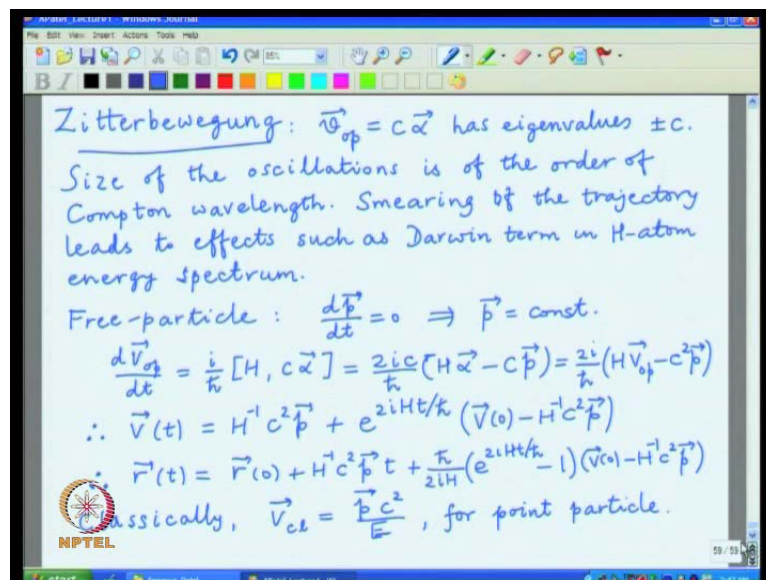


Relativistic Quantum Mechanics
Prof. Apoorva D. Patel
Department of Physics
Indian Institute of Science, Bangalore

Lecture - 12
Zitterbewegung, Hole Theory and antiparticles

In the last lecture, I described how a rapid change of the potential over a distance of Compton wavelength give rise to pair production process is and dealing with relativistic quantum systems. Today, we will see another consequence of relativistic systems when one tries to probe distances is which are of the order of Compton wavelength or smaller.

(Refer Slide Time: 00:54)



And this process is called Zitterbewegung; this is actually a German word and its pronunciation will be more like Zitterbewegung. But these words have entered the standard lexicon of quantum field theories for the simple reason that much of the development of quantum mechanics took place in Germany. And all the original papers of those days are published in German journals starting from Planck and Einstein to Sommerfeld, Heisenberg, Pauli, Schrodinger etcetera. And so it is natural; that the language would have its effect on a terminology; that was created through English translation of this word will be jittering along the way. And that illustrates that the trajectory of a relativistic quantum particle is not going to be a simple straight line as in classical mechanics. But it will have a lot of oscillations.

And, one way to see this effect qualitatively in terms of the machinery which we have already developed; one can look at the velocity operator which we constructed it was just c times the matrix α . And has Eigen value plus or minus c on the other hand the particle actually moves with a velocity less than c when it has some mass. So, how does that come about? Well, the only way we can put both these things together is instead of particle moving in a straight forward fashion from the initial point to a final point; which will give an average velocity less than c ; the particle goes lot of back and forth movements. And then the average velocity will be lower though the instantaneous velocity can be higher. And this back and forth movement or oscillations or jittering as it is called here is then something; which becomes a characteristic of the relativistic quantum dynamics.

One can try to see what is the size of this jittering; and we would roughly expect that the size of oscillations is of the order of the typical scale which we have in this problem which is a Compton wavelength. And this leads to smearing of the trajectory it is cannot be just written as a point particle trajectory. And the smearing of the trajectory leads to the type of physical effect which we have already seen in the case of hydrogen atom which was called the Darwin term. So, now we want to see this little bit explicitly and for that we will again look at a simpler problem than the hydrogen atom problem just a free particle.

And, see what kind of trajectory it describes. So, free particle we have a simple description as far as the momentum itself is concerned; that it will have no acceleration and momentum is constant. But we have seen that the velocity operator is different than just the momentum operator divided by mass it has a completely different structure. And so we will have to obtain the position for such a particle by going back to the definition of the velocity operator and integrating it to get the position.

