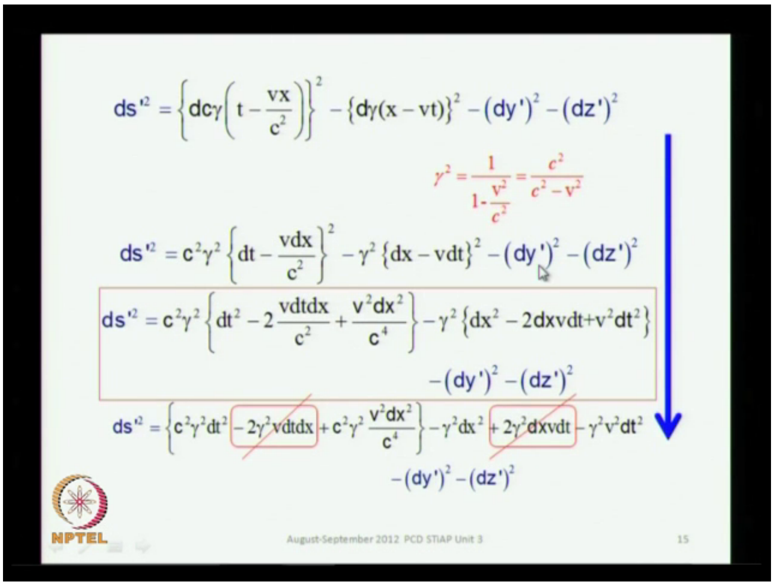

And do some simple analysis, which I will not spend any time on working out for you, this is something that you will do very easily.

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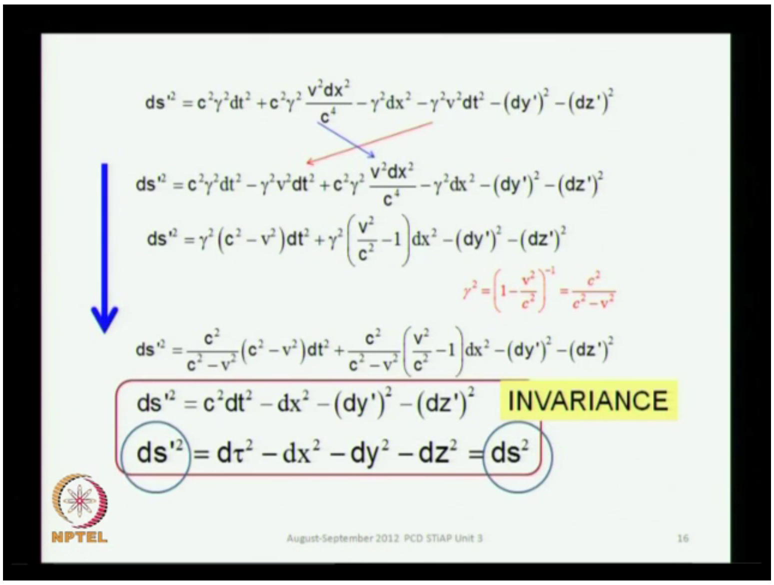

And if you just do this substitution and simplify the terms, your conclusion will be that this d s prime square is exactly equal to d s square, which is how you demonstrate that this is an invariant quantity under Lorentz transformations, so this is our invariant Quantity.

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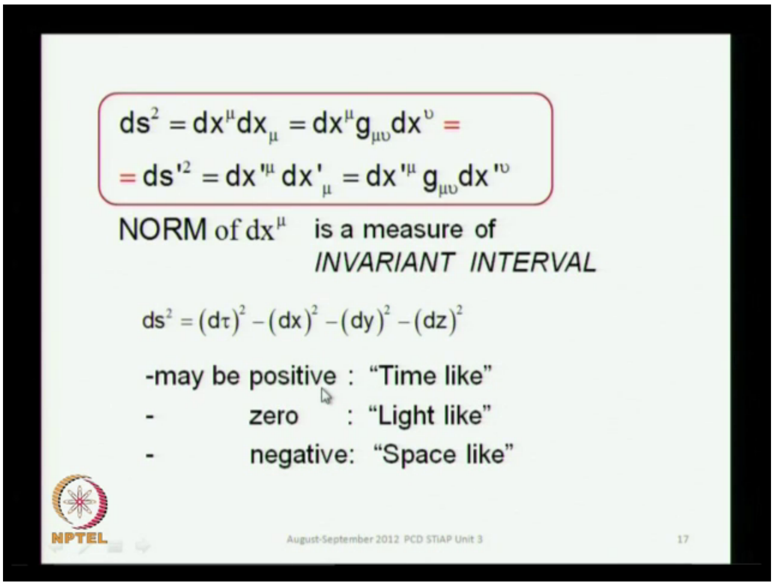

It is a measure of the, what we called as an interval between two events and of course, because each quantity is a square of a number and the first term is positive and other three terms are negative, this quantity you can of course, be either positive or 0 or negative. And depending on what it is, it has got different names, it is called as time like, light like, space like.

