Select/Special Topics in Atomic Physics
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Lecture -22
Many Electron Atoms: Hartree Fock self Consistent Field Formalism

Greetings, we have our catch 22 Hartree Fock problem, and we have made some progress in planning our strategy about how to solve this issue.

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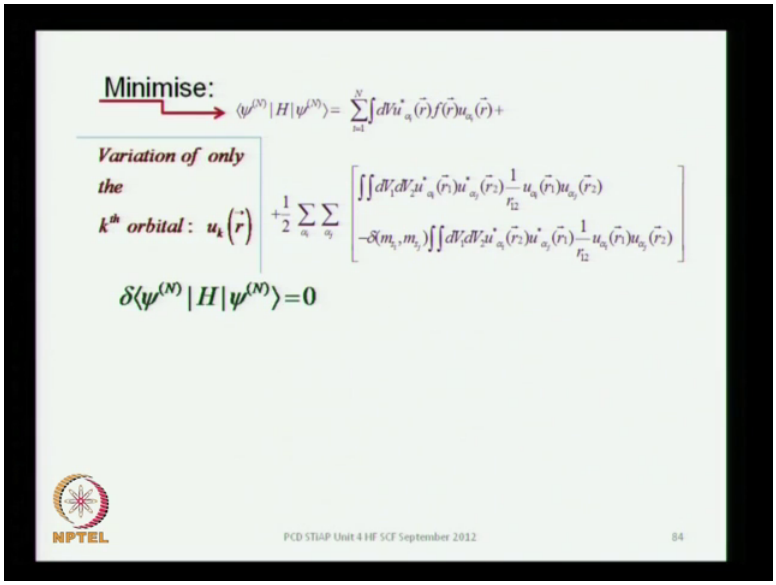

So, our strategy is to minimize expectation value of the hamiltonian, which we wrote in terms of the one electron and the two electron integrals, the two electron integrals being the coulomb and the exchange. Subject to the variations in one orbital at a time, which is the flows orbital approximation that we are referring, all the other orbital's would not be varied, only one orbital at a time. So, subject to this we seek that the expectation value of the hamiltonian in the n electrons later determinantal anti-cemeteries wave function is an extremum. The constraints of course are that each one electron are orbital remains normalized and orthoganal to every other, so these are our constraints.

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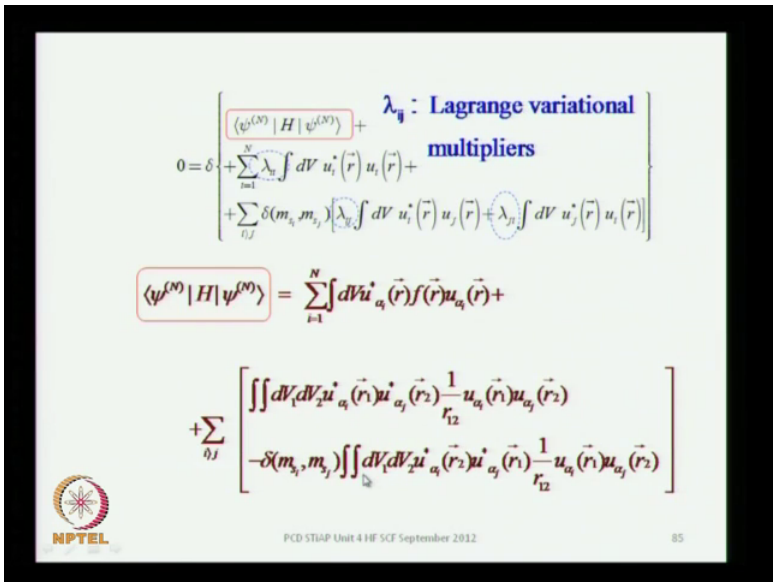

Now, this is what our condition boils down to, that because of this constraints we incorporate this constraints, why are the method of variation multipliers, which is the Lagrange method. And we introduce this method in the previous class, that the condition that particular function is extremum, subject to cert constraints is completely equivalent to seeking the extremum of a different function.

In which the terms, which go in the equation of constraint are multiplied by this parameters, which are known as Lagrange parameters or variation parameters. And accordingly we have this lambda i i, for each ith orbital, there are n of these corresponding to the normalization condition. And then, there are this lambda i j, in the lambda j i corresponding to orthogonality constraints, now these parameters we also know something little more about the Lagrange multipliers.

We know that if you write this variation multipliers has made fixed elements like lambda 1 1 lambda 1 2 lambda 1 3 in the first row, and the lambda 2 1 lambda 2 2 in the second row. The matrix that you would generate the n by n matrix lambda would generate would be Hermetian method, that is something that we have found out in our previous class. Now, if you look at the first term here alone, which is in this red lope over here, this is the sum of this single particle integrals, and the two particle integrals the coulomb minus exchange.

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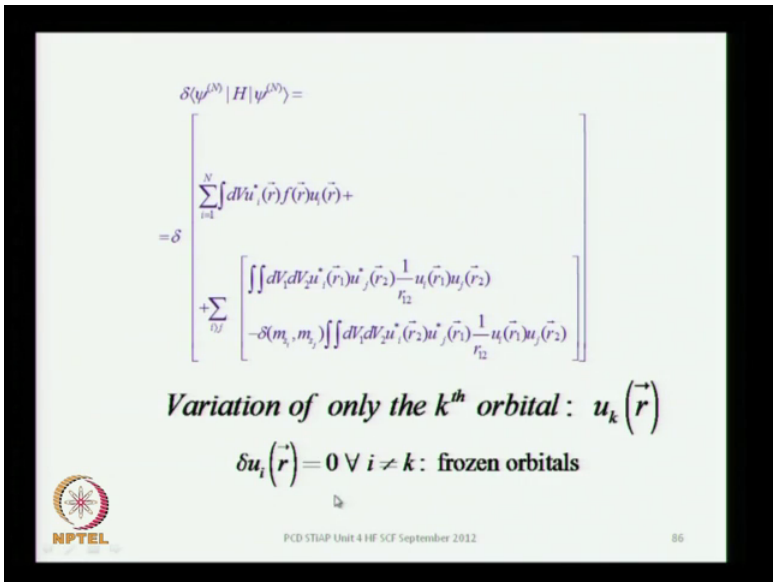

So, I am looking only at the variation in this expectation value of hamiltonian, which is made up of this one particle and two particle integrals, one centre and two centre integrals. We know that there are additional terms, which will come from the Lagrange multipliers, so they will be plugged in later. At this point, I am focusing attention only variation and the expectation value hamiltonian alone, because they all come as additive terms have we have seen in the previous line.

