Relativistic Quantum Mechanics
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Lecture - 8
The Frobenius method Solution, Energy Levels and wavefunctions

In the last lecture I started discussing the solution of the hydrogen atom problem in case of the Dirac equation. We separated the differential operator into radial and polar coordinates, replaced the polar part of the operator by its Eigenvalues, and then obtained the radial equations which were coupled between the positive and negative energy components of the 4 component Dirac spinners.

Now, this equation has singularities at r equal to 0, and at r equal to infinity. The singularity at infinity was easily taken care of by solving the asymptotic part of the equation. And, we impose the boundary conditions necessary for bound state that the solution falls off exponentially with the radial coordinate. Then, the remaining singularity has to be tackled by a series expansion near r equal to 0. And, this is the standard Frobenius method which I will describe today giving rise to the explicit solution.

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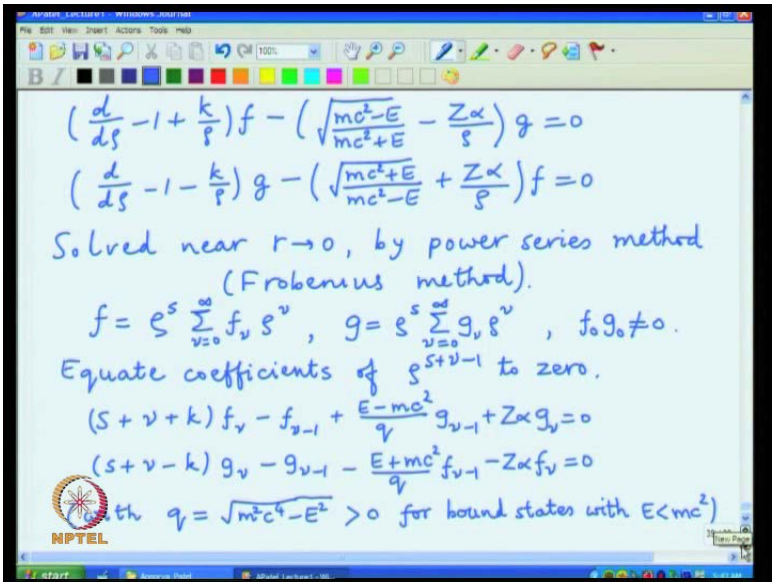

So, the Frobenius method is a written by a convention where the function f is a sum power of the coordinate multiplied by a series. And, we will use the series where the

leading term is always non 0. Now, the same exponent, leading exponent s is used for both f and g; could s can be seen in the equation, the power of f and g which are involved here. The lowest power corresponding to the coefficient of d by d rho, or 1 over rho are identical for both of them. So, the leading term, rho raise to s, happens to be the same for both these functions, f and g.

And now, one can substitute these equations, and equate the coefficient of various powers of rho to 0, term by term. And, it can be written with a little bit redefinitions of certain variables to save some writing. So, equate coefficient of rho raise to s plus nu minus 1 which is a lowest coefficient appearing inside this operator, and that gives rise to the 2 coupled equations now, in terms of the coefficients. This is one equation. And, the other equation has a same structure except for some change of signs. And, here I have chosen a simplification for notation with this variable q is m square c raise to 4 minus e square. It is positive for bound states with energy less than m c square.

So, now we have to solve for this various coefficients from this particular equation. The first step is to go to the lowest order in this infinite series which corresponds to nu equal to 0, and find the terms which contribute to it. Certain terms do not contribute to it. For example, the coefficients of 1 over rho do contribute, but the coefficients of constant terms do not contribute to that particular order. And, that equation is a little bit simpler than this coupled equations, and which can be solved easily, and the result is a determination of the power s.

