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

Lecture - 3 Coupling to Electromagnetism, Solution of the Coulomb Problem

In the previous lecture, I described the Klein-Gordon equation and how its degrees of freedom can be separated in the two component language, which were identified with particle and antiparticle modes. Now, this is a generic feature of relativistic quantum mechanics that with every particle mode, an antiparticle mode necessarily appears. But historically, it was a lesson learnt over many years, the simple reason being that when these equations were developed, none of the antiparticles were experimentally observed. And...

(Refer Slide Time: 01:11)

K) (24 1001 O O O 2. 1. 7. 8 2 8 Electric potential CA. modifies time-derivative with coefficient 1. Coefficient of mc2 15 of. gy is shifted in opposite direction E>0 and ELO solutions, when electric potential is introduced. confirms opposite values of charge ticle and antiparticle Same mass, But all charges are opposite

So, what I describe is the modern understanding of what we call particles and antiparticles. And they have an important relation between the properties, which can be just summarized as these objects have the same value of the mass, but all charge values are opposite. And for that reason, which one we call particle and which one we call antiparticle is sometimes a matter of convention. Most often the objects, which are observed quite frequently in our world – they are called particles; and everything which is rare is put in the antiparticle label. And for example, an electron is a particle and a

positron is antiparticle or a proton will be called a particle and antiproton will be called antiparticle.

Now, it should be noted that, though the masses are the same for both these objects, all the charges are opposite; and the charges may come in many different types. For example, I was discussing electromagnetism; and so the electric charges will have opposite values. If I am discussing weak interactions, the weak charges will have opposite values. If I am discussing strong interactions, the color charge will have opposite values. Sometimes the charges are not associated with any interactions, but they will still have opposite values like baryon number or a lepton number. And this is always associated with a symmetry between particle and antiparticles that, you flip the signs of all possible charges, which may come. If some charges are flipped, the other ones are not flipped; that will not be called an antiparticle. And this is our modern understanding or the modern referring system of how do we associate these objects with each other.

And, the only way we can have objects, which do not have this kind of association is when all charges are exactly 0. And in that particular case, there is no possibility of creating of another object, which has opposite charges. And in such cases, the objects will be necessarily all neutral with respect to all the charges. And in such cases, we may as well refer to them as particle and antiparticle referred to the same object. Or, in other words, the object – it happens to be its own antiparticle. And there are few example of this category. For example, photon is completely neutral with respect to all the charges and we can refer to photon being its own antiparticle.

Now, this emergence of antiparticle solution is a very important lesson of reactivity. But, in the early days, that was not what people studied heavily. The important point of development of quantum mechanics was that, it has to match with observed phenomenon in atomic physics. And that was the essential point of developing the subject. And we have to have a theory, which can explain all the experimental observations described in various atomic phenomena, energy levels, quantization of radiations and transitions, how the levels change in presence of external fields, etcetera, etcetera. And what we learn in quantum mechanics today at the beginning like a particle in a box or harmonic oscillator, which are much simpler problems; they were not the ones, which were historically analyzed first, because the theory had its meaning only if it could match with experiments. So, everything was tested against observations in atomic physics. And the

bench mark of the test was the solution of the hydrogen atom problem. If the theory could explain the hydrogen atom spectrum and its various properties, then it was worthwhile studying.

So, now, I move on to discussing the solution of the hydrogen atom problem with the Klein-Gordon equation. And that is what Schrodinger tried at the beginning after writing down the equation; it was rather unfortunate that, he obtained the solution, but he had to discard it, because it did not match with experiment as well as he had expected, but that is a little bit of twist of history. And I will give the explanation little more after describing the solution.

