Relativistic Quantum Mechanics

Prof. Apoorva D. Patel
Department of Physics
Indian Institute of Science, Bangalore

Lecture - 1
Introduction, the Klein-Gordon Equation

This is a course on relativistic quantum mechanics. Relativity – I mean specifically special relativity and quantum mechanics have been two very highly successful theories of our twentieth century. And what this subject amounts to is combining the two theories in a very successful manner and working out the predictions. Now, it is not a priori clear why to take two very separate theories based on very different principles that, they should be compatible with each other. But, in this particular, it turns out that it is indeed the case. Relativity essentially follows from the property that speed of light in vacuum is an invariant quantity. And mathematically, that is extended to the principle of the Lorentz transformations – one transforming from one physical frame to another. Quantum mechanics tells that nature is discrete at a small scale and its formulation is based on unitary evolution of quantities known as wave functions or states.

Now, these two theories have been successful on their own also. And they have been extended in their own way. For example, special relativity can be extended to general relativity, and quantum mechanics also can be extended to nonlinear versions or other kind of higher order theories. It turns out that, these extensions are not compatible with the earlier versions of either side of the two theories. For example, general relativity is not easily compatible with quantum mechanics or rather one has not found a way to do it yet. And extensions of quantum mechanics do not necessarily agree with relativity. So, relativistic quantum mechanics is just on the border line of merging relativity and quantum mechanics, and it offers many consequences as a result. And in this course, we will explore those consequences.

In particularly, I will try to follow the historical development of the subject to some extent, not give the final product at the beginning, but describe some of the problems, which people encountered and then struggles to fix those problems, various dead ends as well as quite a open conjectures. They both will come out and many times the problems are fixed iteratively that you get something right, but something else goes wrong, and you try to fix that one again and something else will come out.

And the purpose of giving this historical development is also to motivate people to do research in a particular way. When you are doing research, you do not necessarily get everything right in one shot; you struggle, you find various solutions and then in some particular way, they may be able to be put together in a consistent fashion and then you have a well-defined theory. And that approach I think helps explain the subject in a much more clearer way than giving a final product in one shot, where you can work out the algebra, but you do not get much insight in the science of how to tackle problems, which are still open. So, let me begin.

The principle of relativity and quantum mechanics – when they were originally combined together, one discovered that… One just cannot stop at combining these two things just for the reason of self-consistency; one has to take the next step. And that next step turns out what we today called as a today quantum field theory. One cannot talk about relativity and quantum mechanics of just one particle or one object as it is very common in dealing with non-relativistic quantum mechanics, where you can talk about one object in a great detail and workout all kind of different consequences. But, one is not compelled to generalize it to a many object theory or what is called a many body physics.

In case of relativistic quantum mechanics that jump from a dealing with a single object to many object, is kind of compulsory; one just cannot start talking at level of one object and stop there. For self-consistency, one has to immediately extend it to much body system. And that many body system is now what we call quantum field theory. And the relativistic quantum mechanics, which we are going to talk about; the outcome of that many body system is a field theory, which has been tremendously successful; and now, we call it quantum electrodynamics. Similar field theories were subsequently created for other kind of electro dynamical systems very similar to electrodynamics, but based on different kind of interactions.

And, putting all of them together is construction, which we today refer to as the standard model. But, quantum electrodynamics is essentially combining relativity and quantum mechanics for the subject of electro dynamical interactions – basically, interaction of the electromagnetic field and charged particles. And most of the course, which I will talk about, will gradually take it from relativistic quantum mechanics towards the theory of quantum electrodynamics. We will go step by step starting with the first wave equations of relativistic quantum mechanics; then various kind of consequences, which follow from Lorentz invariance, classification of the various systems according to symmetries; and then finally, doing some calculations in detail about interactions of charged particles and the electromagnetic field.