So, let us now write down the evaluation equation for the velocity operator itself. And that is just the Commutator with the Hamiltonian. And this has to be now evaluated Hamiltonian has both α and β matrices. And most of these terms inside are going to anticommute with the second α matrix. So, when you do the calculation most of the term actually just get doubled. Because the Anticommutation rule the extra term with a minus α H essentially produces plus H α the only point is the terms in H with commute with the part in α those terms will produce 0. And we can reinstate them

explicitly by putting on those terms; and which happen to be a diagonal terms; I mean by that that the contribution from this α will have an different part; when the matrix inside H is the same as that in α .

So, when the matrices are different you just get the twice the result; which is H times α the 2 is explicitly put outside. But that miscounts the diagonal terms and we will get rid of that miscounting by subtracting of that extra part and when the 2 terms are equal α square basically gives 1. And so what we have is just the momentum operator left multiplied by c and subtracting of that part produces this minus c times p as a extra term. So, now we have written the derivative of the velocity in terms of velocity itself, because α is the velocity operator. And so we can rewrite this thing is as a operator equation for velocity. And that is this first order linear differential equation; we are going to interpret this equation in the context of Eigen states of momentum as well as energy. So, the formally this H and p as written are operators; we will integrate the equation assuming that they will be replaced in the appropriate state by the corresponding Eigen values.

So, this equation is linear one can actually subtract of c square p on the left side of the equation. So, it becomes essentially a homogenous equation and easily integrate it. So, then if the result is the velocity at time t we have to subtract of c square p divided by H which happens to be a constant in an Eigen state and I will just write it on the other side of the equation. So, it is H inverse c square p plus now an exponential factor described by the coefficient of proportionality appearing in front of v operator. So, that is the part of the solution. And the coefficient of it is now fixed by the initial condition; and we will fix the initial condition. So, that $v(0)$ explicitly appears here; and to get rid of this H inverse c square p we have to remove that particular component.

So, clearly when t equal to 0 the exponent is 1 and we have $v(0)$. And otherwise velocity is varying exponentially with respect to the Hamiltonian; and then there is a additive constant. So, this is now the operator equation for the velocity explicitly solved. And we can now solve these equations once again to get the behavior of position as a function of time well there are constant terms. And there is an exponential both are very easy to integrate integrated out the constant term; just gives a boundary condition $r(0)$ plus a linear term which is H inverse c square p t plus. Now, the integral of this exponential part again adjusted. So, as to make the satisfy the boundary condition at t equal to 0.

So, we will write it as \hbar cross divided by $2i\hbar$ from integrating the exponential the integral is just the same object, but now to satisfy the boundary condition we will put minus 1. So, that it vanishes at t equal to 0. And then the overall proportionality constant remains. So, this is a now a formal solution for what the position will be for a particle with some momentum p . And it has various terms classically the velocity which I will just call v classical is equal to p times c square divided by the energy. So, it is actually p divided by the dynamic mass and the dynamic mass happens to be e divided by c square.

So, this is the term which you would expected for a point particle. And this contribution indeed appears as the first 2 term of this solution for the position; which just describes the particle with a uniform velocity. So, r t is the starting point plus v times t that is the classical result. But in addition we have this μ contribution note that the μ contribution would vanish for a point particle where this $v \neq 0$ and H inverse e square p will actually cancel out. But in quantum theory we know that the point particles are not really practical; what we have actually realized are objects which are best describes are wave packets.

(Refer Slide Time: 14:57)

Size of the oscillations is of the order of Compton wavelength. Smearing of the trajectory leads to effects such as Darwin term in H-atom energy spectrum.

Free-particle: $\frac{d\vec{p}}{dt} = 0 \Rightarrow \vec{p} = \text{const.}$

$$\frac{d\vec{V}_0}{dt} = \frac{i}{\hbar} [H, c\vec{\alpha}] = \frac{2ic}{\hbar} (H\vec{\alpha} - c\vec{p}) = \frac{2i}{\hbar} (H\vec{V}_0 - c^2\vec{p})$$

$$\therefore \vec{V}(t) = H^{-1}c^2\vec{p} + e^{2iHt/\hbar} (\vec{V}(0) - H^{-1}c^2\vec{p})$$

$$\therefore \vec{r}(t) = \vec{r}(0) + H^{-1}c^2\vec{p}t + \frac{\hbar}{2iH} (e^{2iHt/\hbar} - 1) (\vec{V}(0) - H^{-1}c^2\vec{p})$$

Classically, $\vec{V}_{cl} = \frac{\vec{p}c^2}{E}$, for point particle.