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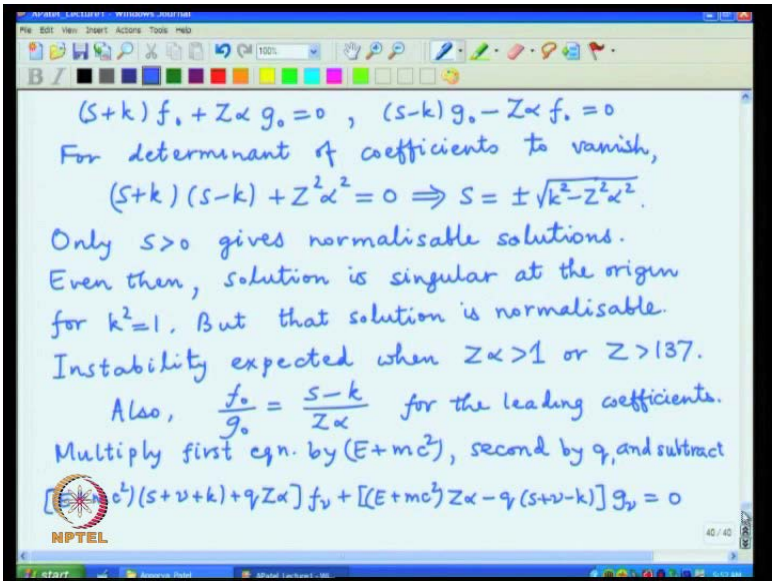

So, for nu equal to 0 in the terminology of Frobenius method, this is also called the indicial equation. We have the simplified version which is relation between f 0 and g 0. There are 2 equations, and they are homogenous equations. And, non trivial solution will exist only if the determinant of the coefficients vanishes, and that determines the values of s; s square root of k square minus z square alpha square.

Only, s greater than 0, gives normalisable solutions because otherwise there will be very strong singularity at the origin. And, so, we have to reject the negative sign of the square root. Even then, the solution is singular at the origin when k square is equal to 1. And, that comes from the fact that in defining the wave function we had written, psi equal to 1 over r times f or g, as the components. And, that 1 over r gives a negative power which is larger than the positive power coming in here, because of this subtraction of z square alpha square.

So, the solution indeed blows up at r equal to 0, but that solution is normalisable because there is a factor of r square in integrating over the 3 dimensional space in normalizing the wave function. So, this is the behavior. And, from the same factor we can expect that something will be peculiar when z alpha becomes greater than 1, in which case the argument of the square root will become negative. And, the imaginary component will indicate, in general, that there is some kind of a behavior which is unstable or uncontrolled growth of certain modes. And, that happens in this particular case where z alpha is greater than 1, or nuclear charge is bigger than 137.

So, that is the determination of this index s. It also gives the leading behavior of the ratio f 0 and g 0, which can be written as s minus k divided by z alpha. And, that essentially tells us which value is larger than the other for the convention which we have chosen; s minus k is going to look like certain integers; and, this is a finite number. So, this is a finite ratio. But, depending on the value of the 2 terms, either f or g can be much larger than the other coefficient, and that will determine which component of the solution dominates over the other.

Now, we can go a step further and try to determine the relation between arbitrary f mu and g mu. It can be done by certain manipulations. And, they are quite straight forward. I will just give the answer that get to equation. And, multiply first equation by E plus m c square, second by q, and then subtract the second from the first one. The result is an equation which eliminates half of the terms, and can be written as.

So, this equation actually now determines the ratio between f and g coefficients, term by term. We still have to solve this. And, for that we observe again the asymptotic behavior of what is the ratio of the f nu coefficient with f of nu minus 1. And, to do that we have to go back and look at the previous equation which involved both f nu and f nu minus 1. In the limit the nu going to infinity, we can drop all the sub leading terms. This term becomes f nu, this term just become f nu minus 1, this term g nu goes to 0, but this g nu minus 1 we can substitute from the next equation which we have derived in terms of f nu minus 1. That is, the behavior for large nu is f and g are proportional upto certain coefficients involving e plus m c square and q.

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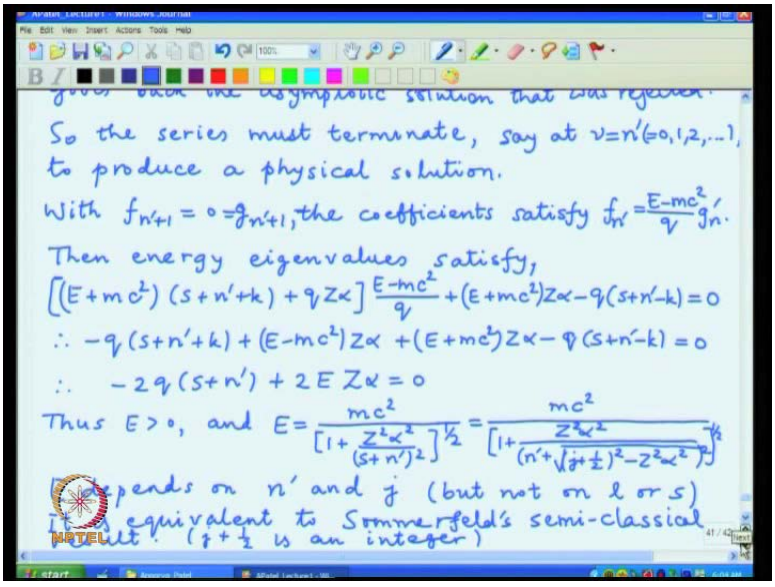