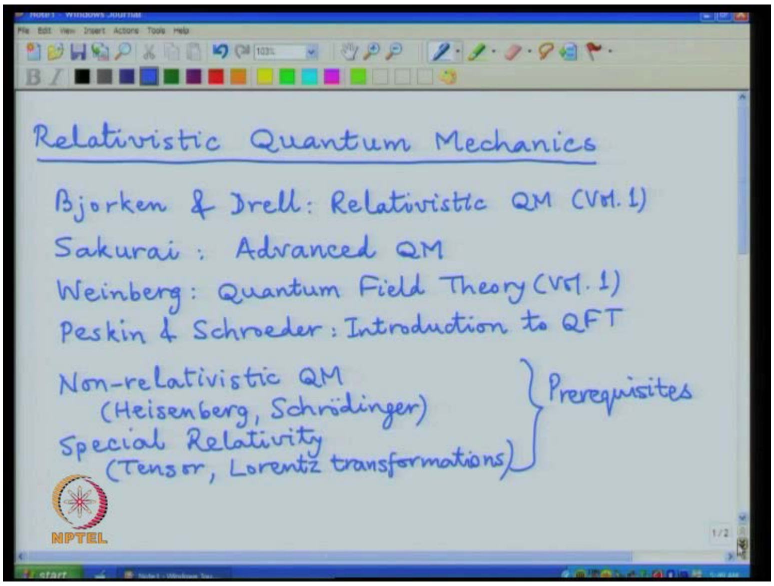
I would also like to mention that, this theory of quantum electrodynamics is a highly successful theory. It has been tested to an accuracy to which no other physical theory has been tested so far. And some of the quantities; for example, the electrons magnetic moment has been measured and theoretically calculated to an accuracy of one part in 10 raise to 10 or 10 raise to 11. And that is accuracy, which is unprecedented in any physical measurement. For instance, such accuracy would determine the distance between Kashmir and Kanyakumari to precision, which is less than the width of a human hair. And that is truly mind boggling that one can measure things to such precision and also have a theory, which works to the same precision.

Let me also add that, just because we have a successful theory like quantum electrodynamics, does not mean that it is the final theory in some sense or the other. What we know is that, at particular scales, which we are working with, we have a certain constraints. In this particular case, those are the constraints of Lorentz transformations and unitary evolution of quantum mechanics. And they dictate that, no matter what the final theory is, at this particular scale, it must look like or it can be very well approximated by quantum electrodynamics. There can be corrections to quantum electrodynamics at a very high scale, which I have not so far been accessed in any experiment. But, what we are left with in our present experiments are certain parameters coming from those unobservable effects.

And, to calculate everything which we have observed in experiments, all we need are the values of these parameters. For example, the mass of the electron or the charge of the electrons and some fundamental constants like Planck’s constant or speed of light in vacuum, etcetera. And as long as we have these few parameters given to us, we can calculate it. And maybe someday if we have a more fundamental theory, it will tell us how these fundamental parameters came to have the value, which we have assigned them.

So, that is the way physics develops and this paradigm is something, which is known as an effective theory. And so quantum electrodynamics is an effective theory; it is a highly successful effective theory. It has a certain number of parameters, which we take from experimental observations. And then based on these parameters, we do calculations, which will result in lots of predictions. And all those predictions can again be tested and verified against the experimental setups. And that gives us the confidence that, this is a correct theory to be used at this particular scale. When we have some new theory, maybe it will explain these parameters. And that is a another story. So, this is the background.

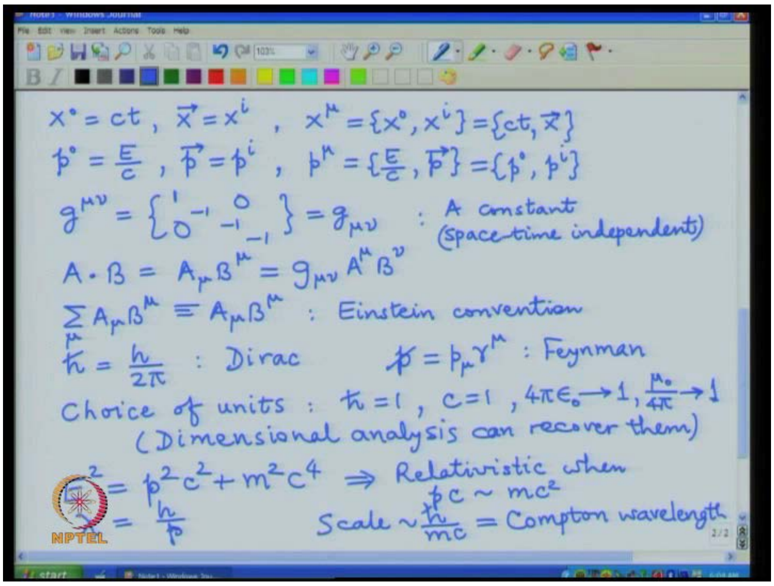
(Refer Slide Time: 11:44)



Now, let me give you a few basic references for this particular subject. As I said, this subject is now close to 100 years old. There are very good text books available, which will discuss many of the things, which I am going to talk about. And these are however easily available now both in print as well as on the web. So, one good text book is by Bjorken and Drell; it is called relativistic quantum mechanics – volume 1. Another good text book is by Sakurai; it is called advanced quantum mechanics. Yet another one is by Weinberg; it is called quantum field theory. And yet another one is by Peskin and Schroeder; it is again called introduction to quantum field theory. So, one can find much of the material, which I am going to talk about in this text book.

