

**Foundation of Quantum Theory: Relativistic Approach**  
**Relativistic Quantum Mechanics 1.1**  
**Prof. Kinjalk Lochan**  
**Department of Physical Sciences**  
**IISER Mohali**

**Klein Gordon Equation I**  
**Lecture- 11**

So, in today's discussion session which we will resume our discussions on the structure of relativistic quantum mechanics and for today we were going to deal with the one set of differential equations which we were found which we had found to be compatible with special relativity which goes by the name of the Klein–Gordon equation. So, remember we were trying to find out replacement of the Schrodinger equation which was first order in time but double derivatives in the spatial derivatives and that was not Lorentz invariant or covariant.

## A relativistic consistent equation ✓

$$-\hbar^2 \left( -\frac{1}{c^2} \frac{\partial^2}{\partial t^2} + \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) \psi = -m^2 c^2 \psi$$

Using method of separation of variables

$$\psi(t, x, y, z) = T(t) X(x) Y(y) Z(z)$$

We would have

$$\frac{X''}{X} = -k_x^2 \quad \frac{Y''}{Y} = -k_y^2 \quad \frac{Z''}{Z} = -k_z^2$$

$$\frac{T''}{T} = - \underbrace{(k_x^2 + k_y^2 + k_z^2 + m^2 c^2)}_{E^2}$$

$$\Rightarrow X = A e^{\pm i k_x x}, \quad Y = B e^{\pm i k_y y}$$

$$Z = C e^{\pm i k_z z}, \quad T = D e^{\pm i E t}$$

$$\Psi(t, \vec{r}) = \Psi_0(\vec{k}) e^{-i(Et + \vec{k} \cdot \vec{r})}$$

or,

$$\Psi(t, \vec{r}) = \Psi_0(\vec{k}) e^{iEt - i\vec{k} \cdot \vec{r}}$$

Relativistic Wave packet

$$\Psi(\vec{x}, t) = \int \frac{d^3 \vec{k}}{E_k} \Psi_0(\vec{k}) e^{-iEt + i\vec{k} \cdot \vec{x}}$$

A relativistic consistent consistent equation

$$-\hbar^2 \left( -\frac{1}{c^2} \frac{\partial^2}{\partial t^2} + \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) \psi = -m^2 c^2 \psi$$

Using method of separation of variables

$$\psi(t,x,y,z) = T(t)X(x)Y(y)Z(z)$$

We would have

$$\frac{X''}{X} = -k_x^2, \frac{Y''}{Y} = -k_y^2, \frac{Z''}{Z} = -k_z^2$$

$$\frac{X''}{X} = -(k_x^2 + k_y^2 + k_z^2 + m^2 c^2)$$

$$\rightarrow X = A e^{\pm k_x x}, Y = B e^{\pm k_y y}, \\ Z = C e^{\pm k_z z}, T = D e^{\pm iEt}$$

$$\psi(t, \vec{r}) = \psi_0(\vec{k}) e^{-(Et + \vec{k} \cdot \vec{r})} \quad \text{or}$$

$$\psi(t, \vec{r}) = \psi_0(\vec{k}) e^{iEt - \vec{k} \cdot \vec{r}}$$

Relativistic wave packet

$$\psi(x, t) = \int \frac{d^3 \vec{k}}{E_k} \psi_0(\vec{k}) e^{-iEt + i\vec{k} \cdot \vec{x}} + c.c.$$

And therefore, we were after some equation which manifestly it is Lorentz covariant structure.

And we ended up getting one potential equation being the Klein-Gordon equation where the D Alambertian which is the double derivative with respect to time and double derivative with respect to the spaces, they hit/the wave function  $\psi$ . So, that is called the Klein-Gordon equation and in today's discussion we will be discussing about the salient properties of the Klein-Gordon equation.

So, the relativistic consistent Klein-Gordon equation when it is written in the partial derivative forms in Cartesian coordinate can be written as  $-\frac{1}{c^2} \frac{\partial^2}{\partial t^2} + \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$  double derivative with respect to  $x$ ,  $y$  and  $z$  hitting together the wave function  $\psi$  with  $-\hbar^2$  which is being multiplied from the left hand side should be equal to some invariant quantity times the wave function. Why invariant quantity?

# Quantum Mechanics I.1

The invariant equation

$$\left( -\frac{\hbar^2}{c^2} \frac{\partial^2}{\partial t^2} + \hbar^2 \frac{\partial^2}{\partial x^2} + \hbar^2 \frac{\partial^2}{\partial y^2} + \hbar^2 \frac{\partial^2}{\partial z^2} \right) \psi = -m^2 c^2 \psi$$

→ Can be converted (or seen as a manifestation of) into

$$p^\mu p_\mu = -m^2 c^2 \Rightarrow -\frac{E^2}{c^2} \psi + \hat{P}^2 \psi = -m^2 c^2 \psi$$

With  $-i\hbar \frac{\partial \psi}{\partial x} = \hat{P}_x \psi$        $-i\hbar \frac{\partial \psi}{\partial y} = \hat{P}_y \psi$

$-i\hbar \frac{\partial \psi}{\partial z} = \hat{P}_z \psi$        $i\hbar \frac{\partial \psi}{\partial t} = \hat{H} \psi = E \psi$   
for stationary solution

$$\Rightarrow \begin{aligned} \hat{P}_x \hat{P}_x \psi &= -i\hbar \partial_x (-i\hbar \partial_x \psi) = -\hbar^2 \partial_x^2 \psi \\ \hat{P}_y \hat{P}_y \psi &= -\hbar^2 \partial_y^2 \psi \\ \hat{P}_z \hat{P}_z \psi &= -\hbar^2 \partial_z^2 \psi \end{aligned}$$

Lastly,  $-\hbar^2 \frac{\partial^2}{\partial t^2} \psi = i\hbar \partial_t (i\hbar \partial_t \psi) = \hat{H} \hat{H} \psi = E^2 \psi$

$$\Rightarrow \frac{E^2}{c^2} \psi - P_x^2 \psi - P_y^2 \psi - P_z^2 \psi = -m^2 c^2 \psi$$