So, now, looking at only the first term, and the variation also in the k th orbital, just one orbital we choose it to be any one of the n orbital let it be the kth orbital just our referencing book keepings purpose. So, it is only the kth orbital it will be vary, all other orbital for i not equal to k will remain frozen.

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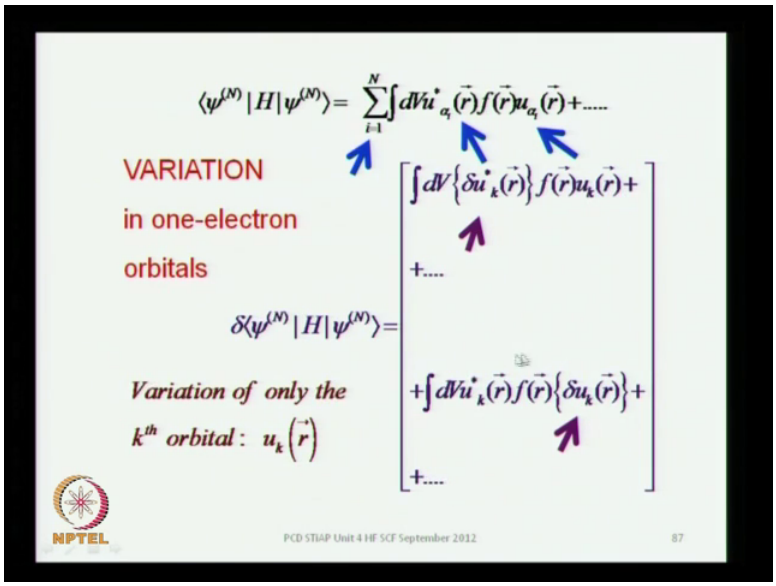

So, let us look at the first term, in this the first term is the single particle integrals and you are seeking a variation in one electron orbital, so this are the one electron orbitals alpha i you must sum over i going from one thought n. And there is one particle orbitals come here, and here and both of these are subject to the variation, so essentially you will have whenever this alpha i does not corresponding to the kth orbital that variation would vanish, and the whole integral would vanish.

The only term that will show up in your analyses is one corresponding to the kth orbital, so from the variation in this you will get the delta u k star r, and then you have the rest of the term, from the first orbital. Then these dots represent all the other terms, which include the two electron integrals likewise, there will be the variation over here, it is only the kth orbital. So, there will be additional terms over here, and you will then write how this terms keep track of each term.

So, we will include all those term, and I will show them on on subsequent slides that we include these terms progressive, so the keep track of the very first term that we are taking care of.

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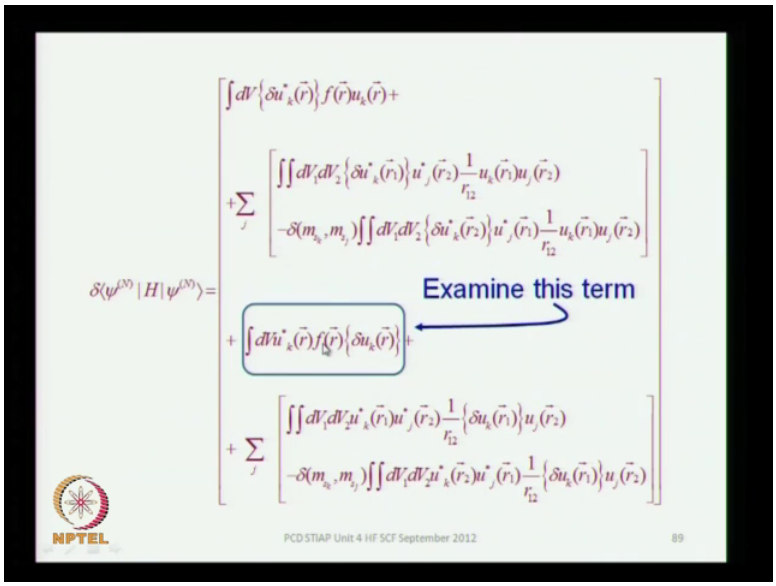

Now, if you look at the variation in the k th orbital, in the two centre two electron integrals, this is the in coulomb and this is in the exchange and you are varied k th orbital alone. You must sum over j, but only the k th orbital is being varied, so any variation in which you refer to a variation in any orbital, it other then the kth orbital, the corresponding two electron integral would vanish.

So, that is not written over here, because it goes to 0, and here you have only the variation in the kth orbital, this is in the coulomb integral, and this is in the exchange integral, then you have a additional terms which are complex conjugate. So, now, you include all of that, so this set has got the complex conjugation, so here you have delta u k star r 1, here you have to delta u k r 1 and so on.

Now, we have got all the terms, now let us see if you can simplify this in something, what is it that this leads has to, but we also have to include the terms coming from the constraints. So, some simplification is possible, if you just examined this term, now look at this term what you know about the operator a f this is the single particle operator.

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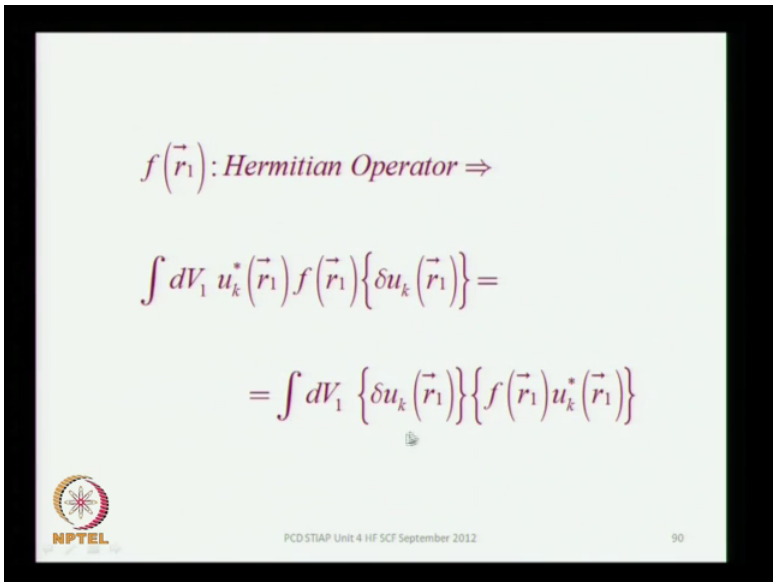

It is a Hermetian operator, so this is the term and this being the Hermetian operator this integrals is completely equivalent to the integrals, which is written here at the bottom, form which delta u k r 1 is the factor, which had appeared in the earlier as well. So, you will then will be able to combine all those terms, let me go back once slide, because here you had delta u k star r, and then you had delta u k star r 1, delta u k star r 2 is here, this is delta u k r, but this is coming in the operant. If you put it behind the operator, then it could be extracted out as a factor, so that you can combine the terms leading to some simplification, still have a look at this that we will use this relation.

