Relativistic Quantum Mechanics
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Lecture - 10
Interpretation of relativistic corrections, Reflection from a potential barrier

In the last lecture I worked out the Foldy Wouthuysen and transformation for the case of hydrogen atom. And to see the various terms, it is a useful to keep in mind the order of the magnitude for this particular problem.

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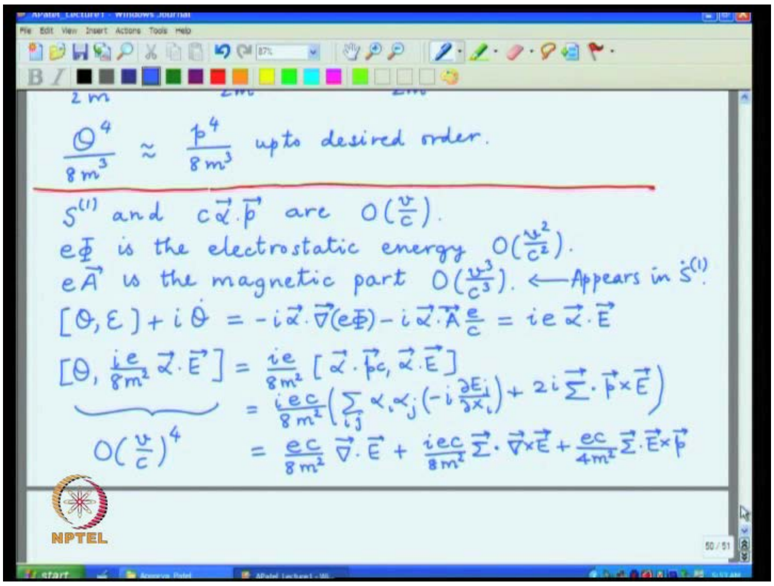

And, to summarize again, the terms which I defined last time, out of them the first are transformation and corresponding part of the Hamiltonian, their order v by c. So, you have to keep upto fourth order terms in the transformation matrix. As on the other hand, the electromagnetic part of the Hamiltonian is not as large as the momentum part. In particular, the electrostatic potential which is of the same order as the kinetic energy in case of hydrogen atom, and its magnitude is order v square by c square.

And, going further down the magnetic part which contributes, which is order v cube by c cube; in particular, it is one order v by c down compared to the electrostatic energy, as is typically the case under Lorentz transformations starting from an electric field. So, these are the various term which appear. And, if you now look at the various contributions, so the magnetic field actually appears in the time derivative of s 1. So, the time derivative is also of the third order in v by c expansion, and that is why we kept many fewer terms involving time derivative than the simple powers of s.

So, with these terms the simple powers of s basically produce the corresponding expansion of square root of p square plus m square, part of the Hamiltonian and the kinetic energy. But, when we include a electromagnetic coupling the same terms also gave rise to this coupling of spin to the magnetic field.

Now, today we will look at the terms which arise completely from the electromagnetic fields. And, they come through the commutators of the operator as with the electromagnetic fields. You can evaluate those things in two parts. The commutator required is actually double commutator.

The first commutator will simplify as commutator of O with electrostatic potential energy E, and it combines with the time derivative of O itself. And, this can be now easily evaluated to be the electrostatic potential energy. The gradient comes by converting momentum to position space representation. And, the second term basically gives rise to alpha dotted with A, and the coefficient of proportionality is e by c.

So, this now can be rewritten as alpha dot e using the general definition of electric field in terms of the potential as well as the time derivative of the vector potential. There is a time derivative acting on this A. So, this is the first commutator which we need.

And, the total part of the Hamiltonian now consists of a second commutator of this quantity with O. And, that amounts to O commutator with i e 8 m square alpha dot E, which can again be worked out by converting the p to a gradient operator acting on this alpha dot E. So, that becomes; here, vector of c here. This can be expanded by the commutators after 2 alpha producing the matrix sigma as well as the contribution of the gradient inside this p acting on E.