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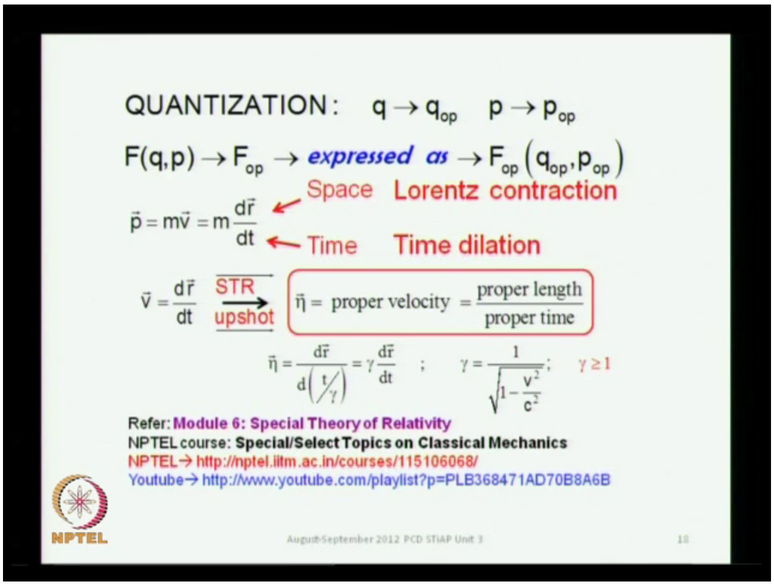

But, we are now interested in quantization, so this is our machinery, this is our tool and our interest is in quantizing the system. We know what quantization is, we have discussed this at length in unit 1 that, you must abandon the dynamical variables q and p and replace them by judicious operators. And dynamical variables, which are functions of q and p get expressed as operators, which in turn or express in terms of the position operator and the momentum operator.

Now, this was our notion of quantization and we expect something similar to be needed to be done in relativistic quantum mechanics. Now, let us see how, we would go about doing it, now momentum is obviously a quantity of specific interest. It is one of the dynamical variables, which specifies the state of the classical system, it is quantization is fundamental to what else we do in quantum mechanics. So, let us have a look at momentum, which to begin with, we defined as mass times velocity, although we have better definitions like the derivative of the Lagrangian and so on.

But, if you look at the mass times velocity then, this velocity is a ratio of space to time in the limit that, the denominator time interval goes to 0. And our concern here is that, the numerator space interval and the denominator time interval, neither of these two quantities is invariant under Lorentz transformations, one undergo dilation, time undergoes dilation and the other undergoes contraction. Now, these are the upshots of special theory of relativity, so obviously we are going to need some special afford to deal with this quantity, which is a velocity.

And then, it will have consequences on, how we define the momentum and furthermore, on how we would quantize it. So, in special theory of relativity what it do, is to construct a ratio of space to time, but you do not take the space and the time in the same system of frame of reference, you take what is called as proper length and proper time and these two are different. And you have met these quantities in your earlier course on special theory of relativity, so I will not define them, I will not spend too much time in discussing it.

I need to introduce this proper velocity, which is a ratio of these two quantities and that is what, that goes into the special theory of relativity. So, this velocity is now not just d r by d t, but d r by d t times gamma, where gamma is this ratio which includes v square over c square and this is not 0, because the speed of light is finite. So, this is now your proper velocity and I have discussed this at some length in another course, which happens to be available on the internet.

So, if you want, you can look it up, it is available in the NPTEL library, it is also available on the YouTube. And I have dealt with some of these ideas, including the ideas of time dilation and length contraction in some detail in those lectures, so I will not repeat any part of it over here.

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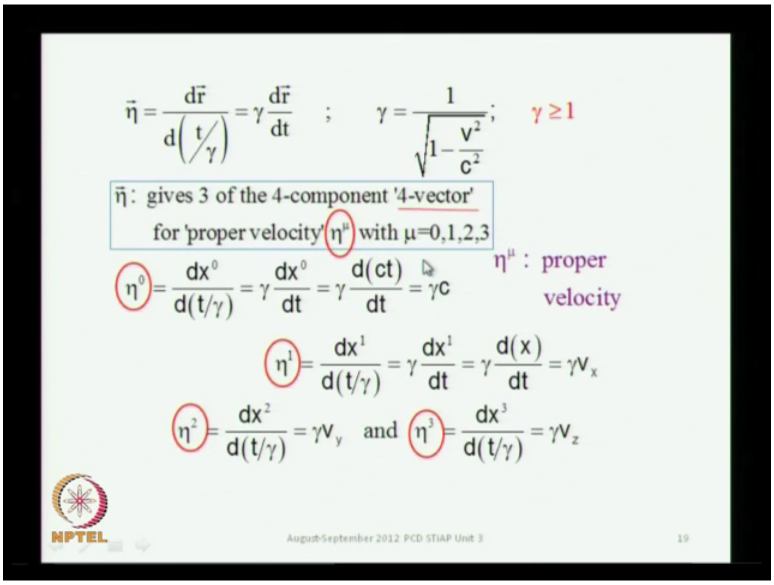

So, this is our introduction to, what we will call as a proper velocity, this gives three of the four components, because events is described by four components, you have got four vectors. So, velocity will also have four components and the fourth component is the natural extension of this. So, the first three components, which we get from this relationship are this eta 1, eta 2 and eta 3, which are gamma times the corresponding components in non relativistic mechanics and eta 0, which is a fourth component is given by the ratio of d x 0 to this quantity over here. So, essentially you rationalize the whole things in a consistent fashion, this is the natural way of doing it and this gives you the four vector, which constitutes the proper velocity.