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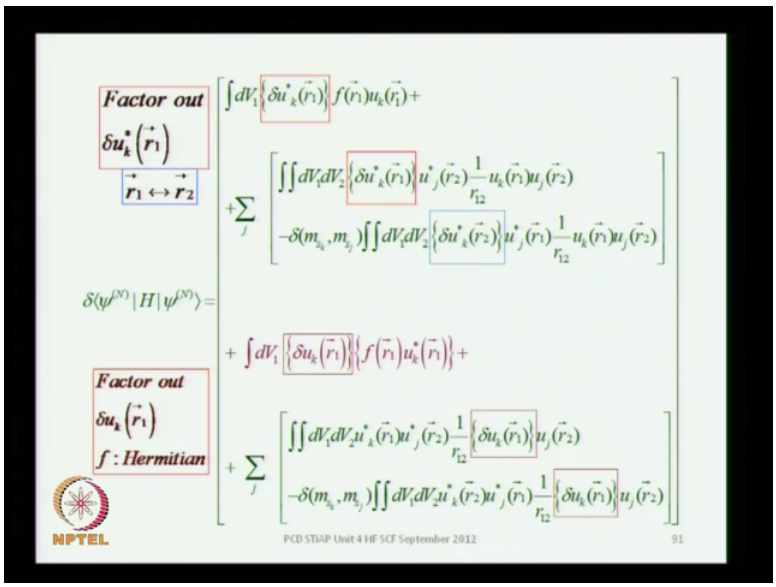

And now, you have used it over here, this delta u k r 1 comes here you have got the f operator operating on a u k star r 1, and now you can look at all those terms, which have got delta u k r 1. So, delta u k r 1 is common over here, you have delta u k r 1 over here and then you have delta u k r 1 over here, and all of this three terms it is only a multiplicative common factor in all the three integrals.

Say you can combine the integrals, over here you have got delta u k r 1 and delta u k r 1 in this two integrals, and this come already this one come already before the operator. So, this operator is not going to affect this part, so you can extract delta u k star r 1 has common in this term and this term, you can factor it out, can you pull it out from this term what do we have here.

The one with the kth label is delta u k star, but the argument is r 2 rather than r 1, say you cannot extracted straightaway, but then both r 1 r 2 get integrated out. This is the double integral over d v 1 and d v 2, both r 1 and r 2 get integrated out, these are dummy labels, so you can write x in place of r 1, and y with in place of r 2 or you can write r 2 in place of r 1 and r 2 you can just interchange r 1 and r 2 labels.

They are dummy labels which get summed over integration is just sum, and they get summed over. So, if you just exchange dummy labels r 1 and r 2, you can extract delta u k star r 1 from this term as well, can you see that and then you can combine all of this 3 terms. Likewise, you can combine all of just three terms in which one can extract delta u k r 1 from here, delta u k r 1 from here, delta u k r 1 from here, from this 3 terms you can extract delta u k r 1.

And then you can write these terms exactly by factoring out by common terms, and there get a very simple form, because now you have a fairly complicated set of terms, but of course, we still have to include the terms coming from the constraints, so we will do that later.

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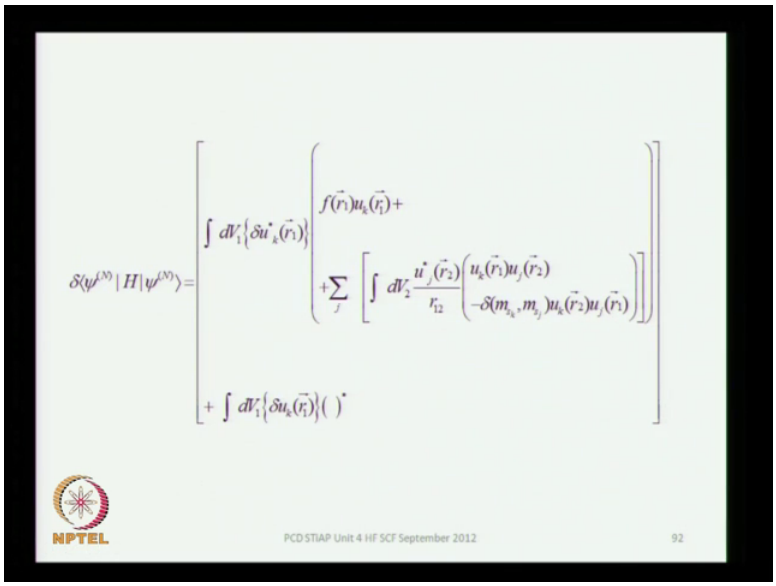

So, here you have factored out this delta u k star r 1, factor out the integration over the element v 1, this is a triple integral mind you, what happened to the summation over this spin variables that has already been carried out. And that gave us ((Refer Time: 12:44)) delta's and all that passes has already been achieved, it has already been completed. So, now, you have integration over v 1, then you factor out delta u k star r 1, and then all the terms involving integration over r 2 or in the coulomb and the exchange term, and you have got the complex conjugate, what is in this bracket over here.

So, here this is integration over v 1, the one factor which is common extracted is delta u k star r 1 and the factor, which is extracted over here is delta u k r 1 and this multiplies the complex conjugate. So, these two terms in the top row and the bottom row, which are added to each other completely equivalent they are just complex conjugate of each other.