The invariant equation

$$\left( -\frac{\hbar^2}{c^2} \frac{\partial^2}{\partial t^2} + \hbar^2 \frac{\partial^2}{\partial x^2} + \hbar^2 \frac{\partial^2}{\partial y^2} + \hbar^2 \frac{\partial^2}{\partial z^2} \right) \psi = -m^2 c^2 \psi$$

→ Can be converted (or seen as manifestation of)

$P^\mu P_\mu$   
with

$$-i\hbar \frac{\partial \psi}{\partial x} = \hat{P}_x \psi$$

$$-i\hbar \frac{\partial \psi}{\partial y} = \hat{P}_y \psi$$

$$-i\hbar \frac{\partial \psi}{\partial z} = \hat{P}_z \psi$$

$$i\hbar \frac{\partial \psi}{\partial t} = \hat{H} \psi = E \psi$$

for stationary solutions

$$\rightarrow \hat{P}_x \hat{P}_x \psi = -i\hbar \partial_x (-i\hbar \partial_x \psi) = -\hbar^2 \partial_x^2 \psi$$

$$\hat{P}_y \hat{P}_y \psi = -\hbar^2 \partial_y^2 \psi$$

$$\hat{P}_z \hat{P}_z \psi = -\hbar^2 \partial_z^2 \psi$$

**Lastly**

$$-\hbar^2 \frac{\partial^2 \psi}{\partial t^2} = i\hbar \partial_t (i\hbar \partial_t) \psi = \hat{H} \hat{H} \psi = E^2 \psi$$

→

$$\frac{E^2}{c^2} \psi - P_x^2 \psi - P_y^2 \psi - P_z^2 \psi = -m^2 c^2 \psi$$

We have written  $m^2$  which was an invariant.  $P^\mu, P^\mu$  was supposed to be  $-m^2 c^2$ . So, this was the invariant quantity which is appearing over here. Why do we want some invariant quantity on the right hand side? Because left hand side this box operator, we have learned in this discussion on special relativity that it has an invariant structure. Box is a low rate invariant operator. Therefore, some invariant object which is operator hits the wave function  $\psi$ . And as I put out that, we should find out something which is also invariant times hitting the wave function  $\psi$

So, this is a Lorentz invariant equation for the wave function  $\psi$ . Now, looking at the structure of this differential equation, where the double derivatives with respect to time  $x, y$  and  $z$  have appeared separately, there are no mixed derivative like  $\partial_t \partial_x$  or  $\partial_x \partial_y$ . And also the coefficients of all these double derivatives are constants.  $1/c^2$  here, 1 over here, 1 over here and 1 over here. There is no coefficient which is a function of  $x, y, z$  or  $t$ . In that case where all the derivatives are separate and all the coefficients of the derivatives are also constants, we can employ something called a method of separation of variables that I can think of the wave function which we are after is a separable function of individual variables  $t, x, y, z$ . So, we have thought of a wave function which has  $x$  dependency,  $y$  dependency,  $z$  dependency and time dependency captured as a separate product functions  $t, t, x, x, y, y, z, z$ . So, this we are looking for a basis of this equation. So, this is a potential solution which can satisfy this equation. And if we are familiar with the method of separation of variables in various differential equation courses or mathematical method courses or even in electrodynamics you might have come across to exact same equations then if I feed up this equation into the differential equation what we get would be the double derivative of time will only see the first function  $T$  because there is no other time dependency anywhere else. The double derivative with respect to  $x$  will only see the  $X$  function because there is no small  $x$  dependency anywhere else in the function. And similarly for double derivative with respect to  $y$  which will see this  $Y$  function and double derivative with respect to  $z$  which will see the  $Z$  function which we have. So, these are individually different functions of different variables and different derivatives will hit/different individual functions. So, once I do that that I feed this  $\psi$  into the differential equation what and the double derivatives have acted/. Then what I can do, I can divide the

whole sides with the wave function  $\psi$  itself. After the double derivative has acted, then I will divide both sides by  $\psi$ . So right hand side will become a constant, which is  $m^2 c^2$ . Left hand side, you will get a structure like  $-\hbar^2/c^2 T''/T + X''/X + Y''/Y + Z''/Z$ . that should be equal to  $-m^2 c^2$ .

Now, once we have this structure, what we can do is to take first this  $\hbar^2$  on the right hand side. So, if I take  $-\hbar^2$  on the right hand side, left hand side will be not having the  $\hbar^2$  and  $\hbar^2$  will come downwards without flipping the sign on the term on the right hand side. Then next what we can do is to take the three spatial derivatives x double primed, y double primed and z double primed terms on the right hand side. So, I take these to this side. So, that would make the differential equation like, so suppose I take all these terms from here and move it on the right hand side. So, they will move to the right hand side with a negative sign. that means I will get  $1/c^2$ , actually it should have been  $-1/c^2$  because the time derivative comes with a  $-$ sign,  $-1/c^2$ . double prime/t should be equal to  $+ m^2 c^2 / \hbar^2 - X''/X, Y''/Y$  and  $Z''/Z$ . So, I would have this kind of structure. So, you see left hand side is only a function of  $t$ , while right hand side is a function of  $x, y, z$ , all these three functions. Actually, what we can do that since this depends on a function only  $t$ , the double derivative is also a function of  $t$ , small  $t$  and the function itself is a function of  $t$ . So, left hand side is only a function of  $t$ , some function of  $t$  and right hand side is some other function of  $x, y, z$  which are coming from this  $X, Y, Z$ . So if that is true, this can only happen if two functions which are functions of two different independent variables, they should agree to each other at all  $x, y, z$  and  $t$ . that is our demand. We are not looking for what  $x$ , what  $y$ , what  $z$  this differential equation is satisfied. We are demanding some functions which satisfy the differential equation at all time and spaces. So, that means this equality which we have just landed up should be true at all  $t, x, y, z$ . So, that means they should better agree to a particular constant. So, let us call this constant as a  $-E^2$ . So,  $-1/c^2$  or  $+ E^2$  we can call it which is the manifestation of the operatorization of this invariant equation.