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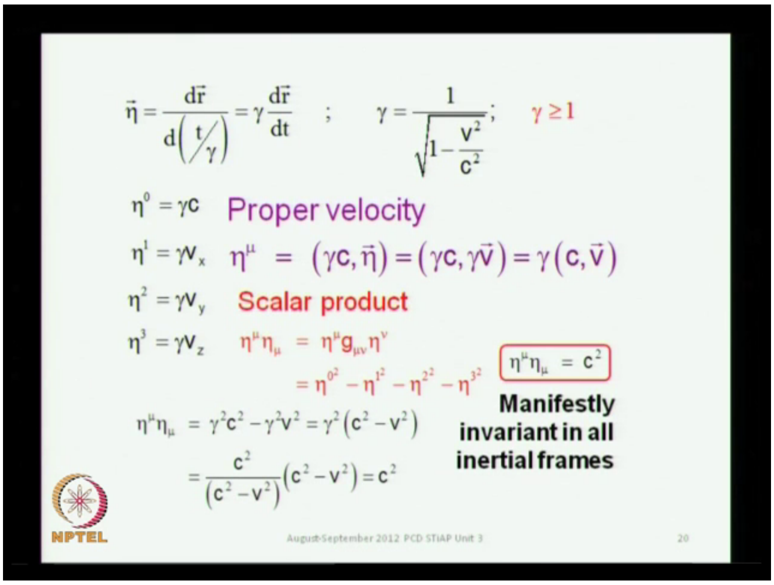

Now, that you have got the proper velocity, you can ask if it is invariant, so you construct this scalar and all you have to do is, to plug in these numbers and determine what this quantity is and it turns out to be the square of the speed of light. So obviously, it is invariant, because we know that the speed of light is invariant under Lorentz transformations.

It is the same for every observer, which satisfies us that, our rather unorthodox way of defining velocity, which is to take the ratio of proper length to proper time. This unorthodox way of defining the velocity is well justified and very rationalized, so this is an obviously invariant quantity in every inertial frame.

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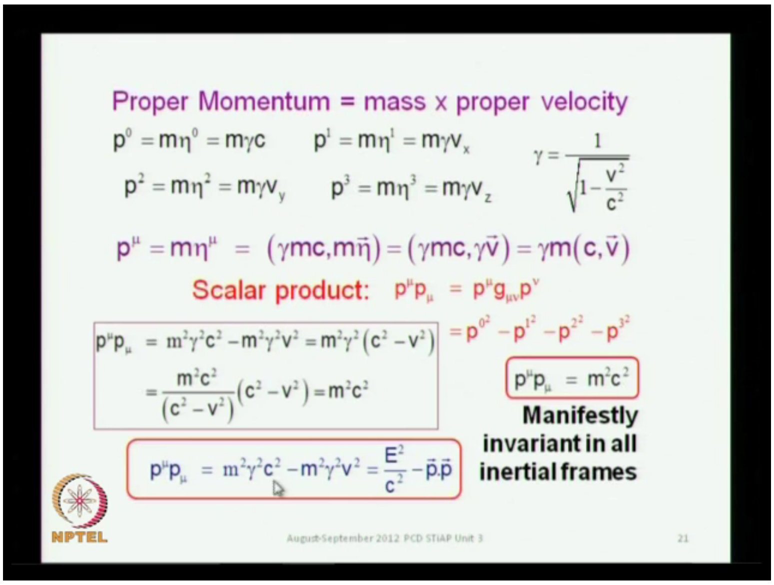

We defined the proper momentum as mass times proper velocity, which is again a straightforward extension of the classical idea. So, you have the proper velocity, you multiply each term by m and you get the proper momentum, which is again it has four components and the first component involves the speed of light. So, this is your description of proper momentum, again you can ask if it is an invariant quantity and you construct the scalar and you find that, it turns out to be m square c square, which is again invariant.

Although one must be careful about, how you define mass and you will see, why it is important to define mass carefully. So, I am use a mass, which is invariant in the Lorentz transformations, it is a same mass at every frame of reference. And this is m square c square, so again this is a manifestly invariant quantity in a every inertial frame of reference. Now, if you look at this expression, it has got two terms, one is the quadratic term in this velocity and the other is quadratic term in the speed of light, and if you take the difference, essentially this is E square by c square minus p square.