And then, we see that the asymptotic behavior roughly looks like f nu is 2 by nu times f nu minus 1, and g nu is a similar structure. This kind of series behavior can be easily solved. And, it is a asymptotic behavior of the exponential functions. The factorial terms basically produces this 1 over nu e facts, and 2 is the same as what is the terminal ratio. And, this behavior is actually not acceptable as a physical counter part of the required solution because it gives back the asymptotic solution that was rejected when we solve for the singularity at infinity, saying that the solution has to behave like e raise to minus rho. And, if you multiply that 2 things together, it will give e raise to plus rho which happens to be a solution, but which is not a physical solution that we want.

So, we cannot allow this series to go on forever. The only way out is to make that series terminate at some value of the index nu. And, this number can be any integer which

appears in the series expansion. And, if the series terminates, the function is like a polynomial and which can be normalized, and it will have a well behavior at infinity because of the factor e raise to minus rho which we have already separated.

And now, with this criteria in hand, we will go back to the equation and impose the condition explicitly. So, the condition is that, with a finite series we will put this coefficient from, f of n plus 1, and, g of n prime plus 1 equal to 0. Then, the proportionality constants basically are determined; 2 of the terms vanish, and the other 2 gives a ratio. So, this is now a condition for the series to terminate.

We can determine now the Eigenvalues for energy by satisfying all the conditions which are imposed simultaneously; one is this ratio. We also obtained a different ratio which was the previous equation coming from the ratio of f and g over here. Equating both these ratios to have the same answers; then, we have the equation for the energy Eigen values become;

This quantity, it is a quadratic equation, but the quadratic term actually drop out in a nice fashion. And, we can reduce it easily to the structure which is now linear equation in energy, and that gives a simple constraint which is this simple relation. And, as the signs show with q greater than 0, we have the straight forward answer that energy is; and, one can put in all the determinations of various indices explicitly to get a result in terms of the quantum numbers.

So, this is the final result, exact solution for the energies of the hydrogen atom problem. And, it depends; this is E depends on n prime which plays the role of the radial quantum number, and j which is the angular quantum number. But, it does not explicitly depend on l or s. And, this particular fact is responsible to leave a degeneracy behind; that j can be obtained in 2 different ways- either j equal to l plus half, or j equal to l minus half. And, the degeneracy between those 2 different ways of obtaining j survives in this particular solution.

On the other hand, this solution is equivalent to Sommerfeld’s semi-classical result with certain redefinition of what is meant by the quantum numbers, in particular j plus half is a integer. So, this is the explicit form. We can compare it now with various forms which we know.

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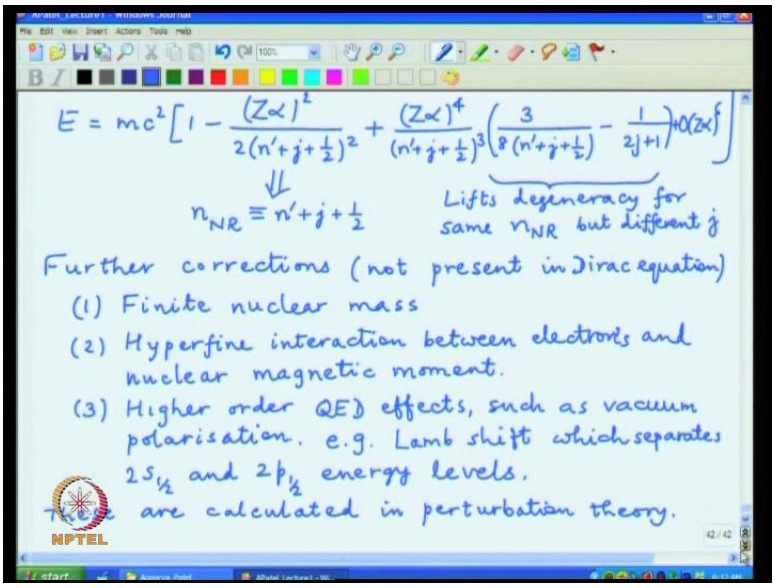