So,  $1/c^2$  or  $+ E^2$  we can call it.  $-1/c^2 T''/T$  should be equal to this combination which is  $m^2 c^2 / \hbar^2 -$  the  $X''/X, Y''/Y$  and  $Z''/Z$  that should be equal to  $E^2$  let us say some constant  $E^2$ . Once that has happened Again the same thing can be played on the right hand side equality meaning this function together should also be equal to the same  $E^2$ . So then what I can do I can take this  $m^2 c^2$  and this double derivative with respect to  $y$  and  $z$  towards the right hand side and I will get a equation like  $x$  double prime/x is equal to  $E^2 - m^2 c^2 / \hbar^2 + Y''/Y + Z''/Z$ . So, therefore, again left hand side is a function of small  $x$ , right hand side is a function of  $y$  and  $z$  and they should agree on all  $x, y, z$  point that means they should better agree to that they are equal to some constant. So,  $x$  double primed/x is equal to some constant let us call it  $-k_x^2$ . So I will get  $X''/X$  is  $-k_x^2$ . Similar game I will play on the remaining quantity

$Y''/Y$  and  $Z''/Z$ . So since this combination is equal to another constant which is  $-k_x^2$ , again I can take this  $Z''$  and this quantity on the right hand side. So  $Y''/Y$  should be equal to some constant which is  $-k_y^2$ . And ultimately you play the same game on the  $z$ th variable itself and you end up getting that  $Z''/Z$  should also be equal to some constant  $-k_z^2$ . So, ultimately the differential structure will break down to four pieces that  $x$  double primed/x should be equal to some constant,  $Y''/Y$  should be some other constant  $Z''/Z$  should be third constant. And then the temporal part should be equal to some constant which is a function of all the three constants which we introduce  $k_x, k_y, k_z$ . Together they determine

what  $e^{1/c^2}$  will. So, there should be  $1/c^2$  which I have missed in this notation. So, this  $1/c^2 T''/T$  agree to.

So  $k_x, k_y, k_z$  determine this  $E$  because they have to satisfy the differential equation. All right, so these all four functions  $X, Y, Z$  and  $T$ , they do satisfy harmonic oscillator kind of differential equation structure. Okay so therefore their solutions would be oscillatory exponential integrals so  $X$  will be some function of  $\pm ik_x x$   $y$  will be  $e^{\pm ik_y y}$  times  $z$  will be  $e^{\pm ik_z z}$  times  $z$  and similarly the temporal part would be  $e^{\pm iEt}$  by  $t$  so these are the four functions which would be making up the  $\psi$  which satisfies the Klein–Gordon equation. Once I combine that means I put all the functions together I can write down the wave functions as product of all function which will become  $e$  to the power either  $+ik_x -ik_y +ik_z$  or any combination of this  $\pm$ . So any combination of  $k_x, k_y, k_z$  with  $+$  or  $-$  sign I am going to call some vector  $k$ . The vector  $k$  component along  $x, y, z$  will be decided/what constant you have chosen for  $k_x$ , what constant you have chosen for  $k_y$  and what constant you have chosen for  $k_z$ . So any constant or any signature together they will generate some special vector  $k$ . So, all the sign differences which are appearing differently, I am saying that can be captured by sum  $k$ . However, for the temporal part, I am going to write it explicitly. There are two possibilities of the temporal part, one with  $+iEt$  and another is  $-iEt$ , which I write separately. First function will be sum  $k$  times  $e^{iEt}$ . And the second set of solution would be  $e^{+iEt}$  and  $e^{-iEt}$ . In these two spatial vectors capture the science of a spatial part, but explicitly I have written  $e$  and  $-e$  because there is no temporal vector I could have written like, but that is how I have decomposed it. The upper thing is called positive energy solution because The energy is typically measured by operation of Hamiltonian, which is effectively  $-i\hbar$ , sorry,  $+i\hbar$  times  $\partial/\partial t \psi$ . If I take the first wave function, this operation gives me a positive  $e$  times  $\psi$  back. So, therefore, in the exponential, if I have a  $-iEt$ , then it is a positive energy eigenfunction. However, when I apply to the second one with a exponential with a positive argument in the exponential, then the Hamiltonian operation  $-i\hbar\partial\psi/\partial t$  for a stationary solution I will get a  $-E\psi$  so this is what the definition of the stationarity even in schrodinger equation we demanded that this should be the definition of stationarity which remains true in the case of Klein–Gordon equation as well so therefore I will have these two solutions possible one with positive  $e$  and one with a negative contrasted to the schrodinger equation there only we had one solution with positive  $Ei\hbar\partial\psi/\partial t$  was  $\hbar\psi$  and that was supposed to be  $E\psi$  only one signature was there here in the relativistic signatures relativistic setting there are two signs which are possible positive energy and negative energy and in general any relativistically valid wave packet can be made from these solutions superposed with different coefficients. So, I will integrate over all  $k$ . So, all vectors in the space can be integrated over all  $\pm$  sign or their value of the constant will be captured by variation of  $d^3 k$ .  $d^3 k$  contains all possible  $e^{ikx}$  and they come up with different weight factors and  $e^{-iEt}$  I am not summing over integrating over  $E$  as well because when I change  $k_x, k_y, k_z, E$  automatically changes.

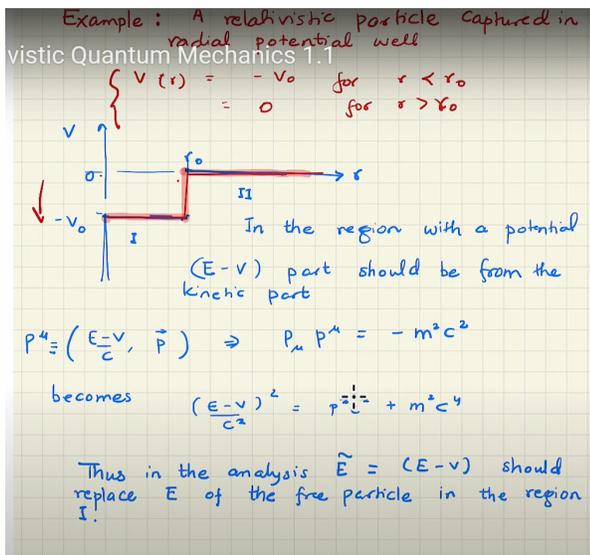
There are two possibilities of the temporal part, one with  $+iEt$  and another  $-iEt$ , which I write separately. It is just a function of  $k_x, k_y, k_z$ . In this process, when I have integrated over all  $k_x, k_y, k_z$ , I have effectively integrated over all possible energies as well. And if I want a relativistic real wave function, I can add a complex conjugate to that as well.