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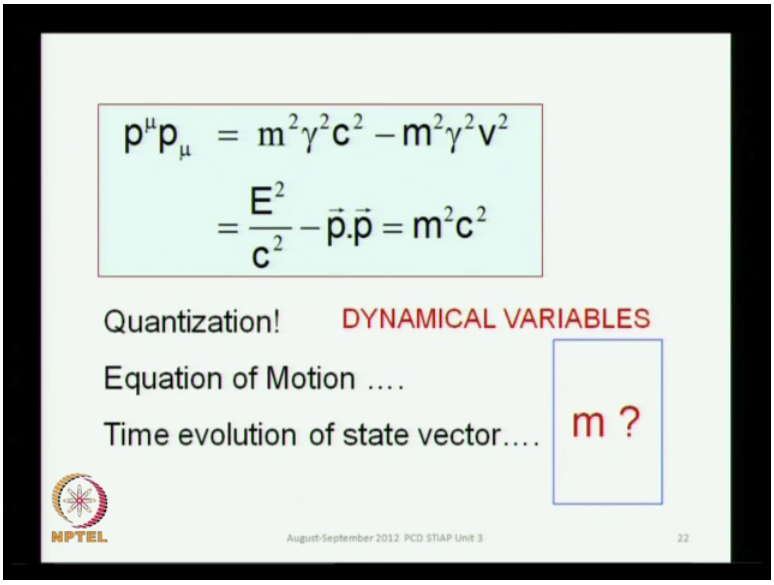

Now, what I am made use of is a certain relativistic well known expression and now we have the dynamical variables with us, we have the momentum, we have got the energy. And we can proceed to find, how to go about quantizing this and then, how to describe a state vector and how the evolution of that state vector to be described. Because, we know that the fundamental problem in mechanics, whether it is classical mechanics, non relativistic quantum mechanics or relativistic quantum mechanics, essentially is the same, how do you describe the state of the system and how does the system evolve with time. So, these are the questions that we are going to discuss, but before we proceed, I will like to remind you, alert you to, what exactly we mean by mass.

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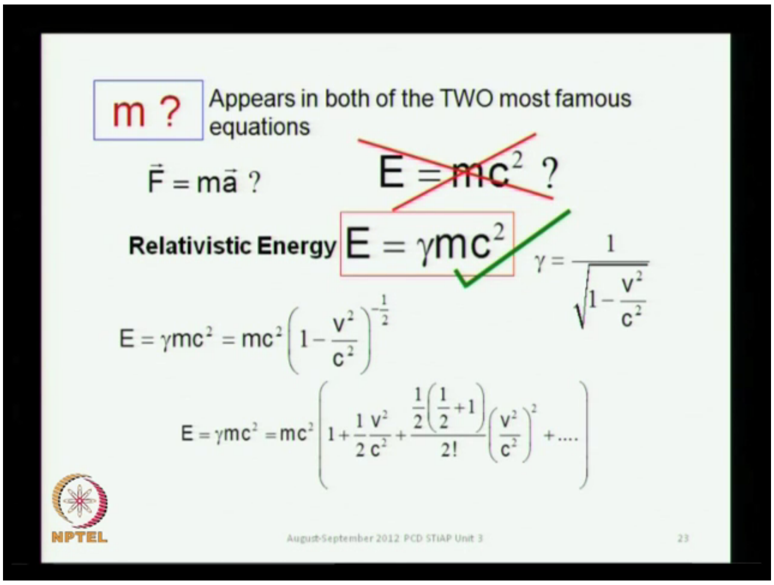

Because, mass obviously appears in two of the most famous equations in physics, one is F equal m a and the other is E equal m c square. I do not think that, anybody would argue that there are any other relations in physics, which are more famous than this, including perhaps Maxwell's equation, that this one is not right. So, first of all, I like to discuss this, because you must understand exactly what you mean by mass. Because, the correct way of writing this expression, which establishes the equivalence between energy and mass.

This whole relationship between energy and mass is about a establishing the equivalence between energy and mass, that it what have you make a bomb. Now, you and I may not be interested in making a bomb, although some of you maybe, who knows.

Student: ((Refer Time: 33:08))

Now, I am going to explain this, there is good reason why I raised this, you will see very soon in next few minutes. It is not the same, because the whole idea of introducing energy and mass and writing this relationship is to be able to convert mass into energy and vice versa. This is to establish the equivalence and if the two are equivalent, you cannot be required to introduce a relativistic energy and the relativistic mass, just one will do, that is the key to understanding this, but I will explain this further.

Let us look at this expression, this is the correct expression, E equal to gamma m c square, rather than E equal to m c square. This is the correct expression and write this as m c square into the factor gamma, which is 1 over this square root factor. Go ahead and expand this 1 minus x to the power minus half, which the little kid on the treadmill perhaps would do and you have various terms.

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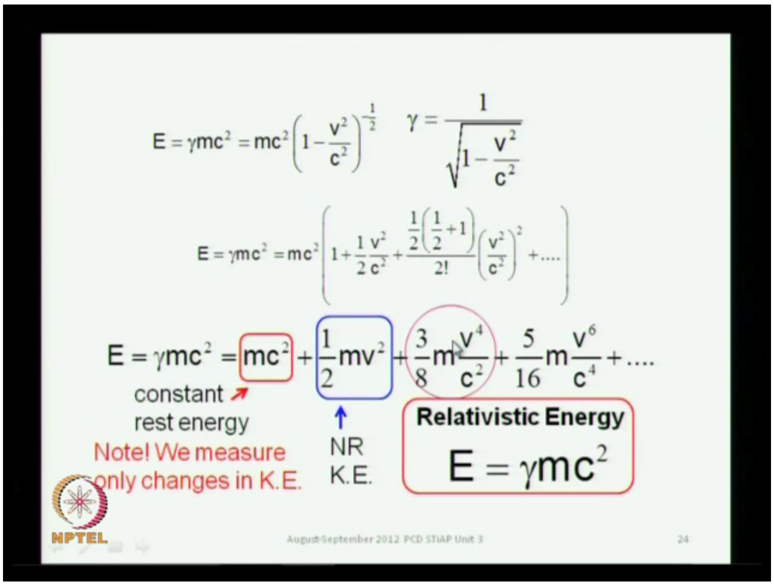