Let me mention some prerequisites as well. And in this particular case, they are going to be familiarity: one with a non-relativistic quantum mechanics, which is for example, the formulations of Heisenberg and Schrodinger; and another is the familiarity with special relativity, which means Tensor notation and as well as Lorentz transformations. So, given this kind of background; and I will give a just a hint of both of these things in the next few minutes. And then we can go on to build on the whole subject. So, non-relativistic quantum mechanics means that, you are familiar with Schrodinger's equation; how to do perturbation theory with it, solve it in a special cases, do scattering analysis, etcetera. Special relativity means that you are familiar with various kind of tensors, contra variant and covariant notations; how to transform from one frame to another; and how to construct objects which are invariant under Lorentz transformation. So, that is essentially as much as I can say about the background required for this course.

(Refer Slide Time: 16:00)



Now, let me move on to the next part of the introduction, which is to give some of the basic notation. And this notation consists of various kind of a variables. For example, we will be extensively dealing with four vectors, which in the position coordinate will be described by various kind of indices; and the time coordinate will be denoted by the index 0; and space coordinate will be denoted by the index i. When all the four are together, we will also use a notation, which is just called x mu denoted by a Greek letter; and it refers to a set of both space and time indices. And the corresponding variables for momentum for example, will be… The 0-th component of momentum will be energy divided by the speed of light; and the space part will be used as itself; and the 4 vector will be accordingly defined as components of E by c and p. So, let me write it in all possible combination and… So, these are the definitions of the fundamental position and momentum variables, which will keep on appearing all the time.

There will be a Lorentz metric describing or also referred to as a Minkowski metric. And the sign convention, which I am going to choose, is 1 for the time component and minus 1 for the space component. And this will also be the same matrix when the indices are lowered. In the case of the tensor transformation, the indices are raised or lowered using this particular metric. You can also contract various indices for example, the inner product of 2, 4-vectors will be written as one index lower, other index upper; and the both having the same value, which can also be rewritten using the metric tensor as the quantity g mu nu A mu B nu. So, this is the way to contract indices or other way to construct inner products.

And, we will be sticking to special relativity, which means this metric tensor is actually constant; it does not vary with space-time. So, I can call it as space-time independent. And that is sufficient for dealing with a special relativity. One will obliviously see some kind of a device or conventions, which saves writing, because otherwise, the descriptions of all the equations in quantum field theory get quite cumbersome and various people over various stages in time decided their own conventions. One of the conventions you have already seen is that repeated indices, where one of them is lower index and other one is upper index is assumed that they are actually summed. So, what I have written is A mu B mu – here is actually the sum over all the values of… So, this was the convention chosen by Einstein.

And, several other things also followed for instance; the quantum theory quite often involves the variable, which is known as a Planck’s constant. And it turns out that, the combination, which occurs much more frequently than Planck’s constant in all the calculation is something which is called h bar or h cross; and it is equivalent to the Planck’s constant divided by 2 pi. And this was a short-hand, which was used heavily by Dirac and it has now become kind of automatic; and both h and h bar are often referred to as Planck’s constant. The notation of this 2 pi – whether it is divided or not, is reduced to putting a slash. Similar device will appear in construction with a contraction of vectors with what are called gamma matrices. And that was the convention again slashing up letter and which stands for taking the 4 vector and combining with this object known as a gamma matrices. And this was introduced by Feynman. All these are kind of tricks to save writing, because otherwise, the calculations and the equations really look too cumbersome; and people who are to follow them often do not like to write complicated things, because it kinds of hides the real physics or the insight into the problem. So, these are the abbreviations.