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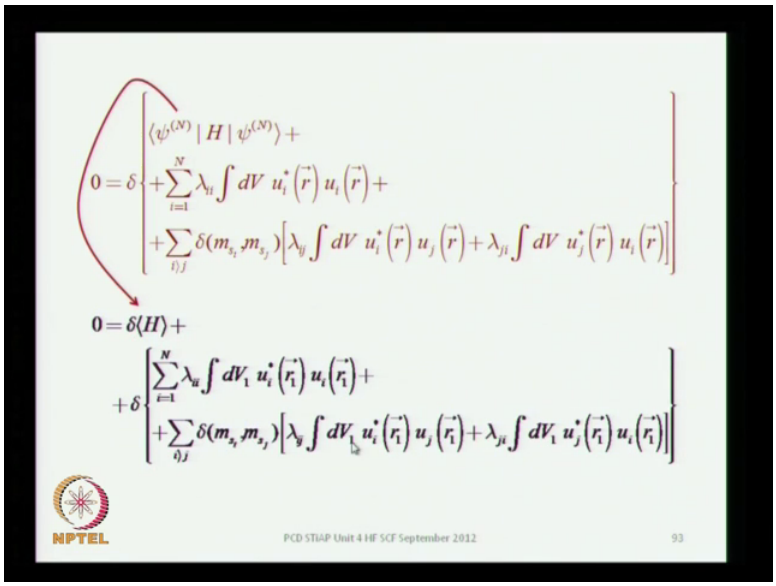

Now, let us include the terms coming from the constraints, say what this terms coming from the constraints this is coming from the normalization constraints, this is coming from the orthogonality of i with j, and this one j with i. These are complex function, and the real part and imaginary part can be varied independently, so you have the lambda matrix generated with which is the Hermetian matrix. And just for brevity have now written this expectation value of Hamiltonian has in this notation which is completely equivalent to this, the rest of the terms are written d r.

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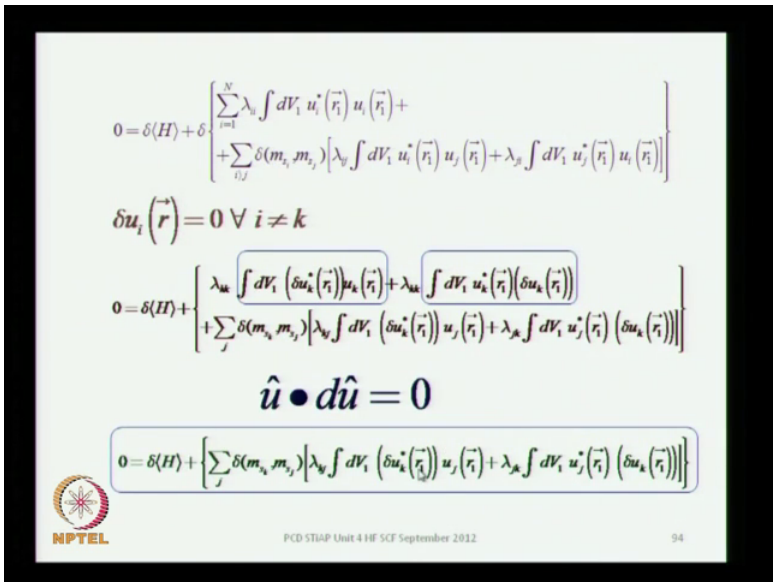

At this is what we have we have got the variation in the expectation value of the hamiltonian, which is the average value, and then to this you must add the variation in the term coming from the constraints. And there are the normalization constraint and the orthogonalitic constraint, we also know that all orbitals other than the k th orbital are not changed, so this is our constraint. So, here you are varying all of this i th orbital, but any variation in i not equal to k would vanish, therefore the terms which you must include are only those for which i is equal to k.

So, here you have got the delta u k star r 1 u k, whenever i is not equal to k the term would vanish. So, out of this n terms you have only one corresponding to the kth term, which is allowed to be varied under the flows orbital approximation all the other n minus 1 orbital are frozen. And therefore, variations in those n minus one orbital would vanish, so this is coming from the variation of delta u k star r 1, and this is coming from the variation in delta u k which is the complex conjugate.

So, there are two terms coming from here, from the variation of this is the product of two function, you must see variation in both, then in the coulomb exchange terms like wise you have only the variation in the kth orbital. So, delta u k star r 1, and then over here you have got the delta u k r 1, this is coming from the orthogonality constraints. So, this is coming from the normalization constraint, this is coming from the orthogonality constraints, and the variations in the single particle the one electron integral, the two electron integral, those are already setting over here.

So, now you have to right all of this term together, now notice that if you look at this terms, this is the variation in the kth orbital, and in the direct notation are in the vector notation this is completely like the inner product of the unit vector on it is change. Delta u k star is a variation, and any variation has to be orthogonal to the original orbital otherwise, it is not a variation at all. For delta u k to be variation, it has to be orthogonal to the original orbital, if it is as a any component along original orbital, it would not even mean a variation.

And we know it from your ordinary vector algebra if you take spherical polo coordinates or cylindrical polo coordinates, any coordinates system you have got this unit vectors which change. From point to point you know that the change in any unit vector delta u is always orthogonal to the original vector, so it is the same idea over here. And these two terms which

represent the norm or the inner product of a base function with it is change this integral would vanish in both of these terms easy, that y also.

So, that simplifies the number of terms that we are working with, and now we can eliminate these two terms, and write our condition as the variation in the expectation value of the hamiltonian. And now you have to worry only about the terms coming from the orthogonalitic constraints, and not from the terms corresponding from the normalization, so that makes our relationship rather simple to be analyzed.

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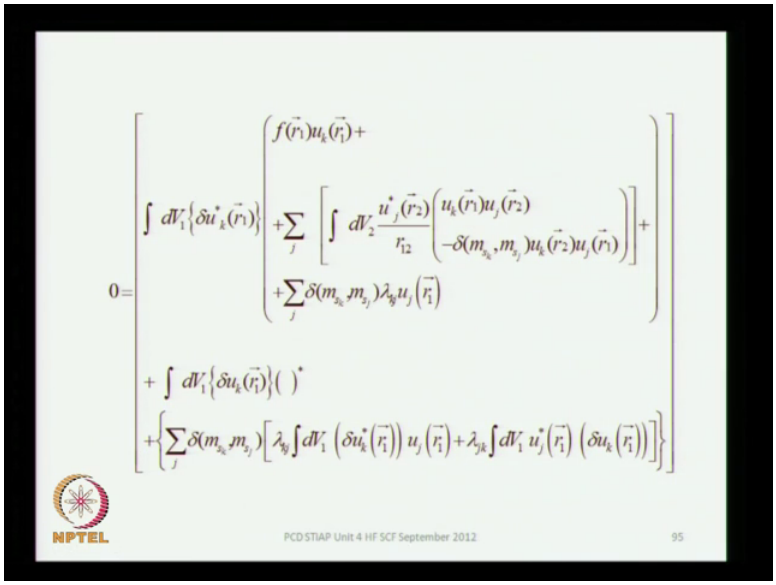

So, let us have a further look at the consequence, we have now combined all those terms these are the basic terms that we work with, so here you have got the terms corresponding from the orthogonalitic constraints. And these are the terms coming from the seeking, the extremum of the expectation value of the hamiltonian itself. Now, everything is here you see all the terms, you have got the one electron integrals, the two electron integrals, and then you have got the constraints, everything is put in.