And if you look at the first term, that is what gives you m c square, if you look at the second term, you get the non relativistic kinetic energy, which is half m v square. And then, you get corrections of various orders, which go in multiples of v square over c square. So, with that factor, those subsequent terms become weaker and weaker and you can truncate it as you like.

And depending on the level of the approximation, even the first term which is the half m v square, would be of interest, m c square would not count, because you are going to measure only changes in kinetic energy, so it is a constant quantity for any mass. So, it really does not matter and this in fact, is the correct expression for the equivalence between energy and mass, not E equal to m c square. So, E equal to m c square would give only the constant term in this complete expansion.

Now, the m c square itself does not really matter very much in our observations, I will like you to note the third term, which is the leading term, which is leading relativistic correction to this, goes as a fourth power of the velocity or the fourth power of momentum, I am going to come back to this much later. But, I want to draw your attention to this, because it will be of some importance at a later point.

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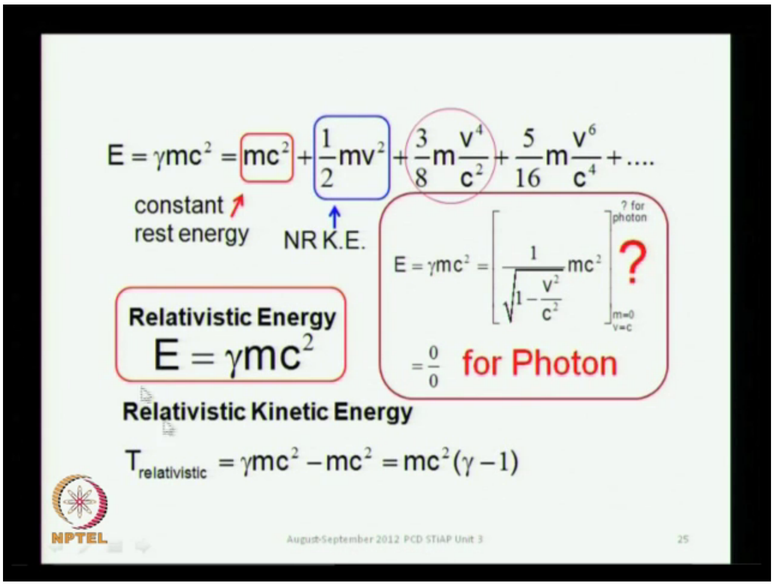

Now, look at the expression for this energy gamma m c square, if you are looking applying this relation for a photon. Now, the photon is the mass less particle, which moves at the speed of light, it always does, if it exists and moves at the speed of light. So, v is equal to c for the photon, so this is 1 minus c square by c square, so the denominator goes to 0, the numerator m goes to 0, because it is a mass less particle.

So, you get 0 over 0, that would make it impossible to define energy for a photon, but the photon has energy, you know it. In fact, you and I live, because we get this energy from the light, we get from sun light. So, photon has energy and this expression would give you 0 over 0, which is indeterminate.

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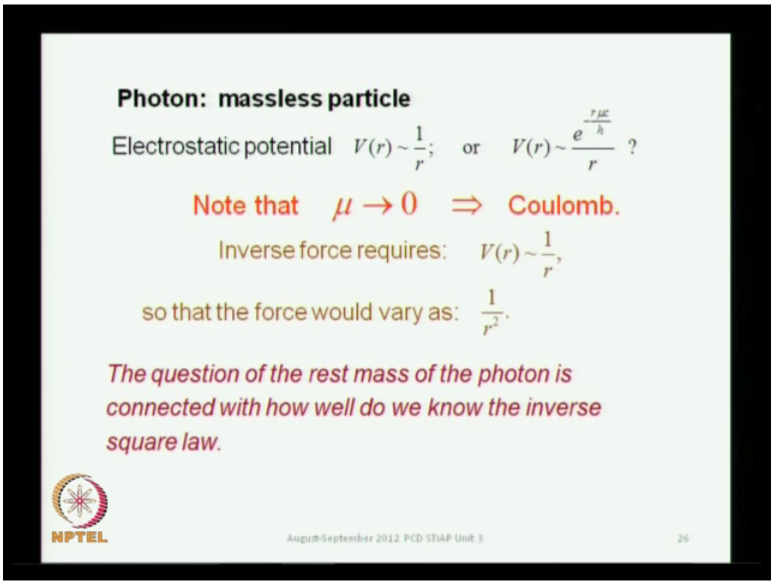

Now, it turns out that, the question of whether the photon is a mass less particle or not, is intimately linked to, how well we know the Coulomb's law, the inverse square law. These two are the same questions, consider this, look at the Coulomb potential, the inverse square tells you that, the potential goes as 1 over r. The 1 over r potential is what gives you the inverse square law, take a different kind of potential like the Yukawa potential.