On top of that, we will also use many times certain units, which simplifies the calculation further. For example, it is quite common in field theory calculation to choose units such that Planck's constant is set equal to 1; the speed of light in certain vacuum is also 1. And on top of that, there are other constants, which often one deals within electrodynamics; for example, the objects like 4pi epsilon 0 is reduced to 1 or equivalently mu 0 by 4pi is also reduced to 1. These are short-hand conventions. And the units can be chosen in this way. And whenever you need the actual detail values for some object in what you use practical units, these can be recovered by just doing dimensional analysis; which means we will reset the values of the units of space, time and length to our conventional measureable values. And that will tell us how you would insert the factors of h cross or c or 4pi epsilon 0, etcetera in our formula. And… But, it is quite convenient to just do the whole algebra without carrying around these symbols.

In the initial stages of this course, I will actually keep track of the factors of Planck's constant and speed of light, because it helps keeping track of the equations and gives some insight about various kind of scales involved. But, at some stage, I will drop these things to simplify the structure of the equations. So, the next thing is to understand when should we use this framework of relativistic quantum mechanics; what are the stages where either relativity or quantum mechanics is not necessary; and what stage we are forced to include them. So, the conventional classical mechanics works very well in our everyday experience. Relativity becomes necessary when objects start moving close of the speed of light. And quantum mechanics appears when we have to look at the structure of the objects at a mix scale. So, that roughly defines when we should get relativity and when we should get quantum mechanics. And relativity and quantum mechanics both are needed together when we are looking at the objects at atomic scale, but which are also moving close to the speed of the light.

And, that object can be compared by writing down the well-known dispersion relations for relativistic object, where the energy E square is equal to p square c square plus m square c raise to 4. And that means relativity must be included when the momentum becomes comparable to mass time the speed of light. And this basically tells us two special cases: one is when the objects involves themselves are massless. For example, the photons. And in this particular case, mass is automatically 0, while the photon will have some momentum and some energy, and they will always have to be treated relativistically. There is no non relativistic description for a photon. On the other hand, when a particle has a certain mass, we have to look at what is the value of momentum if the momentum is comparable to the mass time the speed of the light; we can no longer treat the whole system in a non-relativistic fashion; and we must include the corrections, which come from a relativistic description.

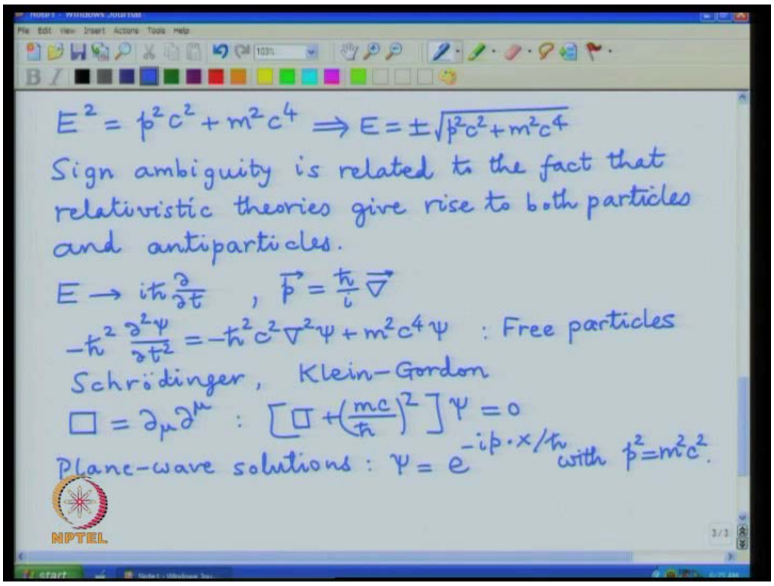
Going further, the scale which is required now to describe the atomic physics is dictated by the so-called de Broglie wavelength and which tells us that, when you are looking at particles at a scale, which is comparable to Planck's constant divided by this momentum, you must include quantum effects. And the de Broglie wavelength gives the wavelength of the particle with a certain mass and it is given in terms of Planck's constant by its momentum. And again for a massless particle, momentum is trivially related to energy. And the wavelength for example, is just the wavelength of the light when you are talking about electromagnetic waves. For a massive particle; however, this relation translates to something else; and one will have both relativity and quantum mechanics required when the scale will be given by the quantity, which is known as Compton wavelength. And it is nothing but Planck's constant divided by mass times the speed of light. And if you are looking at a quantum object at a scale comparable to Compton wavelength, you must treat those Compton objects relativistically. And that is the region in which relativistic quantum mechanics is absolutely necessary.