So now, once we have a solution of all the components of the wave equation, the invariant wave equation, we can try to see what kind of structure emerges out of it. So we had this equation at hand where the double derivative of time, double derivative with  $x$ , double derivative with  $y$  and double derivative with  $z$ . We are hitting the wave function and ultimately giving you a  $-m^2 c^2$  of  $\psi$ . Now one can see that this equation can be converted in terms of some meaningful operators which we are familiar with. And what are those?

So first of all we have demanded that the wave function which we are looking for can be separated in  $x, y, z$  and  $t$  as well. So therefore we can think of looking at this equation which is present over here in some sense as the manifestation of the invariant equation  $P^\mu P_\mu$  is equal to  $m^2 c^2$ . Remember in special relativity we learned that  $P^\mu P_\mu$  is supposed to be  $-m^2 c^2$ . Okay, this is invariant and this because of its contraction, this upper index, lower index repeated and summed over, we know that this is also invariant quantity. So, now we can see that this object and these objects are invariant objects. And if I convert things into the components, let us say, It had a component  $P^0 P^0$  which can be written as  $-E^2/c^2$  if you recall. And if I convert things into the components, let us say, It had a component  $P^0 P^0$  which can be written as  $-E^2/c^2$  if you recall. So ultimately what we have is  $-E^2/c^2$  hitting the  $\psi^+$  vector  $p^2$  operator now this time is equal to hitting on  $\psi$  is equal to  $-m^2 c^2 \psi$ .

Now, we know in quantum mechanics  $P_x$  operator is the spatial derivative of wave function with a  $\hbar$  factor. Similarly, for  $y$ ,  $P_y$  will be  $\hbar$  factor times the  $\partial/\partial y$  operator and similarly for  $z$  as well. So,  $z$  operator is also  $\partial/\partial z$  operator with  $\hbar$  factor. Now remaining over here for stationary states we know the energy which appears is also the temporal derivative which hits the  $\psi$ . The Hamiltonian for the stationary states it so happens that  $\hbar$  of  $\psi$  which is for stationary state  $e$  times  $\psi$  can be represented as the temporal derivative of time. So therefore whatever elements appearing here or whatever operators appearing here they can be converted into differential operators. I have two of  $P$ 's appearing here, special  $P_x$  square. So special  $P_x$  square will be written as  $P_x$  times  $P_x$ . And I know  $P_x$  operator is this. And two times  $P_x$  hitting the  $\psi$  will be equivalent to  $-\hbar^2$  partial derivative hitting twice the wave function  $\psi$ . And similarly for  $P_y$  will be  $-\hbar^2 \partial^2/\partial y^2$  hitting the  $\psi$ .  $P_z^2$  will be  $\hbar^2 \partial^2/\partial z^2$  square hitting the  $\psi$ . Lastly we have the energy thing which  $E^2/c^2$  was appearing we know now that energy has also be to be written as  $\pm i\hbar$  this time  $d\psi/dt$  and therefore the  $E^2$  will be this quantity hitting twice will be just  $E^2 \psi$  you can verify that I have written  $i\hbar \partial_t$  twice  $i\hbar \partial_t$  itself is equivalent to Hamiltonian so it is  $\hbar \psi$  and this operator this becomes a new wave function  $\psi'$  eigen wave function  $E\psi$ .  $E$  will come out and the second second derivative operator will hit the Hamiltonian will hit and again another  $e$  will be popped out so  $E^2/\psi$  so ultimately the invariant equation which was  $-E^2/c^2 \psi +$  all the spatial derivative  $P_x^2 P_y^2 \psi - m^2 c^2 \psi$ .

So, whatever we had as a invariant equation in temporal derivatives, spatial derivatives can be converted into respective operators with  $E$  replacing the temporal derivative and spatial derivatives being replaced by the  $P$  operators. So, that is another manifestation of writing the quantum operator in the relativistic regime. So, this is equation which one should be solving for relativistic particle. This is a good replacement of a Schrodinger equation, so to say. Let us see this through an example. Again, we are all familiar with the step problem or the quantum well problem where there is a quantum well and a particle is supposed to live in that well and we want to know what is the probability of the wave function being in the regime 2 or regime 1 depending/the depth of the potential well. So, again we set up the same problem.



Example : A relativistic particle captured in radial potential well

$$\left\{ \begin{aligned} V(r) &= -V_0 \text{ for } r < r_0 \text{ and} \\ &= 0 \text{ for } r > r_0 \end{aligned} \right\}$$

In the region with a potential  $(E-V)$  part should be from the kinetic part.

$$P^\mu = \left( \frac{E-V}{c}, \vec{P} \right) \rightarrow P_\mu P^\mu = -m^2 c^2$$

becomes  $\left( \frac{E-V}{c} \right)^2 = p^2 + m^2 c^2$

Thus in the analysis  $\tilde{E} = (E-V)$  should replace  $E$  of free particle in the region I.

There is a potential well which goes up to the depth of  $-V_0$  between 0 to  $R_0$  and is zero afterwards so this is the usual step problem only thing is that this time we will not solve this equation through schrodinger equation but we will try to solve it using the the relativistic equation which we have which is over here all right.

So, the thing we should worry about, we should be careful about is there are two regimes region 1, region 2.

In both the regimes quantum equations has to be solved while potential remains constant in both the regimes, but not at the same value. In this regime it is value 0, in this regime it is value  $-V_0$ . So, if I go to regime 1 first, in regime 1 you can see it is the energy of the particle total energy of the particle will be increased by  $E+V_0$  it becomes a constant shift will add to the energies equation if you write down so therefore the free energy of the particle or the  $P^0$  part of the momenta should be treated as  $E-V$  it so happens that  $V$  is already negative of  $-V_0$  so it will ultimately will become  $E+V_0/c$ . So, it is almost like a free particle in this regime with extra energy supplied to it through a negative potential. So, its zeroth component of momenta will become  $E+V_0$  or equivalently  $E-V$ .  $E-V$  is equivalent to  $E+V_0$  divided by  $c$  and usual the three momentum  $F$ . And they have to satisfy the same wave equation  $P^\mu P_\mu$  is equal to  $m^2 c^2$  the equation which we have written over here. This is the relativistic description. So, let us open it up, write it down, zeroth component is this. All the special component in this equation come with negative sign. So, they can be taken on the right hand side of the equation..