And, we can write those things quite explicitly as i e c by 8 m square, that is the overall coefficient. Then, the various part- one is the p directly acting on E which will contribute with the coefficients of alpha. So, it will be summed over say indices i and j, alpha i, alpha j, and then gradient gives minus i, derivative of E j with respect to x i. So, this is a contribution for p acting on E.

And then, the alphas may not commute, and that produces a term which is the sigma matrix. And, the contribution of that thing is 2 i matrix sigma dotted with p cross E, with the understanding that the gradient in p does not act on E. And, this now can be rewritten in symmetric and antisymmetric combinations, which amounts to various terms, which I will separate out.

The symmetric part of this alpha i, alpha j, produces a chronicle delta. And, that just produces divergence of e, and that contribution is then e c by 8 m square divergence of E. Then, the antisymmetric part produces the same contribution as inside here, but it has a different coefficient. And, it can be now written as a, i e c by 8 m square, sigma dotted with curl E. And, the last term can be written with change of sign which makes a little identification easier. So, it is, plus e c by 4 m square, sigma dot E cross p.

So, this is the final electromagnetic terms appearing with the Hamiltonian. In particular, these are all of the order v by c to the power 4, because the first part was order v by c cube, and then one more commutator reduces it to v by c to the fourth. So, the question now is to find a physical interpretation of this various pieces. And, we come to that in steps.

The first step is to combine the term involving the sigma matrices together, and then they make a Hermitian contribution. So, let me just reiterate it. The sigma dot curly, and sigma dot e cross p, the p is actually the gradient. In taking Hermitian conjugate of these terms, we just keep track of the order of operators and the cross product, and Hermitian conjugate comes back to the same terms. The factors of H cross i, I have left out in writing down this expression completely. I will insert them soon to get a completely dimension, full result.

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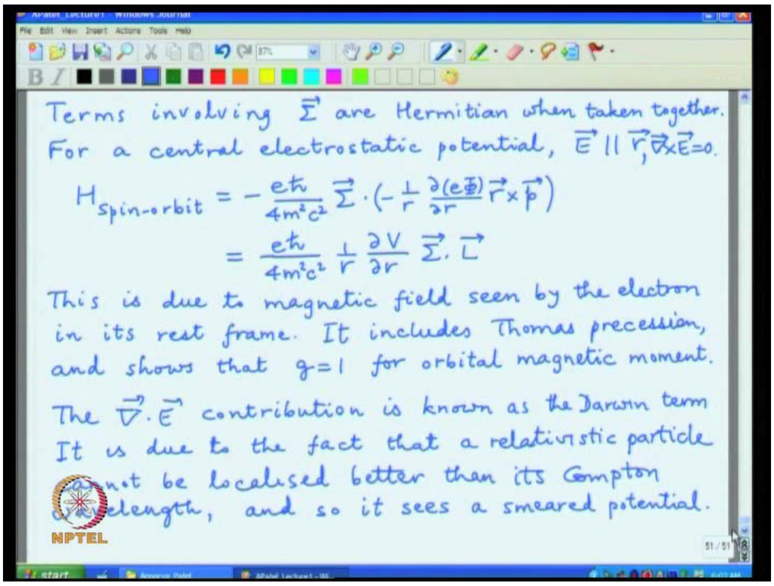

So, the terms involving sigma are Hermitian when taken together. And, they have a particular interpretation, if you take the electrostatic potential to a particular form. So, for a central we have the electric field parallel to the vector r, and then we can simplify the results a little bit. And, one more property which is useful is, the curl of E happens to be 0. So, the operators p and e, one can write it in any order without much conflict.

And then, the two terms basically reduce to what is known as a spin orbit interaction. And, that contribution to the Hamiltonian is the two terms, and the previous expression combined together factor of two comes from writing it in two different ways. And, electric field now can be explicitly written as gradients of a potential which is, expresses a vector parallel to r; the gradient and the magnitude of r is explicitly factored out; and, this now can be rewritten as the orbital angular momentum.