Now, let me say a few more historical things. One is that, relativity was well-established when quantum mechanics came along. Lorentz transformations are older than Planck's hypothesis; Einstein had completed his special relativity by the time Bohr constructed his model of the atom. And by the time Heisenberg and Schrödinger formulated quantum mechanics, special relativity was experimentally well-tested in lots of different areas as well. So, the question kind of arises that, why did not everybody include relativity from the beginning in quantum mechanics when it was already a well-established theory? Some part of it is historical, but some part of it is also instructive in the sense that, the very first atoms to just write down a relativistic quantum theory did not quite work.

And, what succeeded first was the non-relativistic description; and then gradually, people got experience with non-relativistic quantum theory to include and generalize it to include relativistic corrections as well in perturbation theory as well as in a full fledge Lorentz covariant framework. And that is also the history of how gradually we understood the structure of atom. Experimentally, various phenomena were discovered; and then theory explained those phenomena term by term by including first several extensions in perturbation theory and then constructing a full fledge framework, where all those perturbation calculations just came out of the general framework. And I will try to explain them gradually in the next few lectures.

So, let me begin. The way we construct quantum mechanics is either convert the objects of space and time and also momentum energy from just numbers to operators and develop an algebra of those particular operators, which is a procedure, which Heisenberg followed. The other procedure was to write down the relation obeyed by this particular numbers, which is nothing but the dispersion relation for energy and momentum; and then convert this dispersion relation into a wave equation, where the numbers are replaced again by operators. And that was the approach followed by Schrödinger in constructing his famous wave equation. And I will first follow the wave equation approach in dealing with relativistic quantum mechanics and then come back later to the operator-based formulation.

(Refer Slide Time: 33:51)



So, let me write down what are the corresponding quantities, which look like once it start with the dispersion relation and convert this into an operator. So, the relativistic dispersion relation for a single particle is what I wrote down earlier, is E square is equal to p square c square plus m square c raise to 4. And this produces two solutions for energy just because we are forced to take a square root in determining the energy.

And, this already indicates a problem; positive energy is something, which physical theories are quite comfortable with it; but negative energies – in this particular case, energy is going all the way to minus infinity, because p can be increased without limit arbitrarily and the sign is sitting in front of the square root. That negative energy is problematic, because it means that, whole system is unstable; it will just keep on going down in energy and emitting those difference in energy or some kind of radiation or whatever; but it indicates instability. And this ambiguity in the square root turns out to be very fundamental in a relativistic field theory; and it took a while for lot of clever people to understand the meaning of these sign ambiguity in the energy. And we will see thing cropping up every time we solve a relativistic quantum mechanics.

And, the sign ambiguity is nowadays related to the fact that, relativistic theories give rise to both particles and what are called antiparticles. And this actually was a great prediction of combining relativistic theories with unitarity of quantum mechanics; particles which we are quite familiar with it are what make up our everyday materials and which we try to understand in non-relativistic quantum mechanics all the time. But, antiparticles is something, which the founders of quantum mechanics were not familiar with it. They came out of this relativistic generalization of the theory and were discovered later.

So, in some sense, the prediction of antiparticles was a great success of relativistic quantum mechanics. And at the basis of it lies this very simple ambiguity in taking a square root of the dispersion relations. Antiparticles are interpreted as manifestation of the negative energy solutions in a way, so that the energy does not remain unbounded from below. So, you try to define new variables, so that the energy has a lower bound and the matter does not become unstable at the fundamental scale. And antiparticles defined properly will take care of this particular feature. But, that will always appear in these calculations and we will see how to deal with this negative energy solutions and interpret them appropriately in terms of antiparticles.

What people had hoped earlier while wondering about relativity and including in quantum mechanics is another unexpected feature, which showed up in the experiment. And that was the property that electrons and protons seem to have an intrinsic spin. They are both known as fermions or what we more explicitly call them as spin-half particles. They came with this internal degree of freedom labeled spin; and the spin could be either up or down; it had two particular values. That degree of freedom did not exist in the quantum mechanics, which was formulated by Heisenberg and Schrodinger. And to include it, one had to add an extra degree of freedom by hand into those equations. What people had hoped that, somehow this spin degree of freedom will automatically come out of relativistic generalization of quantum mechanics; it turns out that, that is not exactly the case; spin does occur as a specific possibility in case of relativistic quantum mechanics, but the value of the spin is left open by the relativistic theory. And in particular, one has many different allowed values of spins possible. And for every value of the spin, there is a corresponding different wave equation, which one writes down.