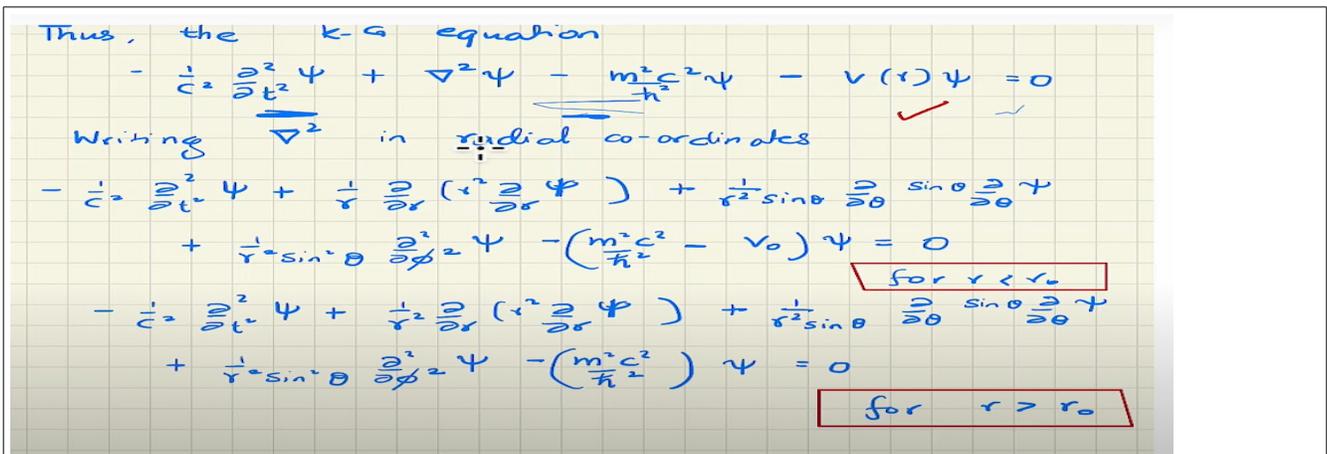
So, that is what we do. So, just a second. Yeah.

So, that is what we can do. Actually, in this equation, if I write down, there was an overall  $-$  sign over here. If I flip the sign, this should come with a positive sign. So, let me fix it first. There should be a

positive sign over here. And therefore, the equation which we are looking for,  $P^\mu P_\mu$  is equal to  $+$ , depending/which we write. If we write  $E^0$  with a  $-$  sign,  $P^0$  with a  $-$  sign, then it remains a  $-$  sign here. If I write a  $+$  sign here, which is like this, then it should appear as a  $+$  sign over here, which is good. So

therefore, I took all the  $P$  operator, the square of  $P$  operator to the right hand side. It added to the  $m^2 c^2$  already present over there. And left hand side would be left with  $P^0$  only.

$P^0$  is  $E - V_n$ . So, therefore, the equation which I have to solve is  $(E - V)^2$  divided by  $c^2$  is  $p^2 + E^2 c^2 + m^2 c^4$ . This is the effective momenta energy relation for region 1. We can call this quantity  $E - V$  as  $\tilde{E}$  and that is a free particle with energy  $\tilde{E}$  equation.  $\tilde{E}^2$  divided by  $c^2$  is equal to the  $p^2 c^2 +$  the  $p^2 c^2$ , the spatial  $p^2 c^2 +$  the mass of the particle. So, as we discussed in the region 1, the energy shifted to  $\tilde{E}$ . Okay. So, if I write down the Klein-Gordon equation which we had initially started with, ultimately it is a wave equation, the temporal derivative and the spatial derivative are appearing. As again we can write down the wave function into radial part just like we had previously decomposed into x, y, z, we can decompose it into radial angular part as well. So, write down the Laplacian the spatial Laplacian which is appearing over here into the spherical polar coordinate system. I know that becomes double derivative with respect to r in a particular way, double derivative of  $\theta$  in a particular way and double derivative with respect to  $\phi$  in a particular way.



Thus the K-G equation

$$\frac{-1}{c^2} \frac{\partial^2 \psi}{\partial t^2} + \nabla^2 \psi - \frac{m^2 c^2}{\hbar^2} \psi - V(r) \psi = 0$$

Writing  $\nabla^2$  in radial co-ordinates

$$\frac{-1}{c^2} \frac{\partial^2 \psi}{\partial t^2} + \frac{1}{r} \frac{\partial}{\partial r} \left( r^2 \frac{\partial \psi}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial \psi}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2 \psi}{\partial \phi^2} - \left( \frac{m^2 c^2}{\hbar^2} - V_0 \right) \psi = 0$$

for  $r < r_0$

$$\frac{1}{c^2} \frac{\partial^2 \psi}{\partial t^2} + \frac{1}{r} \frac{\partial}{\partial r} \left( r^2 \frac{\partial \psi}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial \psi}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2 \psi}{\partial \phi^2} - \left( \frac{m^2 c^2}{\hbar^2} \right) \psi = 0$$

for  $r > r_0$

If we are looking for stationary solution again we can employ method of separation of variables

$$\psi(t, \vec{r}) = \Phi(\vec{r}) e^{-i\tilde{E}t/\hbar}$$

Then the spatial part satisfies

$$\frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial \Phi}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial \Phi}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2 \Phi}{\partial \phi^2} + \frac{\tilde{E}^2}{c^2 \hbar^2} \Phi - \frac{m^2 c^2}{\hbar^2} \Phi = 0$$

If we are looking for stationary solution again we can employ method of separation of variables

$$\psi(t, \vec{r}) = \phi(\vec{r}) e^{-i\tilde{E}t/\hbar}$$

Then the spatial part satisfies

$$\frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial \Phi}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial \Phi}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2 \Phi}{\partial \phi^2} + \frac{\tilde{E}^2}{c^2 \hbar^2} \Phi - \frac{m^2 c^2}{\hbar^2} \Phi = 0$$