So, one is to expand the solution in powers of the fine structure constant to see the explicit effects of various terms. And then, we have the structure. The first term is just the rest mass, and the second term is the so called Rydberg formula which means that we have to identify the non relativistic quantum number as n prime, plus j, plus half. And, then there is a fine structure term. And then, still higher orders can be calculated if necessary. But, in particular, this fine structure term does match with experimental observations. It will separate the degeneracy between same value of; so, this one lifts degeneracy for same; different values of j.

So, the degeneracies are quite easily observed by putting the atom in a magnetic field where all these fine structure separates out, according to Zeeman splitting. One can do actually one far more accurate experiment to see what happens further even at a higher energy scales. And, there it is necessary to include extra effects which are not part of the Dirac equation in order to match the experimentally observed quanta. And, those various effects I can just list right now.

One is the finite value of the nuclear mass. In Schrodinger's equation, this can be included by using a reduced mass for the electron, but that is not possible in case of Dirac equation. And, one has to actually calculate the effect of the finite mass using a perturbation theory calculation; it shifts the energy levels somewhat. The other is a so called hyperfine interaction between the magnetic moment of the electrons and the nucleus. This again can be calculated very easily as a dipole interaction and added in

perturbation theory. And again, it is something which is experimentally quite clearly seen.

The particular effect which is actually more famous than either of them is arising from the full formalism of quantum electrodynamics. And, they include correction to the coulomb potential because the propagators for electrons and photon and the vertices do get modified, once you consider multiple interactions. And, they change again the various energy levels in various ways. And, the famous example of this particular is a something which is known as a lamb shift which separates 2 s and 2 p energy levels.

And historically, this lamb shift provided a very important step in establishing the theory of quantum electrodynamics. It was first observed in experiment, and then the theory had to produce a number which can explain the experimental result. The interesting part is the Dirac equation leaves the energies of 2 s and 2 p states degenerate to any order; the reason being that both these states have the same value of j.

And, the Dirac energy solution depends only on j and not the l is equal to 0 which happens to be the s state, and l is equal to 1 which happens to be the p state. But, experimentally this 2 are separated by many of these things which are calculable. And, these are all calculated in perturbation theory. We can again make certain observation for the ground state because expressions are quite simple.

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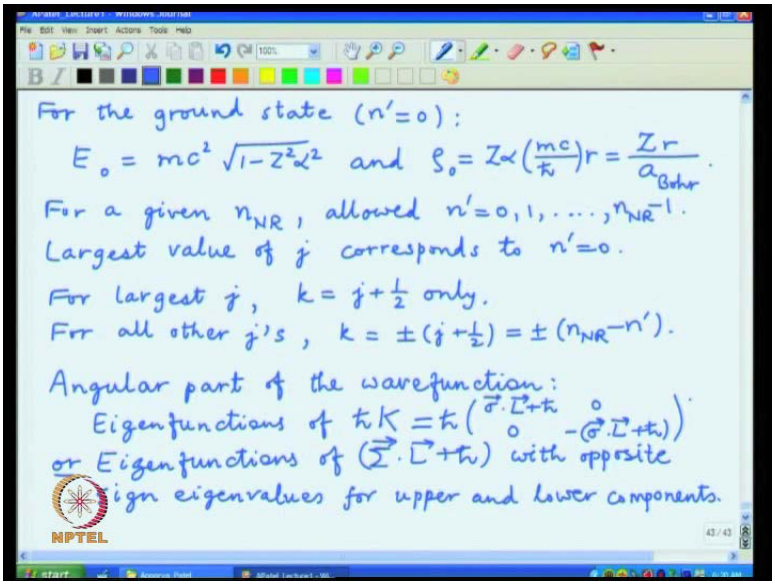

And, the ground state correspond to n prime is equal to 0. And, in that case, the energy drastically simplifies to an expression which is easy to remember. It just a rest mass energy connected by this fine structure effect. And, one can also calculate the exponential fall off which becomes the same as in case of the Schrodinger's equation. In particular, the exponential rate of fall off is determined by the Bohr radius. So, these are the results which one expects. And, they emerge quite naturally from this detailed solution.