Now, I have constructed a numerator here and I am chosen an exponent to include the mass, the speed of light and the angular momentum. So that, the dimensions are m c over h would cancel and you get a number and if you let this mass go to 0, you would get the Coulomb's law. Now, what is interesting is that, the mass going to 0 is linked to the Coulomb's law.

If one of the other was different, you would find some incompatibility between these correlations. And this is what, I applied when I said that, the question of rest mass of a photon is intimately linked to, how accurately we know the Coulomb's law. If it was any different then, it would require a mass, which is non zero.

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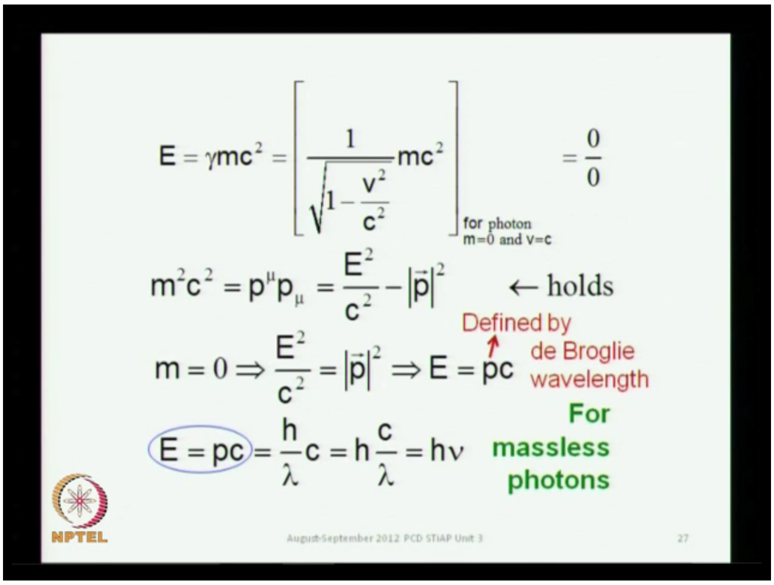

So, if we were to apply this relationship to light, we would get an indeterminate quantity for the energy of the photon, but that is not a worry. Because, this relation that we got from the invariant scalar constructed from the four momentum, it still holds with the difference that, now we should allow m to be 0, no problem. But, let us define the momentum using the de Broglie wave, because if you used p using the de Broglie wavelength, you get E equal to p c, which is h c over lambda, which is h nu and then, you do not have any problem defining the energy of a photon. I have highlighted this, because you could also write this E equal to c p, but I prefer that, you write E equal to p c because then, it associates energy with mine issues.

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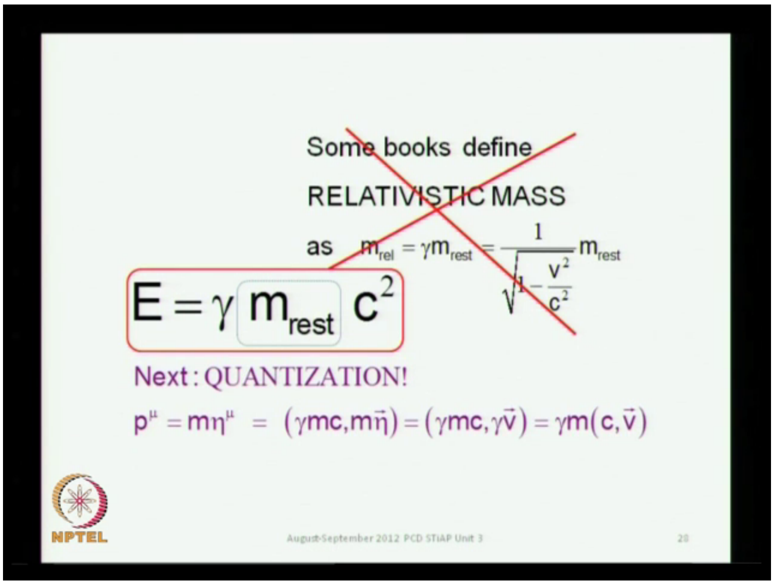

I do the same with the CPT theorem, which I always called as PCT theorem and this brings me to the other relation, why it is not appropriate to define a relativistic mass, which some books and some literature actually do. Because, you really deal with only one mass and you need to deal with only one mass, if mass and energy are equivalent and they are. So, it becomes pointless to introduce another mass, which is gamma times m, they may be mathematically arithmetically equivalent, but this is completely redundant.

And then, you must define E equal to gamma m c square, the only mass that I will always referred to is the rest mass, which is what makes m square c square invariant in all inertial frame of references. It is a conclusion that, we are going to base our formalism on and it also means that, E is equal to gamma m c square, rather than m c square. So, we will proceed with this and now, what we want to do is to quantize the system.