In Quantum Mechanics the wave function is standard (like in hydrogen atom) with  $Y_{lm}(\theta, \phi)$  as eigen functions and  $-l(l+1)$  as eigenvalues

$$\Rightarrow \Phi(\vec{r}) = R_l(r) Y_{lm}(\theta, \phi)$$

With  $R_l(r)$  satisfying

$$\frac{\partial}{\partial r} \left( r^2 \frac{\partial R_l}{\partial r} \right) - l(l+1) R_l + \tilde{k}^2 r^2 R_l = 0$$

with  $\tilde{k}^2 = \frac{1}{\hbar^2} \left( \frac{\tilde{E}^2}{c^2} - m^2 c^2 \right)$

Taking  $\tilde{k}r = u$

$$\left( u^2 \frac{d^2}{du^2} + 2u \frac{d}{du} - l(l+1) + u^2 \right) R_l = 0$$

Bessel Differential Equation

$$\Rightarrow \text{Solutions: } \tilde{N} \tilde{J}_l(\tilde{k}r) + \tilde{M} \tilde{Y}_l(\tilde{k}r)$$

Diverges at  $u=0$

$$R_l(r) = \tilde{N} \tilde{J}_l(\tilde{k}r)$$

The  $(\theta, \phi)$  part of the wave function is standard (like in hydrogen atom) with  $Y_{lm}(\theta, \phi)$  as eigen functions and  $-l(l+1)$  as eigenvalues.

$$\rightarrow \Phi(\vec{r}) = R_l(r) Y_{lm}(\theta, \phi)$$

With  $R_l(r)$  satisfying

$$\frac{\partial}{\partial r} \left( r^2 \frac{\partial R_l}{\partial r} \right) - l(l+1) R_l + \tilde{k}^2 r^2 R_l = 0$$

$$\text{with } \tilde{k}^2 = \frac{1}{\hbar^2} \left( \frac{\tilde{E}^2}{c^2} - m^2 c^2 \right)$$

with

Taking  $\tilde{k}r = u$

$$\left( u^2 \frac{d^2}{du^2} + 2u \frac{d}{du} - l(l+1) + u^2 \right) R_l = 0$$

Bessel Differential Equation

$$\rightarrow \text{Solutions: } \tilde{N} \tilde{J}_l(u) + \tilde{M} \tilde{Y}_l(u) \text{ diverges at } u=0$$

$$R_l(r) = \tilde{N} \tilde{J}_l(\tilde{k}r)$$

$$\tilde{k} = \frac{1}{\hbar} \sqrt{(E + V_0)^2 - m^2 c^4}$$

$$k \approx \frac{i}{\hbar} \sqrt{\frac{(E + V_0)^2}{c^2} - m^2 c^2}$$

And these two quantities can be clubbed as a single object which are all constants, mass and the potential which is appearing over here. Remember  $v$  is  $-V_0$ , so therefore the relative sign difference will appear. okay so for region one which is  $r$  less than  $r_0$  it will be  $V_0$  for region two which is  $r > r_0$   $V_0$  will vanish so both the equations these equations are almost the same only thing is that  $V_0$  is present here with overall positive sign or not depending where region which region you are in so we can look for the stationary state solutions which is some  $\psi(r,t)$  which is dependent on spatial

distribution which we have to figure out but temporal distribution I say that it is in the stationary state that means  $e^{-iEt/\hbar}$  this is eigen state of  $\partial/\partial t$  operator if that is true the derivative temporal derivatives appearing here and here will just throw up  $\tilde{E}^2$  so that will become this times the  $\phi$  all the spatial derivative will hit  $\phi$  as r derivative  $\theta$  derivative and  $\phi$  derivative and we have to figure out what their character is but temporal derivative will hit and bring down  $E^2$  over here so that is what we have done okay in region one  $\tilde{E}$  is  $e + V_0$  in region two  $\tilde{E}$  is  $e$  that's all the what we have to be careful about okay now you can see that if you have solved hydrogen atom problem or any spherical symmetric problem. The  $\theta(\phi)$  part, angular part of this differential equation is to be easily solved because in the potential there is no  $\theta\phi$  dependence. So therefore, angular part is already known to us. And the angular part's eigenstates are  $Y_{lm}(\theta, \phi)$ , the spherical harmonics. So I urge you to refresh your analysis of spherical polar coordinate systems and Laplacian over there by looking at 3D oscillator, harmonic oscillator or hydrogen atom or any spherically symmetric problem like this one. You will realize since this is spherically symmetric problem, you should expect eigenstates of angular coordinates, angular differential operators and  $Y_{lm}(\theta, \phi)$  are those. So, therefore, I know my state which I am looking for  $\phi$  r can have a non-trivial structure in the radial direction, but in the angular direction, it better be  $Y_{lm}(\theta, \phi)$  provide me a good basis and they satisfy the Klein-Gordon equations angular component. So, I decompose the angular and the radial part like that.

Put this uncharged solution into the differential equation which we are after here. There are temporal derivatives, there are angular derivatives here and here which will hit/the  $\phi$  and give me back  $Y_{lm}(\theta, \phi)$  because  $Y_{lm}(\theta, \phi)$  are the eigen states of the angular double derivative operator. And  $Y_{lm}(\theta, \phi)$  being hit/by the angular derivative part come back with the eigenvalue  $l$  into  $l + 1$ . All this you might have seen in 3D systems, spherically symmetric potential, harmonic oscillator or hydrogen atom, there  $l$  into  $l + 1$  came about as the eigenvalue of the  $Y_{lm}(\theta, \phi)$  operator,  $Y_{lm}(\theta, \phi)$  eigenstate corresponding to the operator of the angular derivative. So all these angular derivatives are replaced as  $-$  of  $l$  into  $l + 1$  times the  $Y_{lm}(\theta, \phi)$ . So all the terms will have a  $Y_{lm}(\theta, \phi)$  which I can pull off and the radial part will be left like this. This is the standard business you have done for the spherically symmetric harmonic, spherically symmetric potential in any case. Only the potential structure has changed. Spatial derivative and the temporal derivative structure has slightly changed not completely only thing is that energy square has appeared because Schrodinger equation energy was only coming with  $E$  this time  $E^2$  has appeared. So the  $K$  square which was used to appear previously had an  $E - V$  structure if you recall in the ordinary schrodinger equation this time we are talking about a relativistic version so energy will also appear in the same footing as the other momentum components they will also appear with a square the  $\hat{k}$  square will be  $\tilde{E}^2 - m^2 c^2$  okay so that you can see I have just clubbed these two things as  $\hat{k}^2$  and these two things as  $l$  into  $l + 1$  times the radial part. This is also radial into  $Y_{lm}(\theta, \phi)$ . And this part is giving me  $-l$  into  $l + 1$  times  $RY_{lm}(\theta, \phi)$ . So  $Y_{lm}(\theta, \phi)$  is common to everyone. I pull it out, send it towards on the right hand side of 0 and the radial part is left with this equation.