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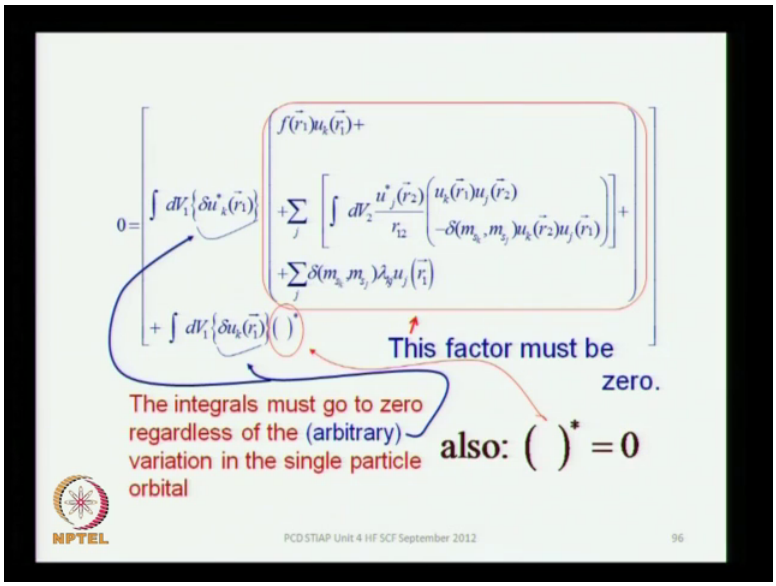

So, let us factor out this terms, and now you have two rather the interesting integral to look at, what is this is a integration over the coordinate 1, this is the orbitary variation in the kth orbital. So, at look at this as a integral of an integrate, the integrate being a product of two factor, one is this factor, and this is the other factor. This is an integration over coordinate 1, integration of what integration of an integrate that integrate is a function of r 1, at that function of r 1 is written as a product of two factor.

One is this, which is in this beautiful bracket, this is the orbital variation in the k th orbital the other factor is what sitting in this bigger bracket from here to here. This is the other factor, this is also a function of r 1 because in this the integration over r 2 is carried out. So, two is a dummy label, once the integration is carried out you have left only with a function of r 1, and you have a similar exercise over here, that you operate on u k r 1 by this one electron operator and you have left with some function of r 1.

So, essentially you are integrating an integrant, which is written as a product of two factors, one of which is an arbitrary variation in delta u, which means that the other factor must vanish. There is no way this integral would vanish, because when you integrant over r 1 the left hand side is 0. So, you must get 0 from this integration, and the only way you can get it is if they other factor is necessarily 0, there is no choice, and this is an important conclusion that you can derive at and this is at very hard of the Hartree Fock formalism.

That our process of seeking the extremum of n electron hamiltonian, in an anti cementrized n electron way function which is the slater determinant. This expectation value would be and extremum subject to the constraint of normalization and orthogonality, if and only if this other factor in the integrant vanishes, because this factor is multiplied by an arbitrary variation no matter what this variation is, this integral must vanish.

So, independence of this factor, you have got the product of two factor, whose integral vanishes mindless of the fact what one factor is, then the other factor has to be 0, so what is inside is red lope must necessarily vanish. Now, this is the conclusion, you can draw from our analysis the one which is complex conjugative, so that will be the other box which will have to be 0.

So, this factor in this red lope must be 0, and what is over here from the other term as you pointing, out this would also be 0 which is just complex conjugative, you have got complex number which must be identically 0. So, it is not surprising, that it is complex conjugative also be 0, and that comes automatically from this analysis, we have already seen that these are complex conjugative of each other. So, both are true and you can walk with either, so this is our conclusion, that what is in this red lope or its complex conjugative must vanish.

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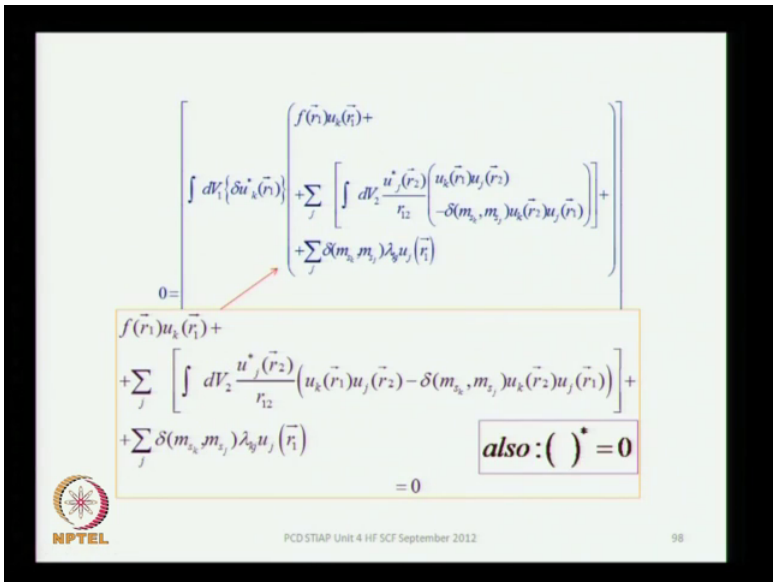

And, let us try this condition, which is subject to the approximation we have employed, which is the single particle approximation, so remember that we have made a certain approximation, in our analysis. This approximation is not completely physically realistic,

because you know that when you vary an orbital your changing the probability amplitude. And therefore, the probability density, therefore the charge density, and any change in the charge density will generate fluctuation in the electron density around it.

So, it is at certain approximation and within the applicability of the frozen orbital approximation, we know that what is inside this red lope must vanish, there is a term corresponding to the complex conjugate which must also vanish. And if this is equal to 0, I take this term to the right side with a negative sign, that is what I have done in the next slide. So, the term involving the variation multipliers is this one, this is the term which goes to the other side of the equation sign with the minus sign.