(Refer Slide Time: 06:55)

coupled to electro magnetic fields prescription: pt- $\int -m^2 c^2 \cdot \int \Psi = 0$ ≠0, B= VXA A.=0. is the same operator rödinger equation term, with

So, let us take now the Klein-Gordon equation and couple it to electromagnetic fields. And that equation when we solve it, we will get a solution of the hydrogen atom problem in a fully relativistic frame work. So, the standard prescription for coupling quantum theory to electromagnetism is so-called minimal prescription; which says that, you take the momentum operator and replaced it by p mu minus A mu; where, A mu is the gauge potential for the electromagnetic field. And if you do that, then the modified equation will describe the particle in the presence of electromagnetic field specified by the potential A mu. And so we have the Klein-Gordon equation now written in terms of a derivative operator or gradient in the particular form – del mu minus A mu whole square minus m square c square multiplied by psi equal to 0. Now, we have to solve this

equation. And in various cases, depending on the field, there will be various kind of solutions. It can be easily seen that, the particular situation, where this differential operator is different compared to Schrodinger equation, is in the time component. The space part of this produces the Laplacian. And that is exactly the same structure as what is happens in the Schrodinger equation. And so one can look at the situation in electric and magnetic field separately.

In case of just a magnetic field, where this vector potential is not 0 and B is defined as curl of A; and we will put this scalar potential equal to 0. In that particular case, what we have in this equation is nothing but the operator, which happens to be the same. And so it produces the same solution and the same spectrum as happens in the case of Schrodinger equation. In particularly, it gives the usual dipole coupling of the electron in presence of a magnetic field, where the dipole is proportional to the orbital angular momentum. Or, in other words, the Gyromagnetic ratio happens to be equal to 1 for this particular interaction. So, this is a standard. And it has been observed in certain situations; but it fails when the electron spin also contributes to the magnetic moment. And that is something, which does not come out from the Klein-Gordon equation. However, this was not the first concern; the magnetic field was known to have a smaller effect than the electric field itself.

And, the particular solution of the hydrogen atom problem corresponds to solving the equation with the coulomb field, where the potential A 0 is essentially Z e by r with presence of a nucleus, which has atomic charge Z e. So, it is not necessarily just the proton, but for any nucleus ((Refer Time: 13:20)) a single electron going around it. And now, the point is now to solve this equation in presence of this coulomb field; and we will put the magnetic field equal to 0. And this case is a simple enough, so that one can directly compare the solution with respect to the non-relativistic case. And we will see term by term what are the changes, which occur. The first thing to observe that, in this particular case, this is a central potential, which implies that, the angular momentum is conserved. And so the equation can be separated into radial and angular parts essentially, because the angular parts, which are associated with the spherical angles theta and phi – they only occur as a part of the Laplacian; and the potential does not produce any term, which depends on those angles.

(Refer Slide Time: 14:45)

So, now, let us write the solution, parameterize the same way as in case of a hydrogen atom. So, I will decompose this general wave function psi into its radial part and an angular part. And since the angular operator only comes as a part of the Laplacian operator, the solutions are the well-known spherical harmonics. And the potential does not do anything to the angular part and we can just use the solutions. The part, which depends on the potential, is the radial wave function.

And now, we can write down the reduced equation for the radial part assuming that, the angular part basically just gives the same value as is well-known in case of quantum angular momentum; it will produce a contribution, which are the eigenvalues of the spherical harmonic and a term, which appears as I times I plus 1 divided by r square. So, the equation, which we have after this separation of variable looks like minus 1 by r square d by dr r square d by dr plus I into I plus 1 by r square into R. This is differential operator, which comes from the radial part of the Laplacian acting on the wave function.

And, the result has to be the other terms in the equation, which are essentially the energy and the radial potential. And then, can be very easily written as the combination E minus A 0 whole square minus the rest mass contribution. And this is the equation, which we have to solve. It helps to compare with the corresponding equation in the non-relativistic case, where the left-hand side is identical; it comes from the same Laplacian operator. But, the right-hand side is different ((Refer Time: 17:35)) the energy part of the equation

is linear in the non-relativistic case.

Now, the comparison can be illustrated by writing down the coefficient of each power of r in these two equations. The differential operator is identical while the other part, which are basically coefficients of 1 over r square, 1 over r and the constant term – they are different in these two particular equations. And by knowing the solution of one, we can actually write the solution for the other by just replacing these appropriate changes in the various terms, which are basically just changes in certain coefficients. So, let me write a little table, which compares this particular coefficient.