So, together this has a interpretation that the overall contribution is sigma r dot L; V is just the electrostatic potential; and, we have a dipole coupling between the spin magnetic moment and the orbital magnetic moment. This can be interpreted is, as the magnetic field seen by the electron in its rest frame. In this frame the nucleus is moving, and that produces a magnetic field. And, the spin of the electron interacts with this magnetic field.

The feature which is specific to special relativity is built inside this, that it includes the effect known as Thomas precession. And, that shows that the gyromagnetic ratio for the orbital part is a 1. So, this is one particular term. We have its interpretation in non relativistic theory. This has to be included by hand. By the same logic you find a effective magnetic field include the Thomas precession correction and then make the spin of the electron interact with that particular magnetic field.

The term which is not at all obvious in non relativistic analysis is the remaining part which involves divergence of the electric field or effectively the laplacian acting on the electrostatic potential. And, that term is known as the Darwin term by the person who explained it. And, it expresses the fact that any relativistic particle cannot be localized better than its Compton wavelength.

And so, what the electrostatic potential it feels, is not the pointwise potential, but it experiences smeared potential. And, this smeared potential is different than the point wise potential, and the difference essentially this Darwin term. It is easily worked out atleast in terms of dimensional analysis, and that we just have to do a little bit of averaging of the potential by very simple Taylor expansions.

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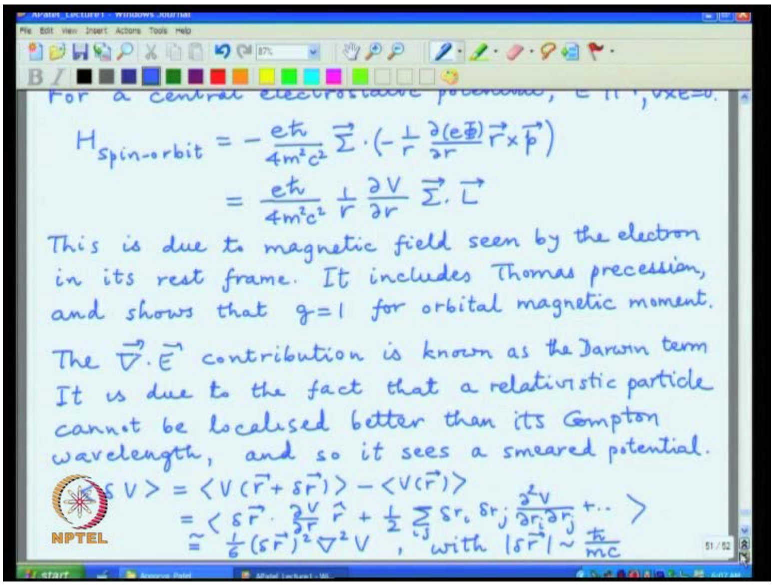

So, suppose I want to smear a potential v over a certain region, so it is can be expressed as some average over a distance delta r. And, that can be expanded. And, for isotropic averaging the delta r contributes to nothing, and this second order term is proportional to chronicle delta means i and j have to be equal. And, that can be then rewritten as delta r in one co-ordinate direction is one third of the total delta r vector square.

And then, this second term basically gives a effect which is delta r square times the laplacian acting on the field r. Here we assumed isotropic distribution for delta r, and then the coefficients of various derivatives in del square we got added together which produces del by del x square, plus del by del y square, plus del by del z square, and so totally they adapt to the laplacian. And, this 1 6, 1 6 factor came in because we use a total delta r, and not the just the individual components.

And then, this term matches with the expression which achieved when we use the value of delta r of the order of Compton wavelength. Then the term which is here exactly turns out to be the expression which we have seen before its divergence of e multiplied by all these various coefficient is nothing but the laplacian suppress with a scale of the order of Compton wavelength.

So, this is the understanding of a various terms which have appeared so far in the hydrogen atom analysis. And, there are peculiar relativistic effects which actually can be observed, and they have been verified in comparing the theoretical expressions with experimental data. But, it helps us understand various relativistic effect and their sources in terms of theoretically well defined contribution; what is spin, what is orbital angular momentum, what is a Compton wavelength scale, and so on and so forth.