So, we have got the momentum and what we did in non relativistic quantum mechanics is to quantize a momentum, replace the momentum by the gradient operator. We discussed, why you need the gradient operator, so we expect something similar, we do expect the gradient operator. After all, non relativistic quantum mechanics is not absurd, it has given us an excellent results. So, it is something that must be corrected for, there is no doubt about it, because it did not take into the account the fact that, the speed of light is finite, no matter how large, it is huge, but it is finite. So, it must reconcile with that and we can borrow many things from non relativistic mechanics, but not everything. So, we are going to be guided by our method of quantizing momentum by expecting a gradient operator.

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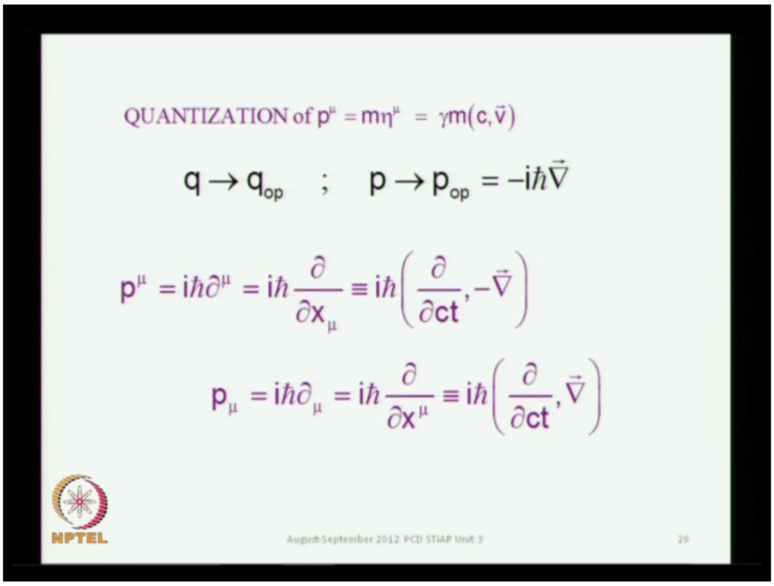

But, we have to be prepared for some modifications and we have to look for quantization of this four momentum, rather than the three momentum that we did in non relativistic quantum mechanics. So, this is our four momentum and this is how, we quantized it in non relativistic quantum mechanics. So now, our four momentum and this mu will take four values 0 1 2 and 3, these are the four values of the index mu.

And there is a gradient derivative operator for each one of them and this is what the operators are, this would be a natural extension of, what we did in non relativistic quantum mechanics. This is the covariant one, this is contravariant one and you have a minus sign here, but a plus sign over here and this you know comes from the fact that, the signature that we have been using is this, plus 1 minus 1 minus 1 minus 1, so it relates to that.

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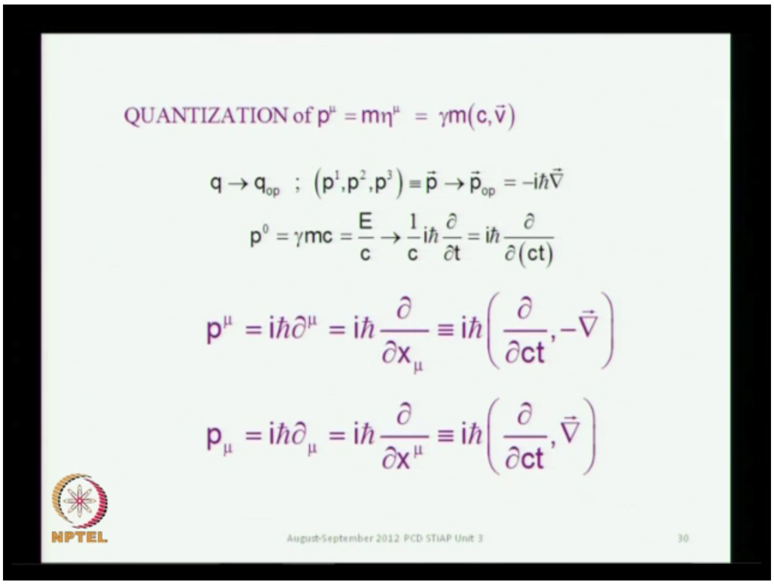

And now, we have the operator p 0, for which the quantum operator would be i h cross del over del c t, you take the corresponding variables and this is your complete quantization prescription. Now, this is how, we would go about quantizing it and then, we are going to have to ask, does it lead us to satisfactory physics. We have followed, we have taken some guidelines from non relativistic quantum mechanics, you have taken guidelines from the special theory of relativity, as introduced in classical mechanics. We have put it together and we have come up with a scheme for quantization.