Actual objects are wavepackets. Spread of the wavefunction oscillates with frequency $\frac{2H}{\hbar}$.

And, wave packets have finite extent and that is related to the fact that we have an uncertainty principle in quantum mechanics; there will be some Δx there will be some Δp . And those measure the size of the wave packet or equivalently the

distribution of the wave function in an appropriate Hilbert space. And because of this the width of the object around the classical trajectory will generically be non-zero.

So, once you go little bit off from the trajectory because the wave function is spread out. The new terms which are $v \approx 0$ minus H inverse c square p will have a different contribution. The typical size of this is again of the order of Compton wavelength that is the spread of this wave function. And once you allow for that little bit spread of the wave function; that spread oscillates with this high frequency given by $2 H t$ divided by \hbar cross. So, the spread of the wave function oscillates with frequencies $2 H$ divided by \hbar cross. And this is a novel feature which has now emerged from the relativistic dynamics; and let us explore these things a little more.

Note that these frequencies are typically quite large. And the reason being that the Hamiltonian corresponds; so the complete energy and it will have at least energy $m c$ square. So, these are frequencies of the order of $2 m c$ square divided by a planck's constant. And which is essentially related to the same size of the oscillation being the Compton wavelength. So, this have naturally emerged from this integration of the equation of motion.

(Refer Slide Time: 17:58)

These oscillations cannot be eliminated from any localised wavepacket. They contribute to physical quantities, e.g. $\vec{j} = c \Psi^\dagger \vec{\alpha} \Psi$. A typical contribution to \vec{j} couples upper and lower components of Ψ (in Dirac basis).

$$\int d^3x \int \frac{d^3p'}{(2\pi)^3} [v(\vec{p}', s) e^{i(Et - \vec{p}' \cdot \vec{x})/\hbar}]^\dagger \vec{\alpha} \int \frac{d^3p}{(2\pi)^3} [u(\vec{p}, s) e^{-i(Et - \vec{p} \cdot \vec{x})/\hbar}]$$

$$= \int \frac{d^3p'}{(2\pi)^3} \int \frac{d^3p}{(2\pi)^3} v^\dagger(\vec{p}', s) \vec{\alpha} u(\vec{p}, s) e^{-i(Et + E')/\hbar} (2\pi)^3 \delta(\vec{p}' + \vec{p})$$

$$= \int \frac{d^3p}{(2\pi)^3} v^\dagger(-\vec{p}, s) \vec{\alpha} u(\vec{p}, s) e^{-2iEt/\hbar}$$

cannot eliminate these oscillation when using complete basis of states involving both positive and negative energy solutions.

And, they cannot be eliminated from any localized wave packet. And to see them one has to go to the size of the Compton wavelength. And there this effect of these high oscillations will be visible together with other effect which we discussed last time; which

is the possibility of creation of particle antiparticle pair roughly at the same scale and both of these appear sort of simultaneously.

Now, one can look at actual expectation values to understand; where exactly these contributions are coming from and they contribute to physical quantities. For example, the current which we defined earlier as just the expectation value of the velocity operator. So, current is a physical observable and if the something is going on and the it will naturally be reflected over here. So, this is just a one particular case there are other manifestation of this particular effect; as well for example, in the spectrum of the hydrogen atom we saw the Darwin term. So, now let us calculate this typical term in such a current and the contribution will come from a coupling between this. So, called upper and lower component of the wave function; because the alpha matrix is an of diagonal matrix in the Dirac basis which we have been using. So, it will couple the upper component of psi to a lower component of psi dagger and a vice versa.

So, let us calculate such a term for a wave packet given by some particular wave function. So, a typical contribution to j couples upper and lower components of psi. And that is defined in the Dirac basis we can give a example. So, that is this explicitly write down this term. And I am going to call the upper component u and the lower component v in defining this cross term. So, term will correspond to the integral of j over the distribution of the wave packet. So, there is a d to the power of 3 x ; and we will write the wave function in momentum space, because that is where we are choosing them to Eigen state of some particular value of energy and momentum. So, typical Fourier transformation factors and psi dagger will contribute the say the lower component. And I am choosing the explicit convention where the lower components have opposite value of energy and momenta compared to the upper component.