If you have not, this easy step you can follow. You can use another variable  $u$ , which is just  $r$  up to a multiplication of the  $\hat{k}$ , which we have defined over here. Square root of this quantity multiplied with  $r$ . I go and define  $u$ . that is just a method of calling this object as  $u$  squared. And therefore, all other quantities which are appearing over here can be returned into variable of  $u$ . If you do that successfully, this is again straightforward algebraic exercise, you will realize that differential equation which we are writing is just the Bessel differential equation in  $u$ . So, what I did, I just called  $\hat{k} r$  as  $u$ , converted every  $r$  appearing over here as  $u$ . And you will see that this becomes automatically a Bessel differential equation. Since I have written in terms of  $\hat{k}$ , the  $\tilde{E}$  has appeared over here.  $\tilde{E}$  was  $E - V$ , which is equivalent to  $E + V_0$  in the region 1 and equal to  $E$  in the region 2 that is all.

And the Bessel differential equation you might have seen or if you have not just look it up. The solutions are the Bessel functions of various kinds. So, I am writing in terms of Bessel and Neumann

functions if you are interested about knowing the nomenclature, but Bessel functions of two kinds  $J_l$ s and  $N_l$ s. If you follow the literature of the Bessel equation, This equation you might have, this differential equation you might have solved, for example, in solving the electromagnetic wave equation or the electric potential, electrostatic potential in cylindrical boundary conditions as well. There the same equation comes about and the same two solutions appear. It so happens that one piece of the solution, which is  $N_l$ , it diverges at  $u$  is equal to 0 at the center. I do not want that. I want my solutions or the wave function to be regular everywhere inside. So therefore this term should not appear. that means  $\tilde{m}$  should be 0. So all I am left with is the first piece. The radial part should be just the  $j_l \hat{k} r$  where  $\hat{k}$  is this.  $\tilde{n}$  is some normalization function which I will put. So overall wave function will become this radial times  $Y_{lm}(\theta, \phi)$ . Okay.

This is for region 1. For region 2, which is the exterior region, you can do this analysis once more and you can try to see that  $\hat{k}$  will be replaced by  $k$ ,  $V_0$  will vanish to 0 and I have this equation. Again, you can see here I can use a identification  $k_0$  which is  $-i$  times  $k$  that is just a variable substitution what i'm trying to do okay if I do that the solution in the outside region will again be  $J_l$ 's and  $N_l$ 's since I'm talking about outside region I should not take  $kr$  tending to 0 which was supposed to be valid for interior region so there is no danger of things diverging over here because I am not supposed to go towards  $r$  tending to zero with this solution however these solutions which are  $J_l$ 's and  $N_l$ 's can be rewritten in terms of two other Bessel kind of function which is Henkel function. This is all again differential equation exercise if you know you just look at look it up solutions of Bessel's equation. Two linearly independent solutions are  $J_l$  and  $N_l$  and their combinations are also you can see this is the combination and the second one is the complex conjugate of that. I can write in terms of  $J_l$  and  $N_l$  or in terms of  $H_l$  and  $H_{l1}$  and  $H_{l2}$ . This is equivalent to If a harmonic oscillator solution you are looking at, it can be written as  $\cos$  and  $\sin$  or  $e^{i\omega t}$  to the  $e^{-i\omega t}$ . Both of these things can be combined into each other. So equivalently, I can write this, the same thing.

<p>In the exterior region</p> $\tilde{k} \rightarrow k = \frac{i}{\hbar} \sqrt{\frac{E^2}{c^2} - m^2 c^2}$ <p>Thus the solution with <math>k_0 = -ik</math></p> $R_0(r) = N J_l(\tilde{k} r) + M n_l(\tilde{k} r)$ <p>or equivalently</p> $= N' H_e^{(1)}(ik_0 r) + M' H_e^{(2)}(ik_0 r)$ $H_e^{(1)}(ik_0 r) = J_l(ik_0 r) + i n_l(ik_0 r)$ <p>Since <math>H_e^{(2)}(ik_0 r) \rightarrow \infty</math> for <math>r \rightarrow \infty</math> for normalizable wavefunctions <math>M' = 0</math></p> $R_0(r) = N' (H_e^{(1)}(ik_0 r)) \quad \checkmark$ <p>For smooth matching across <math>r_0</math></p> $R_i(r_0) = R_o(r_0)$ $R_i'(r_0) = R_o'(r_0)$ <p>Equivalently,</p> $\tilde{N} J_l(\tilde{k} r_0) = N' H_e^{(1)}(ik_0 r_0)$ <p>and</p> $\tilde{N} J_l'(\tilde{k} r_0) = N' H_e^{(1)'}(ik_0 r_0)$	<p>In the exterior region</p> $\tilde{k} \rightarrow k = \frac{i}{\hbar} \sqrt{\frac{E^2}{c^2} - m^2 c^2}$ <p>Thus the solution with <math>k_0 = -ik_0</math></p> $R_0(r) = N J_l(ik_0 r) + M n_l(ik_0 r)$ <p>or equivalently</p> $= N' H_l^{(1)}(ik_0 r) + M' H_l^{(2)}(ik_0 r)$ <p>Since <math>H_l^{(2)}(ik_0 r) \rightarrow \infty</math> for <math>r \rightarrow \infty</math> for normalization wavefunctions <math>M' = 0</math></p> $R_0(r) = N' (H_l^{(1)}(ik_0 r))$ <p>For smooth matching across <math>r_0</math></p> $R_i(r_0) = R_o(r_0)$ $R_i'(r_0) = R_o'(r_0)$ <p>Equivalently <math>\tilde{N} J_l(\tilde{k} r_0) = N' H_l^{(1)}(ik_0 r_0)</math> and <math>\tilde{N} J_l'(\tilde{k} r_0) = N' H_l^{(1)'}(ik_0 r_0)</math></p>
---	---

and  $N_{l,2}(kr_0) = \dots$

$$\frac{J_l'(kr_0)}{J_l(kr_0)} = \frac{H_l^{(1)'}(ik_0 r_0)}{H_l^{(1)}(ik_0 r_0)}$$

Ex: Obtain the matching condition for  $l=0$ .