So, let me denote the two cases here: relativistic and the non relativistic cases. The coefficients of 1 over r square in these two situations happen to be this – the non-relativistic case of layered l into l plus 1. But, here you got an extra term, which comes from A 0 square. The coefficient of linear term in 1 over r; in one case, it comes from the cross product of this expansion of the square; in another case, it is purely the contribution of A 0. So, this is...

And then, there is a constant piece, which does not depend on r and which essentially is a function of the eigenvalue energy. And all we have to do is write the general solution of the non-relativistic equation in terms of these coefficients and then replace those coefficients by the corresponding relativistic answers. And we automatically have a solution for the relativistic case. So, the solution of these equations are the so-called Associated Laguerre functions, which are essentially an exponential fall off multiplied by a finite order polynomial. And the order of the polynomial is related to the radial quantum number.

Now, one can look at these various quantum numbers in an explicit case by writing down a general solution. But, many behaviors are kind of well-known and I will just point them out rather easily. So, one feature is that, the solutions behave r is to l prime near the origin, where l prime is determined by solving this particular coefficient in the same way as this particular structure. And this is a quadratic equation, which can be easily solved. And the answer is easily written in terms of this solution involving a square root. There are things, which I have implicitly assumed in this solution. One of them is that, the negative sign in front of the square root is discarded for this solution of the quadratic equation, because otherwise, the solution will not be normalizable; it will blow up as r goes to 0 with a large negative power.

So, we are forced to take the plus sign to make the function well-behaved as r goes to 0. The other feature happens if the second correction, which is 4 z square alpha square exceeds the first term. In this particular case, the number will become imaginary; and that applies or indicates to an unstable problem. And in that case, we must have to do some thinking and reinterpreting what the solution means, because as long as this number is a positive number, things are fine. But, if it either turns negative or becomes imaginary, something is not physical in the solution, which it produces.

(Refer Slide Time: 24:49)

bility expected when $Z > \frac{137}{2}$ dral quantum number is n', a non-negative intege quantum no: $n_R = n' + l' + 1$. $n_R = \frac{2EZe^2}{\hbar^2 c^2} \cdot \frac{1}{2} \frac{\hbar c}{\sqrt{IE^2 - m^2 c^4 I}} = \frac{E \propto Z}{\sqrt{IE^2 - m^2 c^4 I}}$ $n_{R} = \frac{2EZe^{2}}{\kappa^{2}c^{2}} \cdot \frac{1}{2} \frac{\hbar c}{\sqrt{le^{2}-m^{2}c^{4}}} \sqrt{le^{2}-m^{2}c^{4}}$ $n_{R} = \frac{Ze^{2} \cdot 2m}{\kappa^{2}} \cdot \frac{1}{2} \frac{\pi}{\sqrt{2mlel}} = \frac{Ze^{2}}{\pi} \sqrt{\frac{m}{2lel}} = n'+l+1$ $mc^{2} \left(1 + \frac{Z^{2}\alpha^{2}}{n_{R}}\right)^{-\frac{1}{2}} \qquad NR : E = mc^{2} \left(-\frac{Z^{2}\alpha^{2}}{2n_{R}}\right)$ $(1 + n_{R}) = \frac{\pi}{n_{R}} \sqrt{le^{2} + n_{R}} \qquad (1 + n_{R}) = \frac{\pi}{n_{R}} \sqrt{le^{2} + n_{R}}$ $(1 + n_{R}) = \frac{\pi}{n_{R}} \sqrt{le^{2} + n_{R}} \sqrt{le^{2} + n_{R}}$

So, let me state the first condition, which is already included in by discarding one of the signs of the square root. But, the other condition is at... There is an instability expected when the atomic charge is larger than 137 by 2. This is a problem in the sense that, there are lots of nuclei, which we know which are experimentally observed, which satisfy this particular condition. So, something goes wrong with this solution; and clearly, this is one case, where it does not match with experimental observation. But, let me just continue and construct the complete solution and we will come back to this situation after that. And that remaining part – the angular quantum number now has gotten fixed and we have to find a radial quantum number.