So, this is the contribution coming from psi dagger then there is a alpha. And then there is a second contribution written again in the Fourier language; which is the upper component of the psi. So, full contribution will be this whole quantity plus it is conjugate, but I am not writing both the parts explicitly. So, it will have again the same structure, but with the energy momentum signs which are different. So, this is a typical term in the expectation value of the current. And it can be evaluated in a straight forward manner; the x integral can be easily done it has only exponentials involved and it produces a delta function.

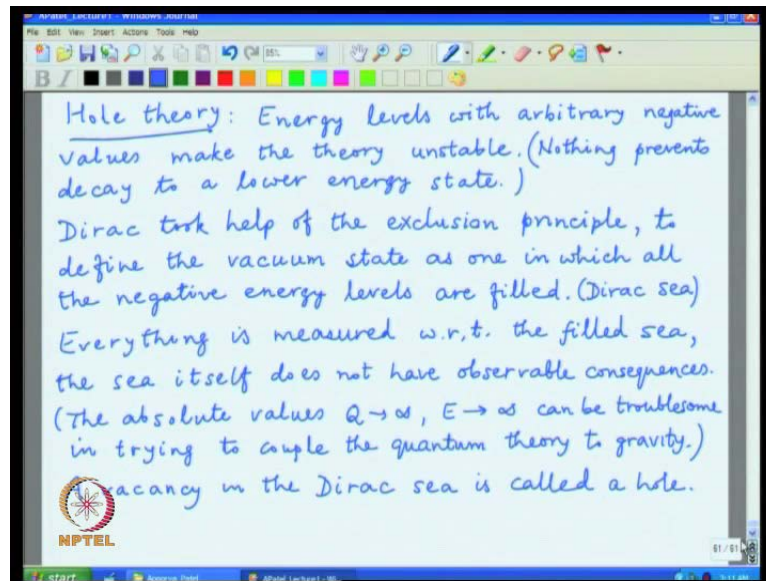
So, now we have $v \dagger p \prime s \alpha u$ of p and s then there is energy term which is $e \text{ plus } e \text{ prime}$ by \hbar cross and then there is a phase integral which produces a delta function. And, we can integrate over the delta function to remove one of the momentum integral. And so final result looks like $v \dagger$ minus $p \text{ s}$ this is $\prime \alpha u$ p and s and then e raise to minus $2 i e t$ divided by \hbar cross, because the momentum have equal magnitude the 2 energies will be the same from the dispersion relation.

So, this is a term which appears in the expectation value of the current. And we see that it will have some answer which comes from evaluating this overlap integral between $v \dagger$ and u , but then it has a time dependence which is highly oscillatory. And again we see a exponential factor involving $2 i e t$ by \hbar cross. So, the frequency will be $2 e$ divided by \hbar cross of the order of $2 m c \text{ square}$ divided by \hbar cross once we go to a Compton wavelength scale.

So, it does contribute to physical quantities and it does oscillate with a high frequency; and that is where the name is quite appropriate jittering along the way. And this high frequency s oscillation will always be there. So, as we have seen this we can cannot eliminate these oscillations when using complete basis of states involving both positive and negative energy solution. And that is essentially the crux of the matter that relativity produces both positive and negative energy solutions.

And, this duality leaves behind certain new effects which are not seen in classical physics ok. So, how does one now interpret this troublesome fact that there are states of negative energy which also produce certain physical effects and Dirac had to think very hard to fix his theory? So, that this negative energy solutions do not create a too much trouble.

(Refer Slide Time: 28:24)



And, that attempt now is known as hole theory; what Dirac was worried about is that the solution of the equation allows negative energy states. And this negative energy states are actually unbounded from below in the sense that you can keep on going to more and more negative energy levels. And if that is literally possible then one can always have a particle going further and further bound in energy; all the way to minus infinity in the process it will radiate photons or any other things; which it can couple to which release this change of energy in the transition process. And the since the process is unbounded it will make the hole theory unstable.

So, energy levels with arbitrary negative values make the theory unstable in the sense that it can keep on decaying. And there is no end to it nothing prevents decay to a lower energy state. And so one has to produce a fix and Dirac tried at first to identify this negative energy solutions as protons; that did not work in the sense that the theory unambiguously predicts that the both the positive and the negative energy solutions have to have the same mass. And certainly electron and protons do not have the same mass. So, that is not an able. And the choice which was left was to predict an antiparticle which has the same mass as the electron, but with opposite charge; and that is what Dirac labeled as the positron. And it was indeed discovered a few years after Dirac is development of this hole theory.