One can also determine various energy states, and the degeneracies, etcetera, by looking at all the integer values allowed inside here. And, it is now easy to classify the same way as we did it in case of non relativistic state. So, you take a given value of NR, then allowed n prime, then we will go from 0, 1, all the way to n non relativistic minus 1. The largest value of j, it corresponds to n prime equal to 0.

And then, one can ask the allowed values of k which are basically 2 signs; so, which values occur for which value of j. And, the 2 signs of k certainly does not occur for all the values of j. The degeneracy has to match as the same case in case of non relativistic atom; and, so, one of them remains unpaired. So, for largest j turns out that k only takes 1 particular value, and for all the other k takes both the values which can be written as; And, this will now count all the allowed degeneracy of the various states correctly; how the different values of l and s combine with other.

Now, we are ready to look at the angular part of the wave functions. And, we had separated them out. These are Eigen functions of the operator h cross times K. Or, equivalently after taking out the factor of beta from the K, they are Eigen function of sigma dot L plus h cross; but they have opposite signs for upper and lower components. One can rewrite it in a same way that the operator involved in here is sigma dot L plus h cross 0, 0, and minus sigma dot L plus h cross.

So, now we have to find the Eigen states of this particular operator sigma dot L. It is easy to do in the non relativistic language. We know the sigma represents a spin half, L represents the spherical harmonics. And, this operator combines the 2 things together; those things can be worked out.

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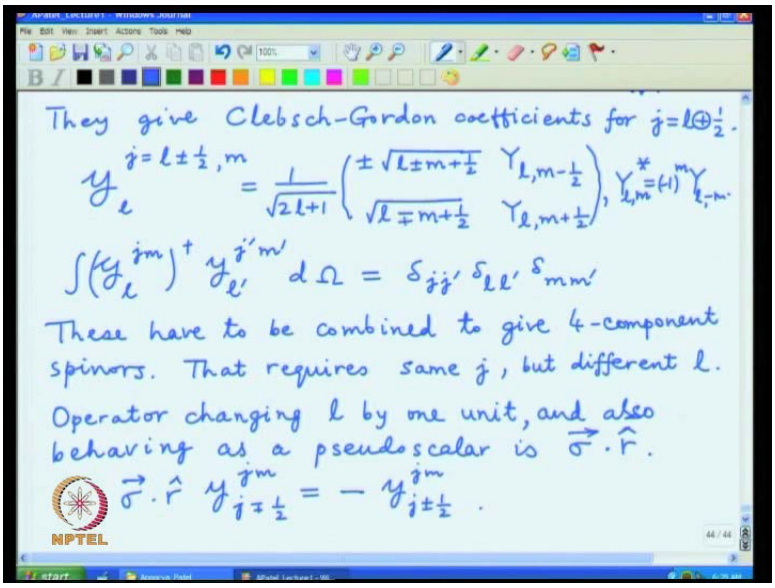

And, the results for non relativistic case are well known obtained by doing a tensor product in the angular momentum algebra which one can schematically write as a spherical harmonics multiplied by the up and down components. And, these are results can be expressed in terms of the Clebsch-Gordon coefficients, for j is equal to addition of l and half. So, when l is non 0, it produces 2 states- j l is equal to l plus half or l minus half; then l is equal to 0, it produces only one state which happens to be j equal to half.

And, these expressions are written in the conventional spherical harmonics basis, as the formula I am writing down. One has to choose a specific sign convention for defining spherical harmonics to be able to determine the Clebsch-Gordon coefficients properly. So, we have an answer. When you add y l m, and then the spin half on top of it, this gives the same value of m for the overall function in both this cases. Here the spin contribution is plus half added to this, and here it is minus half spin added to this.

So, this is a standard result of doing some Clebsch-Gordon algebra. And, it is in the particular convention where a complex conjugate of the spherical harmonics is minus 1 raise to m, times the spherical harmonics with index minus m. So, these are the wave functions which we would like to use to write a Eigen states of the g operator which we want. And, these various Clebsch-Gordon coefficients are determined so as to have the identical normalization conditions which are used for spherical harmonics. And, that in this particular language becomes this overlap integral, and that gives chronicle delta in all the different indices.