Now, let us move on to a different problem. So far we have discussed hydrogen atom solution in great detail and identified various parts, but in a standard course in non relativistic quantum mechanics one does not solve the hydrogen atom problem. First one starts out by solving simpler problems like particle in a box of a harmonic oscillator. And, it is a worth wondering why we did not tackle those kind of problems first before jumping all the way to the hydrogen atom. And, there is a particular reason for that and it is often not mentioned in the text book.

The reason is simple enough that the solution to the problems is of a completely different type. It requires extra ingredient which are not seen in a single particle theories. And, that is possible or that happens when there are potentials which are sort of unbounded or going all the way to infinity. In particular, it does not have to go all the way to infinity, but if the potentials become larger than the rest mass energy of the problem which is m c square, then new effects enter.

And, if you solve the Dirac equation directly without worrying about those kind of effects, and it leads to some puzzling features, and they have been historically called paradoxes. We do not have to interpret now them as paradoxes, we just have to interpret them in a appropriate language and that requires going beyond the description of a single particle theory.

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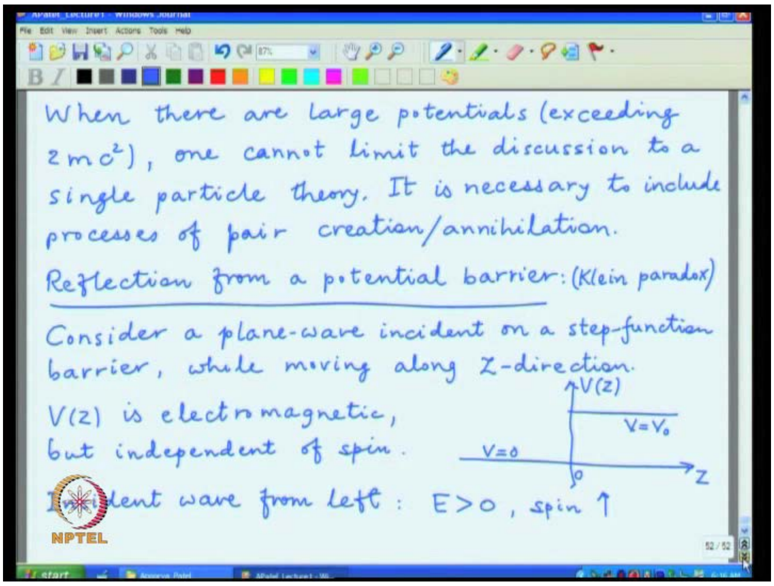

So, when there are large potentials, in particular exceeding 2 m c square, one cannot limit the discussion to a single particle theory. It is necessary to include processes of pair creation and annihilation to understand what exactly goes on. And, this is exactly the reason for leaving out any discussion of a particle in a box or harmonic oscillator. In those particular cases the potential goes all the way to infinity at a large distances, and so that is certainly much larger than 2 m c square, so one gets new effect.

And, before developing the machinery to deal with this pair creation and annihilation we really cannot do full justice to those particular problems. And, that is the crux of why those problems are not discussed and the hydrogen atom problem is worked out in a complete solution. And, what appears in this is, pair processes can be understood by looking at a much simpler problem than a bound state like a potential wall or a harmonic oscillator.

And, that is historically known as the client paradox, and version which I am going to describe is essentially reflection from a potential barrier for a Dirac particle. In particular, we will look at the problem with the barrier height changes, and we will see that something extra will have to be included when the barrier height exceeds 2 m c square.

So, to define a particular scenario just consider essentially a one dimensional problem. There is a plane wave incident on a step function barrier while moving along z direction. And, we will just take to be the simple electromagnetic potential of these types. So, pictorially I can represent as V of z, barrier will be at z equal to 0, or negative value of z I take the potential to be 0, and positive value observed we will take two potential to be v 0. And, this is the origin.

And, the z coordinate is chosen for convenience so that the matrices which appear with the spin part of the wave function are diagonal. So, in this process, as long as the potential is the independent of spin, nothing much will happen to the spin degree of freedom. And, we can directly see the effect of the solutions of positive energy as well as negative energy.