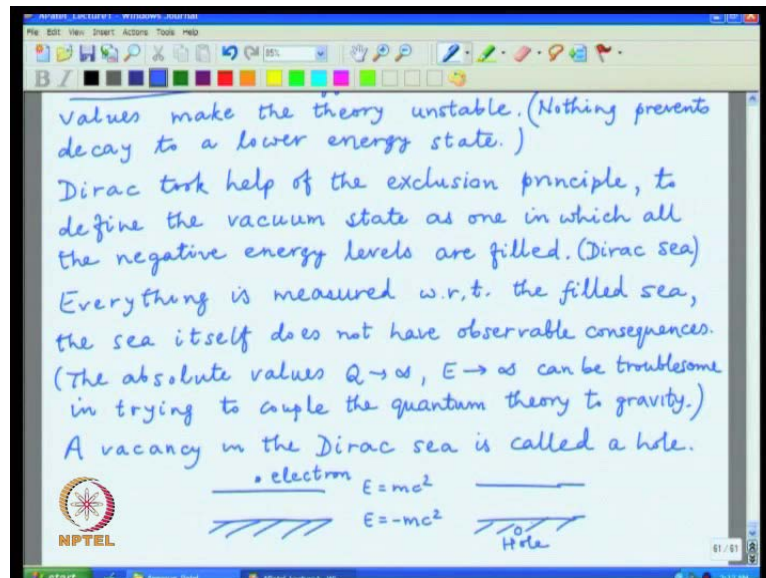
So, let us go through first the argument which Dirac produce to make the positron as a identifiable object. He took this negative energy problem to a solution which is justified as long as the particle obeys Pauli Exclusion Principle. And so Dirac took help of the exclusion principle to define the vacuum state as one in which all the negative energy levels are filled. And this has often referred to as the Dirac Sea. What the introduction of this Dirac Sea? Does is the negative energy states exist, but they are all failed. So, and because the exclusion principle no positive energy particle can now go and fall into those states. Because there is no space available. And this solve the problem by a technical notion set we have to redefine the vacuum.

A vacuum is the one which has all these levels filled it leads to another kind of trouble that; well if there are all these things which are filled then it will have infinite value of charge, infinite value of mass, infinite value of energy s and so for. Because there are so many extra electron filling up the Dirac sea. And Dirac's resolution or his definition was that everything is measured not in an absolute sense, but with respect to this the filled sea. And the sea itself does not have any observable consequences. So, all the properties of various states are defined with respect to the value in the state minus the value in the vacuum. Vacuum has already been defined and this is redefinition all we are measuring are differences. And as long as that is all we measure you will never see the absolute properties of the vacuum. And this actually works very fine when dealing with a quantum field theory.

But this absolute definition where the q goes to infinity or energy goes to infinity can be troublesome; when we try to couple this quantum theory to something else. And coupling the quantum theory to gravity does produce problems in this particular language. Because though the quantum theory measures only differences gravity couples to absolute values of energy. And if there is lot of energy negative energy for this Dirac sea it will produce observable gravitational effects. And one does not have an answer to this particular conundrum. And we will leave that problem aside, because as far as we know we do not really have a theory which merges quantum mechanics and gravity to a satisfactory extent. Dirac by passed the problem by defining an energy sea. And now he had a different interpretation of how we will define various states with respect to this filled a Dirac sea.