I am not supposed to take  $r$  tending to 0. This remains true. But I do not know whether this combination is finite everywhere else or not. And actually, it is not because this becomes very manifest if I write in terms of these variables. Again, the second piece here diverges when  $r$  tends to infinity. At infinitely away, my wave function will diverge. Again, that I do not want. So that means coefficient of this should be 0. So  $m'$  should be 0 and I should be left with only  $n'$  with the first Henkel function. that is equivalent to say if I want  $r_0$ ,  $r$  to be completely regular function in the exterior,  $m$  should be just  $l$  times  $n$  such that I can give this regular function. Okay. So this is the usual quantum mechanics stuff where you throw up the divergent problematic pieces and constitute your solutions accordingly. So inside I have a solutions of  $J_l$ , outside I have solutions of Henkel function. Only thing you have to be careful about. I have done it in a particular way. For the interior case, I had defined a  $\tilde{k}$  which appears in the argument. Ankle with  $i$ . This was just a convenient way of realizing the finiteness or infiniteness. If you kept working with here, you would be working with  $J_l$ s and  $N_l$ s with real argument and whatnot. There you will not be able to figure out so cleanly as you do. The physics is the same if you work in any variable. This is easy to realize, visualize and just a variable transformation. So that is what I am allowed to do. So if you do that, you will get this solution.

Therefore, this was called probability density previously. This time I have to call  $|\psi|^2$  not  $|\psi|^2$ , but  $\psi \psi^*$  with  $\frac{\hbar^2}{2m} \nabla^2 \psi$  as probability density. Now, there is apparent problem with this. First of all, it is a real quantity because this and these are complex conjugate of each other. Therefore, this multiplication makes it real. This is fine. However, the requirement of the probability density is not very acceptable solution. Why do I say so? Because if I just look for stationary solutions, I know there are positive energy solutions or negative energy solutions. So, let us cook up a generic solution, which will be a superposition of a positive energy solution and negative energy solution. So this is a positive energy solution of Klein–Gordon. This is a negative energy solution of Klein–Gordon. So then I can do the superposition with coefficient  $\psi^+$  and  $\psi^-$ . that is also a valid solution for the Klein–Gordon equation. Then I take the first derivative of  $\psi$ , which will give you this quantity. This is simple algebra

you should follow up. Then I calculate the  $\psi \frac{\partial \psi}{\partial t}$ . There is a bit of algebra you have to take the  $\psi^*$  which is the complex conjugate of the  $\psi$  and the derivative of  $\psi$  which we have just evaluated make the product then you will get various terms there will be  $|\psi^+|^2$  of this mod square of that but then there will be cross terms which will be like this the cross terms will be like this that is just simple plane algebra you have to verify and then you have to take in order to get the probability density. You have to take the complex conjugate of that, subtract those things out, multiply with  $i$  times something. So that is what let us do. So I take this quantity which is obtainable over here and this quantity which is also obtainable over here. And when I do the subtraction, the crucial thing is that the cross term if you see are exactly the same, they will cancel out. But there is a relative sign difference between the  $|\psi|^2$  terms. So this is  $-iE\hbar$  and this is  $iE\hbar$ . So when I compute this quantity, the cross term will vanish, cancel each other. But the mod square terms will survive with a sign difference because there is a sign difference between these two. that means the probability density will survive with a sign difference. So therefore, there is a problem at hand because the definition of probability density is coming with a  $A - B$  kind of structure and this is not always necessarily positive semi definite. Remember whenever  $\psi^+$  is greater

than  $\psi^-$ , it is positive.

This is the exterior solution. Again,  $Y_{lm}(\theta\phi)$  will be multiplying to that. And at the boundary from region 1 to region 2, I want things to match very smoothly. So, remember the problem which we are looking at. So, the potential which we have here. At  $R_0$ , I do not want things to diverge again. This should have some functional form here,  $J_l$  functional form and  $H_l$  functional form here. and they should match here. So, I should smoothly go from region 1 to region 2. So, the curve should match, wave function should match, its derivative should also match. So, these two conditions can be written together as the wave function's radial component should match while  $Y_{lm}(\theta\phi)$  anyway is going to match because we are not doing anything to them that are common to both sides. So, radial part should match and its derivative, prime is the derivative with respect to  $r$ . Equivalently,  $n$  should match. The  $J_l$  part inside with normalization  $\tilde{N}H_l$  part outside with normalization  $n'$  should match and their derivative should match. What you can do you can either convert this  $n$  prime as  $\tilde{N}J_l$  divided by  $H_l$  and put it here and then  $\tilde{N}$  on both sides will cancel and you will get this equation. that is just taking care of the normalization which is appearing. Or you can just simply divide equation number 2 to equation number 1 and you will get this equation. So this is the matching condition which is required.  $J_l'$  at the location of matching divided by  $J_l$  at the location of matching should also match to  $H_l'$  divided by  $H_l$  at the location of matching. and this will give me for different different else different different matching conditions will appear so that you can smoothly write down a wave function that will uh so this matching condition will tell you what values  $\hat{k}$  can support to take whether they come in integer non-integer kind of steps so good exercise is to write down what is the matching condition for  $l$  is equal to  $g$  so your exercises

Write down what is  $J_l(\tilde{k}r_0)$  write down its derivative take the ratio and put  $r_0$  and the similar to that side you will obtain there is a matching condition for  $l$  is equal to 0 which I leave you with an exercise for this discussion session okay so we know how to solve differential equations For a relativistic system in a standard scenario, we have solved this problem for non-relativistic particle already in our quantum mechanics course. Now, for relativistic particles, this methodology, the Klein-Gordon equation should dictate the discourse. And the solutions which we obtain is the Henkel functions and the Bessel functions on the two sides and their matching condition for smooth matching. This replaces the standard matching condition which we have obtained in the usual Schrodinger case potential well problem. So, this is a relativistic conditions of the wave function matching. So, I stop over here.