So, now let us try to solve the Dirac equation in this particular geometry. The plane wave has a very simple dispersion relation. So, we will take the incident wave from left to have the property that the energy is positive and spin is pointing up. And now, we have to solve what happens. In particular, how much of the wave is reflected and how much of the wave is transmitted, and then work out the properties and analyse the amount of reflection as well as amount of transmission. So, this can be done rather easily by writing down simple plane wave solution.

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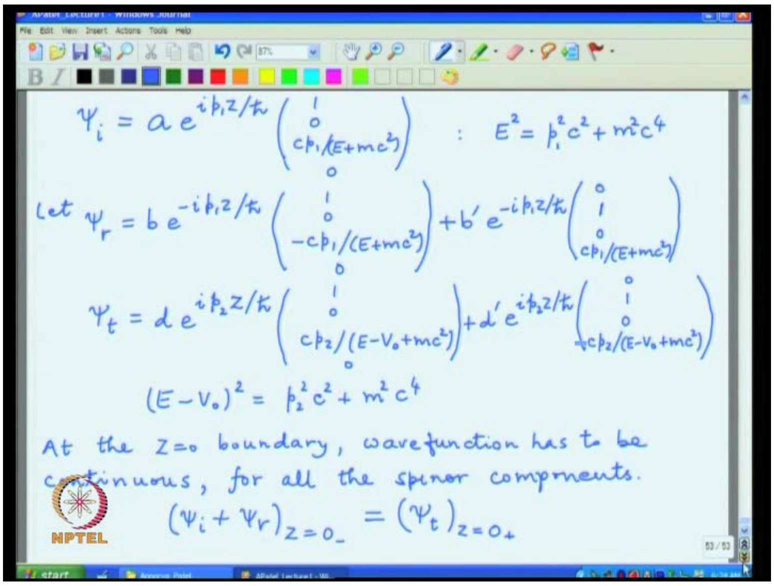

Let me just write down a very general form without worrying too much about normalisations. So, on the incidence part we simply have the wave function 1, 0 for the upper component, and the lower component are decided by the usual non relativistic approximation with which we have seen before. It has the separation of v by c. In particular, this energy momentum dispersions holds the e square is equal to p 1 square c square, plus m square c raise to fourth.

Now, for the reflected and the transmitted part, wave function could have a more general structure. And, we will solve it in generality by imposing the necessary boundary conditions. So, let me take a general expression for the reflected part with one part is moving backwards, and it will have the momentum direction reversed. So, this particular form; and, I am just going to include a possible term which may arise due to spin flip where the wave function will become 0, 1, 0, and then the structure same, but opposite sign. The sign flip comes because the actual operator involved here is sigma dotted with t.

So, this is a general form for a reflected part, and we will again take a similar expression for the transmitted part, such that now it will have a different potential, and so different value of momentum. So, this is the part with the same value of the spin, and a corresponding part which might have a flipped value of the spin. And, of course, p 2 is determined by the same dispersion relation, except that it will now have the form that e minus v 0 square is equal to p 2 square c square plus m square c raise to 4. So, these are the wave functions.

And, to solve the problem we have to match them at the boundary. So, wave function has to be continuous, and in particular for all the spinner components. There is a little difference compared to the Schrödinger equation is solved. Now we have a first order differential equations. So, one boundary condition is enough to solve it, and so just the continuity of the wave function is required at the boundary. We do not have to worry about what happens to the barrieority of the wave function.

On the other hand, the continuity has to be assured for all the different spinner components of the wave function, and that in a sense takes care of the boundary conditions which are impose any Schrödinger equation, both on the wave function and its derivatives. But this is a simple difference which arrives is from the structure of the equation itself.

So, what we need is now incident plus reflected wave on one part at z is equal to 0 on the negative side is equal to the transmitted wave with z on the positive side. And, if you do it for all the 4 components one by one we will get several conditions relating the coefficients a, b, d, b prime, d prime. And, we will have 4 equations. There are 5 unknowns.