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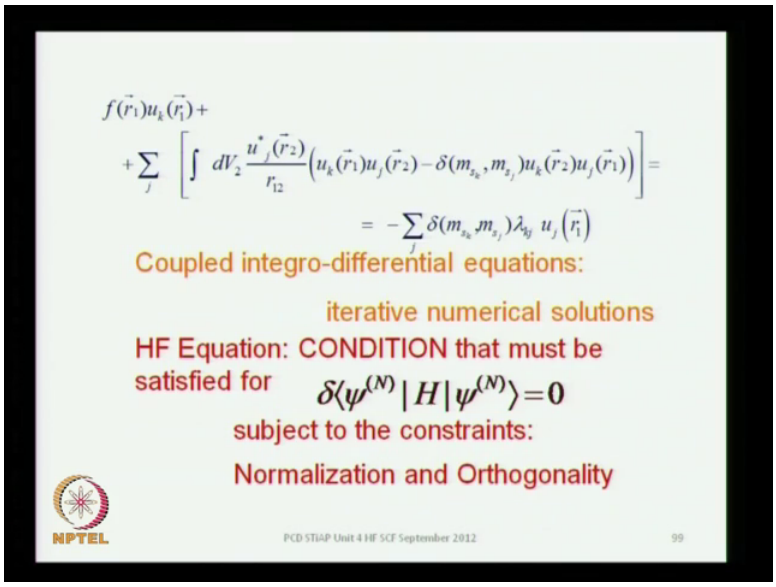

So, that is what is coming on the right hand side, the left-hand side is the remaining terms except for that involving the Lagrange's multipliers, this is the Hartree Fock equation. This equation that you are looking at is what is called as Hartree Fock equation what is it, actually there will be n set equation, because we have written this only for the kth orbital, but k is any index from one through n. So, there will be an equivalent expression for all the remaining n minus 1 terms also, now this is the set of n coupled integro differential equations.

Why coupled, because here you have u k r 1, but you're in this integrant you also have the u j r 2, and these is get summed over j going from 1 through n, so all the other orbital or also included there in some sense. So, these are coupled equation, there are integro differential equation, you can see the integration which is involved there is differentiation is also

involved, because the operator f includes the kinetic energy term, which as got the differential operator.

So, these are coupled integro differential equation, and you can solve them alternatively using numerical methods. So, the Hartree Fock equation are coupled n coupled it is a family of or is a set of n coupled integro differential equations, what do they tell us, their represent the condition that the expectation value the hamiltonian is the extremum subject to the constraint of normalization of each single particle orbital.

And the orthogonality of this orbital with each other, with in the of course, the applicability of the ssingle particle approximation, the frozen orbital approximation, that all the other orbitals, are not varied at it. So, the hartree fock equation emerges has the condition to be satisfied, that this condition must be satisfied that this condition must be satisfied, if this condition is satisfied it is a necessary and sufficient condition if this condition is satisfied you would have achieved your goal.

What was your goal that the expectation value of hamiltonian must be extremum, and that the variations must preserve the normalization and though orthogonality of the single particle orbitals. So, subject to those constraints that the average value of the hamiltonian must be an extremum was our goal, and this goal could be achieved, if this condition is satisfied which is what we call as hartree fock equation.

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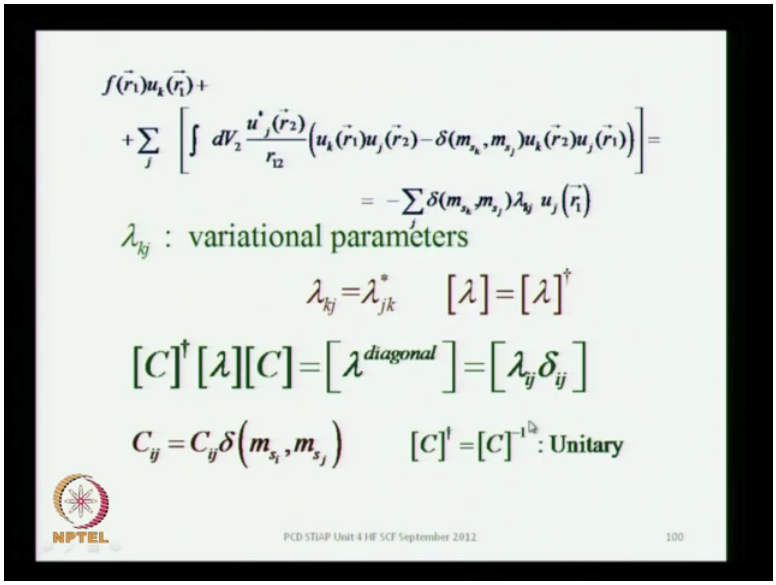

Now, we can simplify this further, because we do know that lambda this variation multipliers are they make up a matrix n by n matrix, which is the hermetain matrix, because lambda k j must be equal to lambda j k star. And therefore, this is the hermetian matrix, if it is hermetian matrix you can find a unitary transformation with diagonal lysis. See you can look for a unitary transformation, which will diagonalysis the matrix of the variation multipliers, that will simplify things further, because in the matrix lambda, you have got n square terms.

And out of this n square terms you really need only n terms, because if you carry out adiagonalizion of a lambda, you have will have non zero elements only along the diagonal, one in each row or each column. And then when you sum over j on the lambda k j, there will be electronical delta, and that will simplify this very significant. So, now, we seek a diagonalizaton and of the matrix lambda through a unitary transformation this unitary transformation is C, so C diagonal lambda C will give you a diagonal matrix.

C diagonal lambda C is a diagonalization process, which will give you diagonal matrix, so that diagonal elements will have a chronicle delta. And the diagonalization what is relevant to the this diagonalization or remember that the orthogonality of the spin part is already taken care of. So, the in dices of C the i and j in dices of C will have nothing to do with spin variable, so implicit to this C i j is a chronicle delta, which guarantees orthogonality of m s i and m s j.

So, it will be orthogonality with respect to other m i s, because that is already taken care of, you are not varying space part of orbital, for a spin part is concerned you already know that the down spin is orthogonal to the up spin.So, there is nothing to vary their there are only two strikes, we also know that this is the unitary transformation, so C diagonal is equal to C inverse.