And, that wave equation predicts the corresponding physical phenomenon related to particle with that particular value of spin. If the spin is different, the equation will be different and the predictions will be different. So, spin is also a new degree of freedom. It will appear in the quantum mechanical extension to relativity, but it will occur in a way different than the appearance of antiparticles, which is just the straightaway square root sign ambiguity. And in particular, it is possible to have particles without spin, but it is not possible to have relativistic particles without the corresponding antiparticles. One little (( )) that if mass happens to be 0 for a particle, the square root can be taken much more easily; and so for this massless particles, a little different interpretation in terms of antiparticles is possible. In particular, the anti particle for the photon is the photon itself. So, it can happen that, the particle and antiparticle degrees of freedom might go inside in some particular cases. But, that is rather simple interpretation and we can easily include that whenever necessary.

So, now, let me convert this fundamental equation using the transformation rules, where I am going to replace energy and momentum by the corresponding operator. And that substitution rule is energy is replaced by I h cross del by del t, while momentum is replaced by h cross by i times the gradient operator. And once you substitute these objects into the dispersion relation, we have the so-called wave equation. And that in this particular case can be written as minus h cross square del square psi by del t square is equal to h cross square c square del square psi plus m square c to the power 4 psi. And in particular, this holds for free particles, because I have not included any term, which would correspond to a potential. The dispersion relation, which I started with it, is nothing but a free particle dispersion relation. And this particular equation was written down by Schrödinger first and then later by Klein and Gordon. And nowadays, it is known as the Klein-Gordon equation.

There also lies a curious story. Schrodinger was very familiar with well-established theory of relativity. So, when he first tried his wave equation, he naturally wrote down this so-called Klein-Gordon equation. But, he did not stop at that; he also solved it; and he solved it for the greatest problem of interest at that particular time, which is the hydrogen atom. And the equation can be as easily solved for the hydrogen atom case as is the Schrödinger equation, which we deal within non-relativistic quantum mechanics. And it gave out certain energy levels and wave functions. Now, what happens was that, the predictions of this particular equation did not quite match with experiment. And the surprise was that, there already existed a formula, which match with experiment quite well. And so Schrödinger was highly disappointed that, I wrote down a very obvious equation incorporating both quantum principles and relativity and it does not work. And so he put these results aside even though we know today that, what he did was perfectly legitimate.

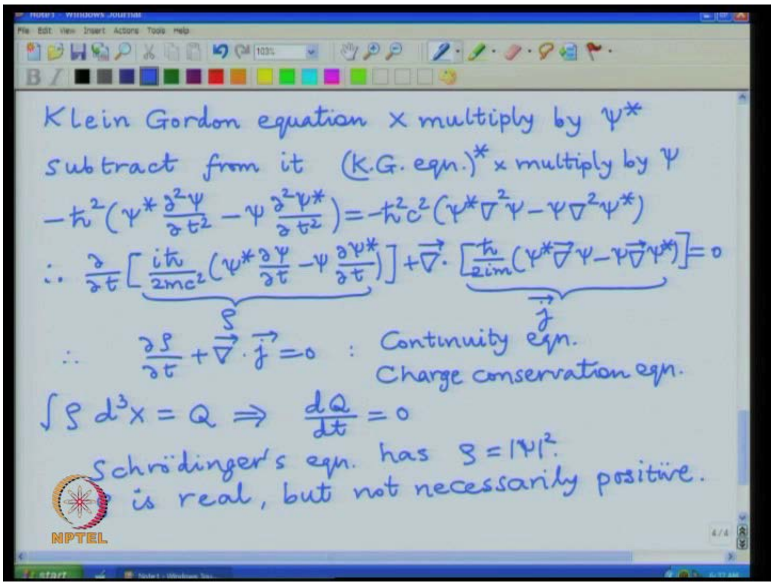
Now, what happened was that, at later stage, Schrödinger thought that if this does not work, I will try something else; and he took the non-relativistic limit of this equation. And that equation again he solved for the case of hydrogen atom. And that equation was very successful in the sense that, it exactly predicted what was observed in experiments. And that is the equation, which is now called as Schrödinger equation and which is the first thing we learn in quantum mechanics nowadays.