The overall normalization of the incident wave remains of re parameter, and all the other 4 will be determined in terms of that incident wave normalization in it. In turn that will allow us to calculate the ratios of probabilities relating to the strength of the incident wave for various kinds of processes that can occur.

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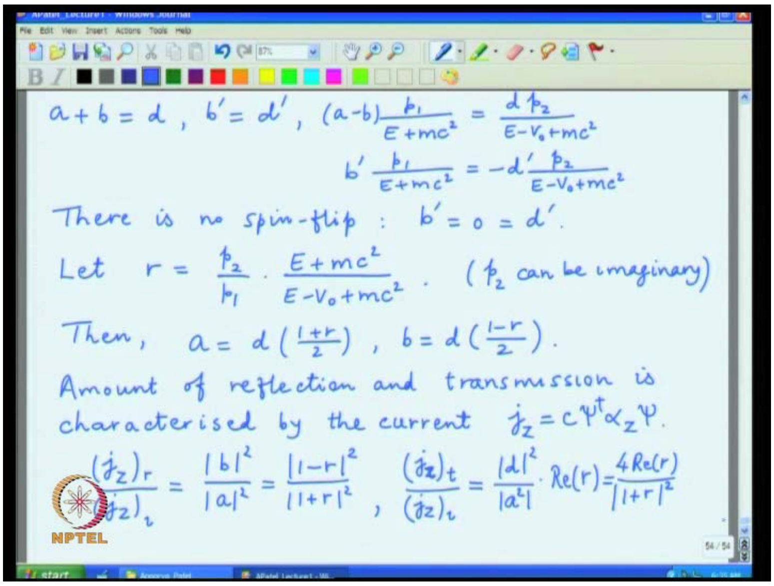

So, let us write down those conditions. Explicitly the upper components gives a very simple conditions which are just that a plus b is equal to d, then b prime is equal to d prime. And, the lower negative energy component give a condition, but with the momentum factors explicitly appearing, and they are therefore, there is a weightage of by these ratios p by E plus m c square on one side, and the other side has a similar ratios with p 2, but now the potentially shifted by v naught. So, that is the condition on a and b. And then, one more arises in a similar structure which is b prime.

So, these are the all the 4 matching condition. In particular, there is a very simple feature that there is no spin flip under this particular process which amounts to the result that b prime and d prime vanish. It is quite straight forward to see that one condition says b prime equal to d prime, and if you substitute anything over there then this is a condition between an p 1 and p 2 which are completely different since the potential is non 0, and you cannot satisfy both of them simultaneously unless the coefficients have all got value 0.

So, we are now left with only the condition on a, b and d. And, it is convenient to define a ratios of this momentum factors to write the result in a simple form. So, like this ratio r be the ratio of these 2 particular factors is p 2 divided by p 1, and the energy factors are E plus m c square and E minus v 0 plus m c square. The thing to keep in mind is, the potential can have different values. And, in particular we can explore the region where the p 2, the momentum becomes imaginary, and then in that case r can also become imaginary, and you have to treat r as a complex number to be able to see all the possible consequences.

And, with this particular thing in mind we can easily workout now what the ratios is a plus b is d, and a minus b will be equal to r times d. And so by simple linear combination we have the results immediately that a is equal to d times 1 plus r by 2, and b is equal to d times 1 minus r by 2. So, this is a general solution valid for all the values of the potentials.

Now, we can look at specific cases which can occur for different components, and for that we will be interested in finding out the amount of reflection and the amount of transmissions. And, these things have to be characterized in terms of the physically observable properties. So, that particular observable which we have seen before as well by the current appropriate to this particular geometry, and we have the waves moving along z direction.

So, this particular current will be the z component, and its expression we have seen- psi dagger alpha psi and the z component of it. And, the value of this objects will tell you how much of the wave is going in one direction, how much is going in the opposite direction, and in particular the current can take both positive and negative value, but it is a physically observable quantity.

So, what we now need are the values of the currents for the 3 different wave functions which we have the incident one the reflected one and the transmitted one. And, in particular, we are going to normalize everything with respect to the incident waves. Now we will look at the ratios of these currents in a various cases. So, they can be very easily derived from this various expressions.