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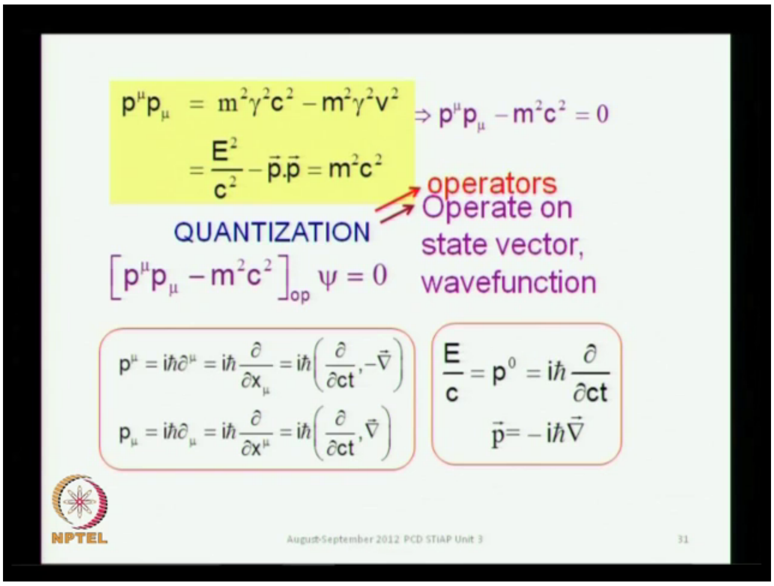

But then, we have to proceed, because we have to describe the state of the physical system and see, how this system would evolve with time. So, the quantization would require these operators, these would need to operate on the state vector of the system or the wave function and then, you come up with a wave equation. So, this is a wave equation that you would get, so this is a quantization scheme.

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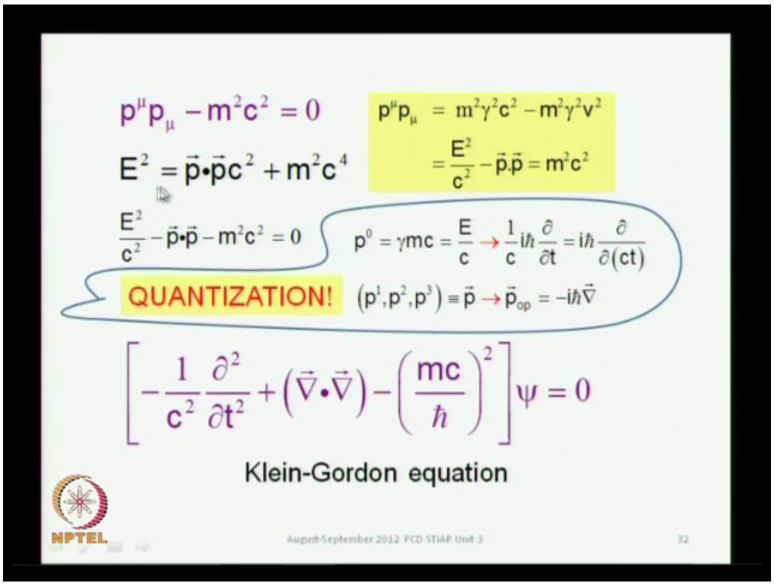

So, far so good, looks fine and when you put in all of these operators in this relation, you get what is called as the Klein Gordon equation. All we have done is to put these operators in this relationship over here, which comes from the Lorentz invariant quantity. So, this is the Klein Gordon equation and this is the relativistic quantum mechanical equation.

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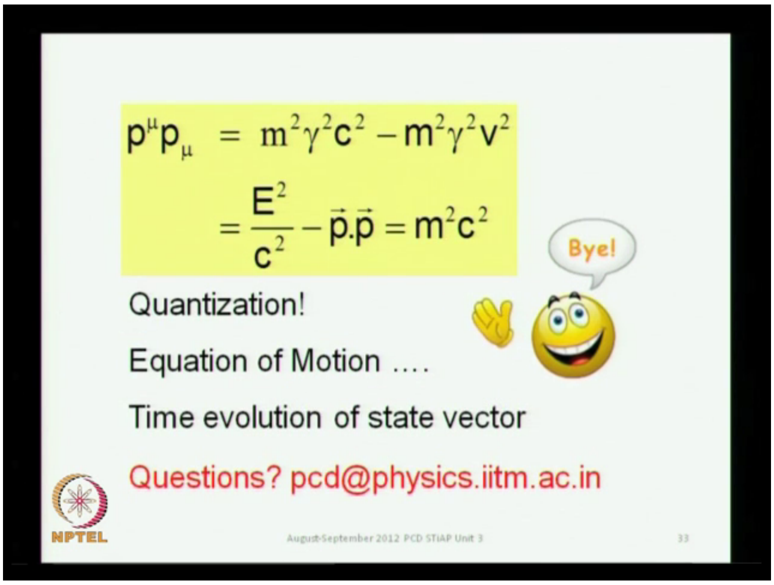

And I am going to conclude today's class over here, tomorrow we begin from here, I will mention certain difficulties with the Klein Gordon equation and quickly go over to the Dirac equation, which is the one of interest was in atomic physics. It is a Dirac equation, which would describe the electron in an atomic system, that is what I would introduce tomorrow. Is there any questions, I will happy to take?

Student: ((Refer Time: 46:53))

It is and it serves well to a certain extent, it also creates some difficulties, I will mention some of it. I would not spend too much time on it, because the relationship of specific interest was for our interest in atomic physics is the Dirac equation, rather than the Klein Gordon, so I will very quickly go over to the Dirac equation.

Student: ((Refer Time: 47:23))

Also by Dirac, I will discuss about these things in the next class, any other question, if not goodbye for now.