And, the radial quantum number is related to the degree of the Laguerre polynomial. And that degree is defined or rather constrained to be a non-negative integer. This is a convention. And it is dictated by the fact that, unless this radial quantum number is not an integer, the polynomial will become an infinite series and the function will then not have a good behavior as r goes to infinity; you must truncate the polynomial and that truncation is enforced by making this number and integer; otherwise, the series of the recurrence relation defining Laguerre functions does not terminate. And then, the final solution is return in terms of a total quantum number, which is a combination of the radial 1, the angular 1 and an extra 1, which is related by all the conventions of where these numbers start and either from 0 or 1. So, this total quantum number is the one which fixes the energy.

And, the relation is that, this number is essentially the ratio of 2 of the terms, which I wrote down on the previous slides. These are coefficients of 1 over r and r-independent term. The l part we have already taken care of and it does not appear anymore. But, these 2 coefficients dictate the value of the energy. And it is essentially is the ratio of those 2 terms; and it can be expressed as 2 E Z e square by h cross square c square into half h cross c divided by square root of mod E square minus m square c to the power 4. This particular expression, which can be simplified after canceling all the constants; and expressing the result in terms of the so-called fine structure constant, which is nothing but e square by h cross c. So, this is a final result.

Just to compare it directly, we can construct the same quantum number in the nonrelativistic case, where the corresponding terms and the ratios evaluate to Z e square into 2m by h cross square into half h cross divided by square root of 2m into mod E is equal to Z e square by h cross into square root of m by 2 mod E. The result that, it is n prime plus l plus 1 in this particular case; which makes up the total quantum number and it has an expression, which is again related to the energy. And the energy levels, which we are familiar with in case of the hydrogen atom problem, are now obtained by inverting this expression. So, E is written as the function of the total quantum number. And that gives the well-known formulae, which are very easily to remember.

And so I will write down those results. So, this energy is a... This is a relativistic case. Energy is m c square 1 plus z square alpha square by n R square is to minus half. And the corresponding version for the non-relativistic case gives the Rydberg formula, where energy is proportional to 1 over the non-relativistic total quantum number square. The difference between the 2 formulae is that, in the relativistic case, we have the rest mass energy m c square, is always part of the solution.

And, if you want to compare the non-relativistic case, you have to subtract out the m c square part and look at the remaining part, which follows from it. Other than that, the results are all identical. So, the non-relativistic case is an energy can be written as m c square into minus Z square alpha square by 2 n NR 2. It is essentially the first term in the expansion of this quantity, but with total quantum number appropriately replaced by its analog; and the difference being that, the value of 1, which appears here is different than the value of 1 prime, which appears there. So, these are the kind of standard results.

And, the question as I said is compare this again with experiments. So, this is the socalled Rydberg formula. And this includes relativistic kinetic energy. And this is exactly what Schrodinger arrived at. He had the Rydberg formula, which actually worked very well in fitting the experimental data. And he thought now he has a more powerful version, which includes the corrections due to relativistic kinetic energy; and so it should be able to explain the observed linear energy levels in particularly the fine structure splitting more accurately than the Rydberg formula.

And, he could just work out the fine structure corrections as a next term in the particular expansions. And surprise was that, it did not work as well as he thought it would; and he was disappointed; he had to put aside his solution, because it did not explain what he thought it would explain. And after some time, he decided to just publish the non-relativistic limit of his particular formulation. And that is the equation, which now carries his name; that is the Schrodinger's equation.