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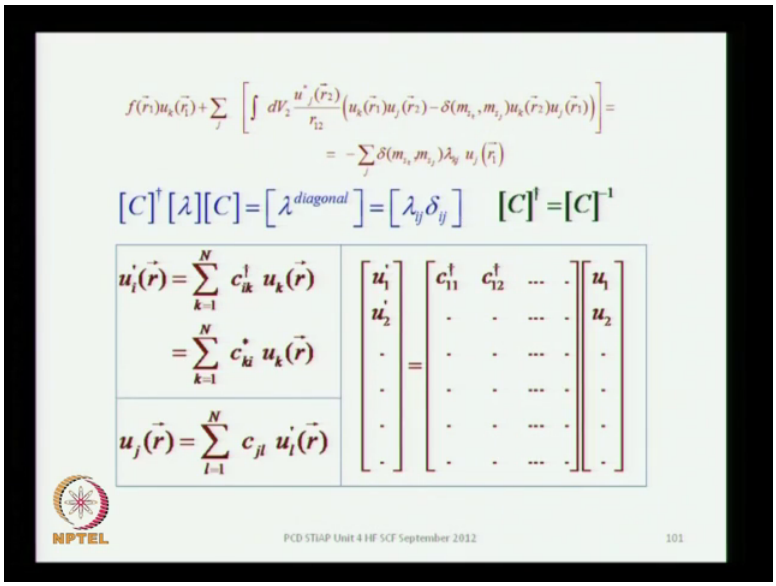

And we can now use this to write this in terms of the bases, in which lambda is diagonal our original hartree fock equation with this year at the top, which emerge as a necessary and sufficient condition. That our expectation value is an extremum subject to the constraints we refer to, this original expression hartree fock equation is in a basis in which lambda was not diagonal.

We can now write it in a bases in which lambda is diagonal, and this basis this is obtained by operating on this unprimed bases by this diagonalizing matrix C, which is C diagonal here. So, C diagonal u will give you the u prime way function, and you can write this in the long form, if you like that every prime function can be obtained has a linear superposition of the unprimed base function.

Because, this will give you a certain basis at, you can always do a linear superposition of this base function to give you new base function, and this is the unitary transformation which will preserve the norms orthogonality. So, you have the invest transformation also, so every u k r 1 over here can be replaced by this summation, and then you will rewrite the hartree fock equation in terms of the primed functions instead of the unprimed function.

So, the hartree fock equation, which appeared as a condition can be rewritten in terms of function, in which the matrix of the variation multipliers is diagonal, so I will let you work that out as an exercise replays each of this unprimed functions by the corresponding prime

function using this inwards transformation. Rewrite the hartree fock equation what will it give you, it will give you an equation in just the primed orbital.

And not the unprimed orbital with the primed orbital are also ortho normal, because you have carried out just a unitary transformation and using the properties of ortho normal functions, you will be able to reduce those multiple sums using the chronicle delta's and you get an equation, which will preserve the form you get an equation in the same form except that it is now primed orbital.

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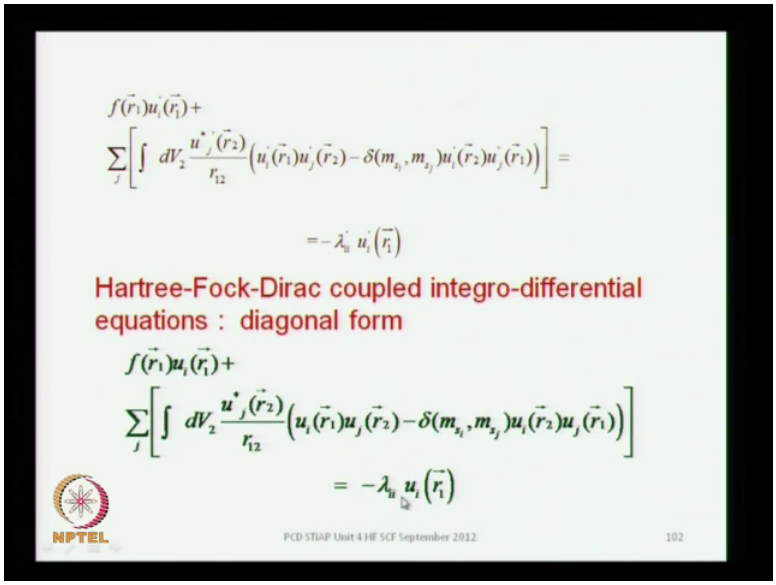

You get an equation completely identical to the previous one except for the fact, that it is now in the terms of primed orbital in which lambda is diagonal, and now why do you need the primes. You need the primes only if you want to distinguish from the un prime in this equation everything as got prime on it, so might have drop it for a simplicity. And having dropped these primes you have this equation, but this is not the original equation that we got, it has the same form, because it has been obtained through a unitary transformation, which preserves the form of the expression.

But, it is now in a form in which the lambda matrix is diagonal, so these are called as hartree fock equation in the diagonal form. Sometime, these are also called as hartree fock dirac, because if the one electron orbitals are not just the spin orbital the two components spin orbital, but even these are four components dirac orbital. You can do this tare analysis an

exactly in same way, an extent this foam formalism from non-relativistic hartree fock, so the relativistic hartree fock which will make the hartree fock dirac formalism.

So, in one go we do the hartrees to the subset to the hartree fock, and we also do the hartree fock dirac are which is the relativistic self consistent feel, which is called as hartree fock dirac. Sometimes, it is very often referred only as dirac fock that will be injustice to hartree, who really set up the whole procedure, so this is called hartree fock dirac. Now, we know that these are the diagonal elements, so the subscripts i and j are equal the row index and the column index both are high for lambda.

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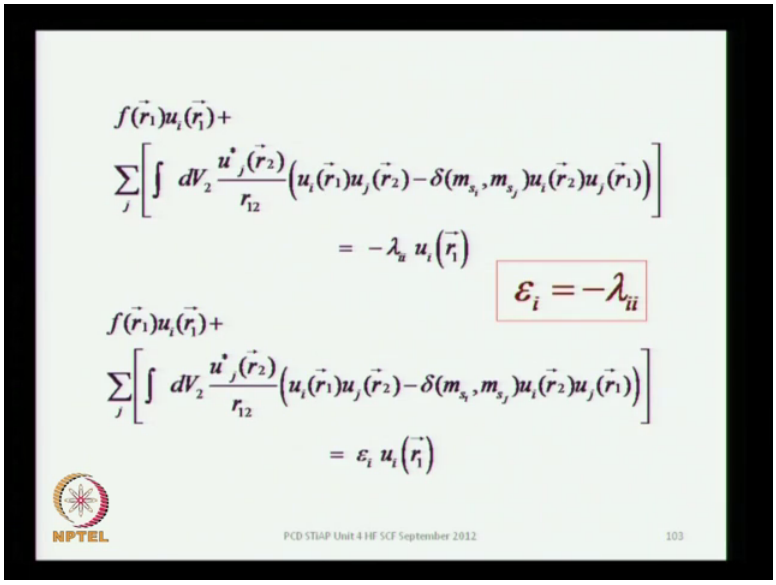

So, you have got the lambda i i on the right-hand side, and since one index is required because the row index and the column index is the sign, you might as well use only one index and we introduce an epsilon i which is minus of lambda i i. So, now, you have an equation which looks to some extent like an Eigen value equation, if you see that way not quite, but it is beginning to look like can diagonal value equation.