So, these have to be now combined to give what we want as 4 component Spinors. There are only 2 components in this script by wave functions, and so we have to use 2 of them. We already saw the effect of upper and lower component contributing with opposite signs, and that was a signature of the parity. And, so, we need to combine solutions with same value of j, but different values of l. In particular, the l values will differ by 1 unit, so as to contribute the compensating factor to gamma 0, to make up an overall parity state.

So, minus 1 raise to l will be the contribution to the parity from the orbital wave function, and minus 1 intrinsic parity will appear for the negative energy components of the Dirac spinner. And, those 2 will just add up nicely. So, the overall parity will be the same for upper and lower components. And, in order to do that, we need to construct an operator which changes l by 1 unit, and also it should have a negative parity. So; is the Pauli matrix sigma dotted with the radial coordinate. These are the only variables available to it.

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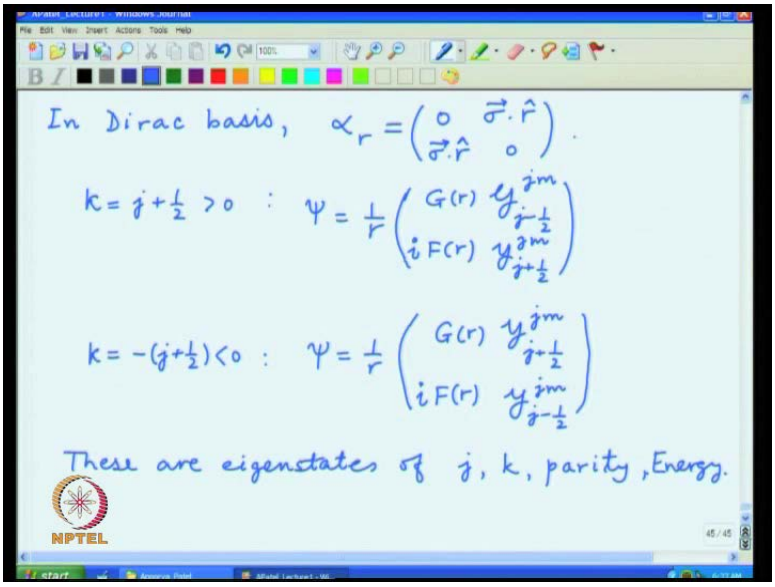

The linearity and the radial variable ensures that the l will change by 1 unit, and the vector can only be dotted with this Pauli matrix to produce a pseudo scalar which will take into account the parity. And, the relation which is useful in understanding the various spherical harmonics is, in this particular basis, there is an identity which says that sigma dot r operating on this script wave functions, changes the l value by 1 to give plus

or minus half. And, the coefficient of proportionality with the all the normalization used is just a negative sign. And, this can be proved in a straight forward manner.

And, it is useful in a completing the solution to the hydrogen atom problem, because now we can go back and look at the original equation that we use the particular form for the matrix alpha r, which was just plus i and minus i in the off diagonal terms. But, if you literally go back to the Dirac basis, then this matrix alpha r is sigma dot unit vector r, on the off diagonal parts.

And now, the solution which was brought out by using just plus or minus i for the entries of alpha r can be re expressed in terms of the solution, in which the how the basis is defined by the sigma dot r. The result is easy to convert, because the sigma dot r is, we have seen is an Eigen operator for this script y spherical harmonics. And so, the solution just have to be converted by replacing that I appropriately with this particular phases.

And then, the final answer can be written in terms of these 2 particular choices of k, what the result look like. And so, we have the various pieces. This was the radial part, and the angular part now gets a corresponding coefficients. We will write this combination as j minus half j m. So, this is the component where orbital and spin part are parallel, and this one is the one which corresponds to those 2 things being anti parallel. And, these coefficients now come exactly with this sigma dot r and the factors of i, which we had inserted earlier boils down to producing this particular structure.

And, similarly, the other wave functions have a similar combination, except the, this indices now are little different. So, the l values are little different for negative and positive k. And again, there is a factor of r appearing over here. And, these are Eigen states of j, k, and parity, and of course, the energy. And, that completes the solution of the hydrogen atom problem in its fully detailed form.

I have not derived each intermediate step in this whole calculation, but they are standard algebraic steps for various angular momentum operator combinations, and they can be easily filled in. And, as you have seen, the expressions for energy match very well with experiments, and the eigen states of angular momentum which are very well classified appear as expected in the appropriate places with correct degeneracies.