That was not the first equation, which he wrote down, but it was his compromise that, the relativistic version did not work. So, he took the non-relativistic limit. And that produced what was expected in the non-relativistic limit. And that then became successful in dealing with lots of problems in atomic physics and chemistry. So, where did this fine structure description go wrong? Let us just work out the details by expanding this object in a Taylor series. The leading part is m c square, which is a rest mass energy. The next term is the Rydberg formula, which is also OK. And we have to go to the still further order in expansion and simultaneously relate the value of the relativistic total quantum number and the non-relativistic one to match the various expressions.

(Refer Slide Time: 36:52)

Sommerfeld's formula Replaces by tained also by includi Kinetic Energy (e.g

So, that relation between the various quantum numbers can be easily worked out by rewriting l prime in terms of l, which turns out to be the non-relativistic quantum number corrected by a small term with denominator 2l plus 1. And now, one can take this expansion again; plug it back into the energy levels and find out what the fine structure splitting is. So, the energy expansion becomes m c square minus m z square e to the power 4 by 2 h cross square n R 2 plus 3 by r m z to the power 4 e to the power 8 by h cross to the power 4 into c square n R 4 minus... And then, you substitute for n R in terms of the non-relativistic constant number. These two terms will give rise to the rest mass and the Rydberg energy, but something will be leftover.

And, that gives a fine structure of these energy levels. And the term is this particular coefficient. But, now, everything rewritten in terms of the non-relativistic quantum numbers. And this is the place, where the detail matching with experiment failed. Schrodinger was not just disappointed, because this thing did not work as well, because there could have been lots of other sources of error. But, he was more disappointed, because the formula, which has matched with the experiment, also existed; and that was already derived in the semi-classical quantization formulation, which Bohr started and Sommerfeld generalized. And that formula essentially gave the very small modification of this particular quantity and it had this number replaced by 2 times k, where k - positive integer.

And, in this particular case, 1 happens to be an integer and 21 plus 1 is an odd positive integer. And the only difference is that, the odd one does not work; the even one works in matching with the experiment. And nowadays, we know the reason for this particular shift; it is just that, what is appearing here is the value of the total angular momentum and not just the orbital part. And the relativistic theory, which includes the new contribution to the angular momentum – essentially, the spin of the particle adds to the value of 1; 1 is an integer; s is half. And once you combine this formula, instead of having an odd integer over here, you will obtain an even integer over here. And this formula now works.

So, Sommerfeld had already derived this particular formula, which met with experiment. And Schrodinger got this slightly different answer; it did not work and he had to put it aside saying that, this is not the correct description of the hydrogen atom. The change from this odd number to even number followed a few years later when Dirac obtained his equation and solved it for the hydrogen atom. That equation automatically included the spin of the electron; and for that reason, shifted this number exactly by this particular amount and arrived at the correct result. So, this is the summary of what all goes on in case of a solution of the hydrogen atom. One can also derive this expression in our modern language. So, the fine structure of the energy level can be obtained by treating. So, this can be obtained also by including the correction to kinetic energy, which happens to be the term in perturbation theory. And this term is nothing but the whatever expansion of square root of p square c square plus m square; the leading term is m c square, which is here.

The next term is p square by 2m, which is already included in the solution, which produces the Rydberg formula. And the third term is this. And if you calculate it in perturbation theory, it exactly produces this fine structure relations. So, we now understand what exactly this thing is coming from; it is the relativistic correction to the kinetic energy. The part, which is missing in this particular formulation, is the spin. And once you combine the spin as well as the relativistic corrections, you get the correct number, which matches with experiment. So, that is the story of a Klein-Gordon equation, its solution for the hydrogen atom problem; and why that was put aside. And Dirac had to look for some other equation, which will describe the hydrogen atom spectrum properly including the fine structure case.

But, let me make a Digration here in the arguments, which led Sommerfeld to derive the correct formula. And it is a little bit unusual that, he could get the correct formula without knowing anything about the spin, because when he derived his formula, spin was not discovered by experiments; and still his answer, which does not include the spin value of the electron at any stage in the derivation matches with experiment. And that was a little bit of a luck in the sense that, there were 2 corrections to the derivation, which he followed as we understand today: one was the spin was left out and another was the correction to the semi-classical quantization, which also was left out. It just happened that, both these effects were equal and they canceled out each other in the formula and he got the final answer correct. And that is a topic of semi-classical quantization.