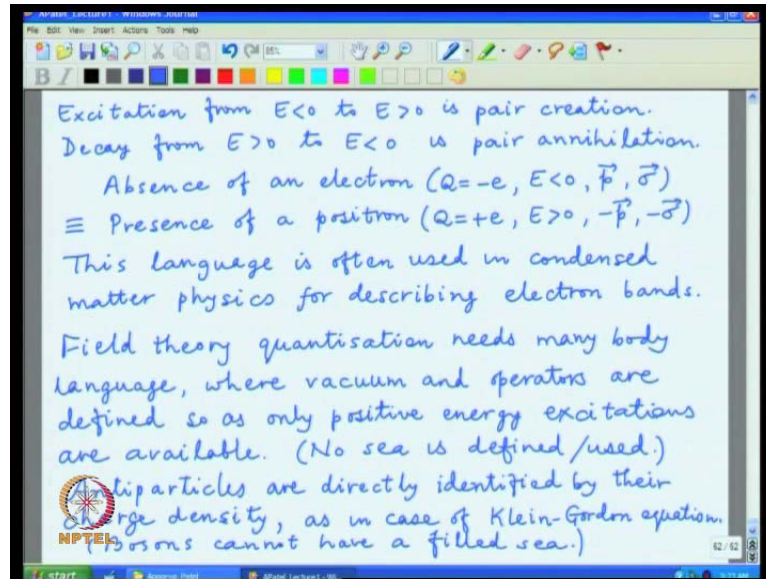
So, the Dirac Sea is filled, but one can have a vacancy in a Dirac sea; which can be created by hitting the Dirac Sea with a photon. And exciting the electron out of the sea to a positive energy value and that particular object can be measured. And it has been labeled as a hole. And then it can be given a little diagrammatic description; where the electron states will be represented by an excitation above the rest mass energy.

(Refer Slide Time: 38:18)



So, this is a electron and the hole will be a state with energy less than minus $m c$ square, but left $m t$. And if you now consider the difference between this state; and the infinite Dirac sea. Then it will correspond to having an energy which can be identified as a single particle state with some value. And so one can have such states described as holes; and now in this language one gets a reinterpretation of what is a creation on of a particle antiparticle pair or what is a annihilation of a particle antiparticle pair?

(Refer Slide Time: 39:59)



And, that is the excitation from energy less than 0 to greater than 0 is a pair creation, because it creates an electron and a hole. And decay from E greater than 0 to E less than 0 is pair annihilation, because then an electron falls into a hole and fills it. So, this new language allowed Dirac to redescribe the particles and antiparticle and associate them with this positive and negative energy solution. And what we now see is a absence of a negative energy state which can be rephrased as presence of a positive energy state. So, let us rewrite it is absence of an electron which has a charge minus e energy less than 0.

And, some value of momentum and some value of spin that is a same as presence of a positron; which will have all these values switched in signs. It will have positive charge, positive energy and momentum and spin pointing in opposite direction. And this objects positrons reach a positive value of charge; and positive energy are now accessible to measurement in experiments. And indeed they were observed after Dirac's reformulation of this negative energy states as a holes and labeling them as positrons with all the properties opposite to that of an electron. And this language of hole theory is actually still used quite often in condensed matter physics for describing electron bands.

So, there are valence bands in this condensed matter physics which are generally empty. And they have electrons floating around in them. And there are field bands which are interpreted as the sea they can once in a while have holes when the electrons from them are knocked out. And these electrons and holes behave in a particular fashion which can

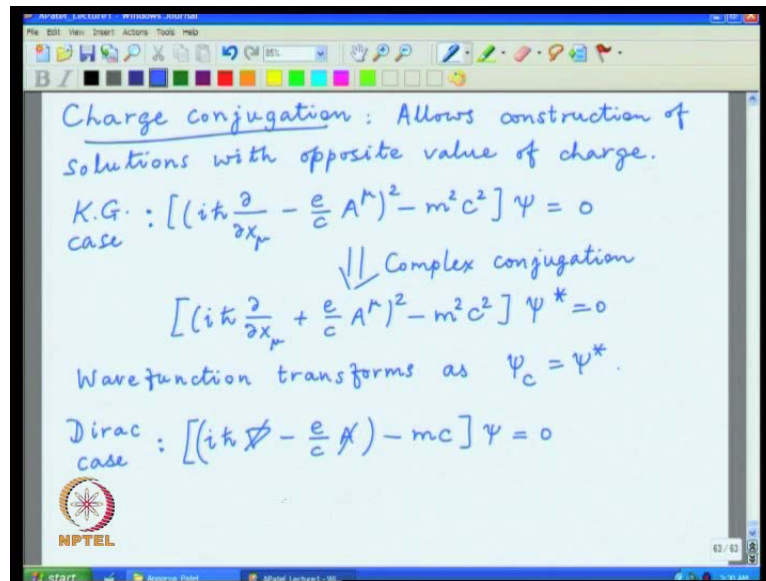
be experimentally detected. The difference from the relativistic physics to this condensed matter physics is that there are a lot of changes in the property of the holes; in due effects which can be called the clouds around the particles or renormalization of certain values. So, the masses the effective masses of the electrons and holes are not the same in condensed matter physics they have different mobilities also and so on and so for.