So, what is j z reflected divided by j z incident; well, the wave functions psi dagger alpha psi essentially have the same structure for both the incident and the reflected wave because all that mattered was the components have the lower components of psi plus p 1 or a minus p 1. And, contribution in psi dagger psi the sine actually gets squared, and we have no other change.

So, this result is actually nothing but mod b square divided by mod a square. And, from the formula above it can be easily written as 1 minus r square divided by 1 plus r square. Note that I have kept the absolute value sign allowing for the possibility that r can be a general complex number.

In case of the transmitted part we have another similar contribution, but now the wave function is little different. In particular, the lower component on one side is p 2 and the other side is p 1. And, if you remember what the alpha z looks like it is a sigma matrix on the off diagonal part which couples the upper component of the, the lower component. So, this value of the current is actually just the product of the magnitude of the upper component and the lower component.

And, looking at the previous expression these two components differ by the value of p 1 and p 2, as well as the potential. If you want to take the ratio this ratio between these two quantity is exactly what defined the quantity which we labelled as r. And so, this object is d square by a square, and the quantity which appears is not just r, but because it is a psi dagger and psi you will get a contribution which is p 2 plus p 2 star for the transmitted wave. And then, divided by p 1 plus p 1 star for the incident wave, and that contribution is equivalent to writing the real part of r. And, now with these particular values we can quickly rewrite this expression as ratio of real part r to 1 plus r by 2 whole thing square. So, this is a quite general result for a current which can be observed in this particular scenario.

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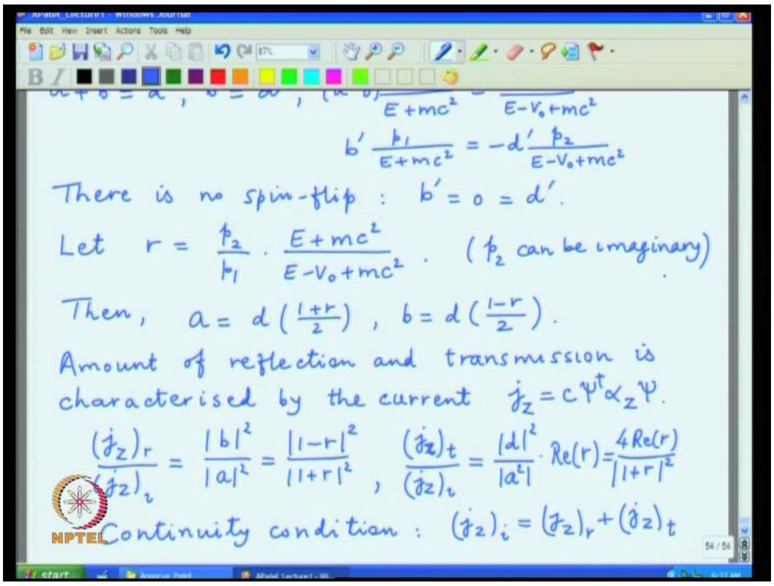

And, since we have done the boundary condition matching, etcetera correctly, we immediately see a consequence that continuity condition is satisfied which just says that the first ratio and the second ratios. If you add them up they add upto 1. Or, equivalently you can write that j z i is equal to j z reflected plus, j z transmitted. One can see that very easily 1 minus r square plus 4 times r, we add them together it just adds up to 1 plus r square. So, this continuity equation is indeed satisfied. And, this is our answer.

Now, what appears is the puzzles when the potential takes different values. And, that corresponds to now changing the value of v 0 relative to the value of e. And, the various cases we are familiar with it. We can now look at what happens when the kinetic energy is bigger than the potential energy, we expect the wave to get transmitted to a large extent.

If the kinetic energy is less than the potential energy we expect the wave to be reflected in non relativistic theory. The reflection will be 100 percent because the wave function on the positive z side will be decaying exponentially. But, something funny happens in this relativistic theory, and we will explicitly see the behaviour in the next lecture.