(Refer Slide Time: 47:10)

Bohr-Sommerfeld quantisation Action-angle variables and phase space. canonically conjugate variables, the period is quantised in units of planck's constant. Adiabatic invariants : opdqi=nih (Separation of variables necessary) Classical behaviour is recovered when n; ->00. Bohr : Circular orbits

And, I will give an outline of this quantization; it is often not given in much detail in text books. But, it is worthwhile to understand the principles of it, because it is useful in connecting classical and quantum mechanics at various different levels and arguments. So, this so-called semi classical or Bohr Sommerfeld quantization follows from the socalled action-angle variable formulation and description of the system in phase space. And what it expresses is that, for canonical formulation, you take the canonically conjugate variables and look at the revolution. And if the evolution is periodic, then the period is quantized in units of Planck's constant. And this was a formulation, which was set up by Bohr. And Sommerfeld expanded it to include many other situations. And the reason that, these kind of objects are quantized, has to do with the behavior of these objects in classical mechanics. And they are the so-called adiabatic invariants. And one can prove that, if you change the parameters of a classical system very slowly, that is where the word adiabatic comes from. This particular quantity do not change. And that is the statement that, integral of p d q over a closed orbit is invariant.

In quantum theory, the rule is that, the area enclosed by the orbit in phase space is an integral multiple of the Planck's constant. This semi-classical rule has two obvious limitations. One of them is that, you can apply it only when the variables go through a periodic behavior. And another one is that, this kind of quantization requires that you will be able to apply it to individual canonically conjugate pair only when the theory or the equations of dynamics can be separated in terms of these variables. And so it can be applied only to, where limited number of possibilities. But, still the formulation was successful, because many of the interesting motions fell into that particular category particularly when the motions are periodic and the variables can be separated. And this is the principle, which Bohr emphasized.

And also, it allowed him to connect classical and quantum mechanics by imposing the condition that, classical behavior is recovered when these quantum numbers become large. And this is named after Bohr as his so-called correspondence principle. So, Bohr applied these arguments to a very simple situation and to get the Rydberg formula. And that was to look at the so-called circular orbits of an electron going around a nucleus. In this particular case, the equations are rather simple; the dynamics just is given by the centripetal force matched to the electromagnetic interaction. And in that case, this particular integral is basically the integral around the circle phi going from 0 to 2pi. And this is the value of r does not change for a circular orbit. One can easily work out what that angular momentum is. And quantization of that in terms of this quantum number immediately produced the result that, the energy is given by the well-known Rydberg formula with the quantization number being an integer. So, this was the first application of a quantization role in atomic system.

(Refer Slide Time: 54:25)



And, since it was successful, Sommerfeld tried to generalize to new situations; and that is where he got inclusion of orbital angular momentum explicitly into this formula; as well as he could include relativity also in this particular formula, because classical dynamics and its relativistic extensions were very well-known. And these two things were included by the well-known results in classical dynamics. One was that, you do not have to stick to only circular orbits; but one can look at elliptic orbits as well, which are again exact solutions of Kepler's problem in classical dynamics. And those elliptic orbiters basically allow the periodices integral to be applied to the radial variable as well, instead of just the angular variable.

And, that basically gives a new quantum number, which now can be written as the one corresponding to the integral of the radial momentum. And it will have values again and starting with a set of integers. The 0 actually corresponds to the object being in a circular orbit, where radial momentum vanishes identically; and after that, there is an integer quantization. And this generalization provided a new rule to Sommerfeld for including contributions to quantization of certain things. And that is where he could get extra levels of the hydrogen atom, which were not there in Bohr's formula. And once the relativistic corrections were included in these integrals, he could obtain the fine structure as well. And that is the formula, which I quoted earlier in relation to the Klein-Gordon equation solution and which matches with experiment. The details of this we will work out next time.