But anyway this is a useful language which has left its mark. I should say that this is not the modern language of the field theoretic machinery, because what explicitly Dirac used in rescuing his theory was the exclusion principle. And that actually does not apply to all the particles; it applies only to fermions. And so one can ask what happens to the negative energy solutions for the bosons; which will be described for example, by the Klein-Gordon equation. So, those particles actually cannot be interpreted in the same hole theory language. And so one actually does have to go to a many body description many body effects are already present here indirectly, because you are using the Dirac Sea. But field theory quantization needs many body language, where vacuum and operators are defined.

So, as only positive energy excitations are available. And no sea is either defined or used, because the sea can be defined only for fermions and not for bosons. And so we have to get around that definitions. So, one does not really have a sea or the associated concept of a hole in the sea when dealing with filled theoretical situations. And then one has a new definition of what are the possible excitations available for the vacuum. And what are the corresponding operators that give rise to that, but it is indeed possible. And we have an alternative description available in terms of how to interpret this negative energy solutions in field theory as well. But right now again I have not going to go into detail of what this does in completely general frame work, but I can see that the physical effect still has to come out.

So, antiparticles are directly identified by the charge density as is the case of Klein-Gordon equation. In Klein-Gordon equation that was a necessity, because there is no possibility of constructing a field sea. But this introduction of a hole theory language was useful. And the words are still often used in a lot of description of relativistic quantum mechanics and also our part of text books and lectures. So, it is a useful thing to know. Let us now go back and construct a particular transformation which turns out to be useful in the context of this hole theory as well as in the context of field theory.

(Refer Slide Time: 50:02)



And that transformation is known as charge conjugations; it allows construction of solutions with opposite value of charge in particular. If you have a solution of the theory for an electron we can use this transformation to construct a solution a matching solution. For a positron under the same structure and in essence these maps the particles to the antiparticles. And so it is a useful symmetry of the relativistic system. And to see this it is much easier to go back and first look at the Klein-Gordon equation where the solution is easily seen. So, there we have a differential equation which looks like $\Delta \psi - \mu^2 \psi = 0$.

So, suppose this as a solution for a particle with charge e we want to construct a solution or a particle in the same field $n u$, but which has an opposite charge and that can be now easily done by flipping the sign of this operator Δ versus μ . And the sign of the mass term does not really changed. And this can easily be done by finding an transformation which changes the relative sign between the these 2 terms the absolute sign does not matter, because the whole thing get squared. And we can quite straight forwardly guess that this sign can be flipped by taking a complex conjugation of the hole operator. The i changes sign position as well as the vector potential as well as the mass everything is real. And so with the complex conjugation we have the result that ψ^* obeys the equation with an opposite value of the charge. And so the charge conjugation transformation of the wave function is equivalent to taking it is complex conjugate.

So, wave function transforms as ψ^c which is a complex conjugate; ψ^c is used for denoting the charge conjugated states. So, this is a very easy transformation in case of Klein-Gordon equation. And we see all the associated property coming out from this conjugation business, because the phase which involved both energy and the momenta. Once you do this charge conjugation it is going to change in sign and the negative energy a solution obtained from positive energy part. Then can be reinterpreted as contributing an opposite value to the current and so on and so for. So, this is the case in case of Klein-Gordon equation.

In case of Dirac equation the result is little more involved, because what we now have is a slightly different operator; which can be written as $\nabla \cdot \mathbf{A}$; and then $m \psi$ is equal to 0. And simple complex conjugation is not going to work although the relative sign flip coming from complex conjugation of i ; will be useful in changing the relative sign between $\nabla \cdot \mathbf{A}$ and \mathbf{A} ; the reason it is not complete is this slash objects involves gamma matrices. And some of the gamma matrices themselves can be imaginary; when that is the case then they will also transform under complex conjugation. And what we need is a little more general property that matrix structure including the gamma matrices should obey this change of sign; which is necessitated by a particle to antiparticle transformation. And we will see how to do that next time.