So, the non-relativistic Schrödinger equation produced the same energy levels, which were written down by Bohr and which agreed well with experiments; while the relativistic version did not agree with the energy levels predicted by Sommerfeld. And those were the relativistic generalizations of Bohr's calculations. Sommerfeld predicted the energy levels. And I will describe that idea a little bit later. And those generalization actually agreed with the experiment, but the prediction of this relativistic equation did not match with Sommerfeld result. And Schrödinger put aside this calculation, because Sommerfeld's result was agreeing with experiment while his calculation was not.

And, nowadays, since Schrödinger's has his name already for the non-relativistic equation, this exercise, which was repeated later by Klein and Gordon even though they knew that it did not work for hydrogen atom, is named after Klein and Gordon. And that is the equation, which we will analyze first. So, what are all the things to be looked at? One can define various quantities here in terms of Lorentz invariant notation. In particularly, it is quite common to define a generalization of Laplacian to 4 dimensional space, which is conveniently written as this box operator. And in terms of this box operator, this Klein-Gordon equation is more easily written as box plus m c by h cross whole square operating on psi is equal to 0. And here we explicitly see the scale of relativistic quantum mechanics appearing, which is the Compton wavelength. And if the derivatives, which are much larger than the Compton wavelength, we have a really high energy object and the mass can be neglected. If the derivative is as small, we can expand this in a Taylor series and obtain the non-relativistic equation from it.

And, one can easily see that the simplest solutions are the so-called plane wave solutions and which are nothing but e raise to minus i p dot x by h cross with p square is equal to m square c square. And this describes waves propagating with some momentum along some direction. And those are the convenient basics for describing free particle solutions. What we can also see is this equation is second order in time, while Schrödinger's equation was first order in time. And that provides a different category of solutions for this kind of equations. The plane wave solutions are of course common to both Klein-Gordon equation as well as Schrödinger equation. But, in general mathematical category, the second order in time equation will be truly called a wave equation, which is a hyperbolic equation in the language of partial differential equation; while Schrödinger's equation has only a first order derivative in time and it falls in the category of parabolic equations when classifying it in a partial differential equation language. And they have different properties and it does effect in certain sense how the system evolves in time.

(Refer Slide Time: 51:17)



One thing which can be easily obtained from this equation is the property of conservation of current. And that can be very easily obtained by taking this Klein-Gordon equation. We can take the Klein-Gordon equation; multiply by psi star; and then subtract from it the complex conjugate of the equation multiplied by psi. This is the same procedure, which is followed in deriving the current conservation rule from Schrödinger's equation. And what we obtained can be written quite easily as follows. The term which involves mass actually completely cancels out; while the second derivative survives easily. And this equation can be made to look very similar to what happens in case of Schrödinger equation by multiplying with a certain overall constants related to mass.

And, that can be written as overall derivatives of the form del by del t i h cross by 2m c square psi star del psi by del t minus psi del psi star by del t plus del h cross by 2 i m psi star del psi minus psi del psi star is equal to 0. So, it looks like time derivative of something plus divergence of something equal to 0. And there I have inserted the constant, so that the space part is exactly the same object, which is obtained from Schrödinger's equation and is defined as the current corresponding to the particular wave and then the time component now can be defined as the corresponding charge. And so the total equation becomes the so-called continuity equation or sometimes also called the charge conservation equation.

To see the property of charge conservation, it is convenient to define the integral of rho over the whole space as Q; and then for any distribution of charge and current, which vanishes as infinity, one can trivially integrate this equation over the whole space. And it follows that, the time derivative of Q is equal to 0, because the divergence integrated over the whole space gives the surface integral by Gauss's law and that surface integral vanishes. So, this is a very fundamental property that one can define a particular current related to the wave function and there is a conserved charge and it is all very fine.

The difference compared to Schrödinger's equation; so is that, the current now has the same form, but the value of charge density in Schrödinger's equation was completely different. It was mod psi square and this had a very useful interpretation in terms of probability for finding up particular particle at some particular location. What has happened in this relativistic description at that, we have a different value of rho or otherwise a different expression for rho; and we have to understand in more detail, what this expression of rho means. I will only say today that, rho is real, but not necessarily positive. In the next lecture, we will discuss the consequences of this particular calculation for the charge density and the current, and how to interpret it in relativistic quantum mechanics.