You have to be careful because just, because looks like a Eigen value equation does not mean that it has an Eigen value equation, but at least it as got some similarity, and by introducing this epsilon i you write it in a certain simple form. What is this epsilon i, it is the Lagrange multiplier lambda i i it is not the original Lagrange multiplier that we began with, which it is the one you get when you diagonalize original matrix of the lambda multipliers, through the unitary transformation. So, this is the hartree fock equation in the diagonal form, in which

epsilon i takes place of what in Eigen value dose in an Eigen value equation, if this Eigen value equation, let us not assume it is just, because it looks like it, but it is got some similarity with that.

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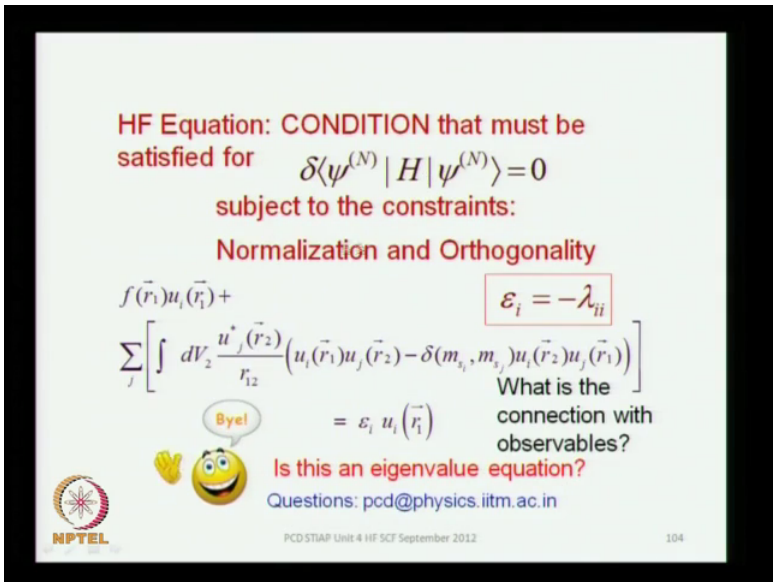

And this is what we recognize as a condition as the necessary and sufficient condition that must be satisfied, now we are going to raise this to questions. One is what is the connection observance, so that all the whole idea of developing a theory is to connect it to experiments to observation that is what physics is about. So, we have done some mathematics, the mathematics that we have done is very elementary all we have done is variation calculates, we have just stated that if you got the function a certain variable.

And if these variables have an extremum then the point at which it is extremum should be such that the tangent to the curve will have 0 slope, that is all we have done. Except, for the fact that we have extended this idea to a function many variables, we are aware that there are certain issue that the mean to be address such as whether this extremum maximum or a minimum or a sidle point. And that point we are yet to discuss we will, but subject to this we have found a way out of catch 22, that the solution.

We are looking for which we did not know how to extract, will result from numerical iterative solution to the n coupled integro differential equations, if we seek iterative numerical solution. If we get solutions in this form and then the question that remains to be answered, and this the two questions actually, many the two important. Questions are what is the

connection of all this with the observations, because that is what the physics is about that is a question will take up in the next class, the other question that I will take up in the next class.

If this is really an Eigen value equation, just looks like this is it an really Eigen value, so you will take up this questions in the next class. And of course, we have two discuss many other aspects of the hartree fock formalism about, whether it is an extremum or minimum or maximum or sidle point, we all we know is that it is a stationary point that it is an extremum, we do not know. And then there are other issues like the consequence, and the implications of the frozen orbital approximation of how good is it and what are it is limitations. So, these are the some of the questions that we will take up for our discussion in the next class, any question for today.

Student: Condition for extremum, and are objective was to find out way function, minimum that we result with the condition which are in the form of n bar integro differential equation matrix form. So, how could we extract way function which will be minimum which will be…

So, you have got n coupled integro differential equation you kick start the process by some trial functions, and then solve them alternatively till you get the self consistency. You understand what is meant by self consistency, this was the original idea that discussed in the context of the catch 22 problem. That your hartree fock equation h i is equal to e psi, where h and psi are respectively n electron hamiltonian and the way function.

Normally, if this was just a single particle problem, you get the psi by solving the differential equation s psi equal to e psi is a differential equation, you know how to solve a differential equation subject to the boundary condition, you get the solution and the problem is done. In many electron problem the operator h requires the solutions, you cannot set up the operator, and less you know what is the solution that was the catch 22.

Now, what they are found out is at this catch 22 is completely equivalent to solving this n coupled integro differential equations, because what has come out as an equivalent criteria. That the solution should be such, that the n electron hamiltonian must have a extremum for expectation value subject to constraints, that condition is represented by the hartree fock equation.

This is the condition hartree fock equation is essentially a condition it must be fulfilled, it is a necessary insufficient condition. Condition for what that the variation in this expectation

value of hamiltonian is 0, subject to the constraints of the normalization and orthogonality within the frozen orbital approximation. So, there will be certain limitations, so we can and we will discuss the scope and the limitations of this frozen orbital approximation.

We will do it in the next class, but essentially we have got a necessary insufficient condition, which is completely equivalent to the statement of the problem itself, so we have restated the problem in a different form, but the original form psi equal to e psi did not give us star. So, how are we going to solve this problem, now we have a star, because the same problem has been posed in an alternative and equivalent fashion, what is this alternative form that the n coupled integro differential equation must be satisfied self consistency.

If you solve one of them, it is not enough the solution to one will disturb the other n minus 1 equations, why will it do, so because they are coupled integro differential equation. You take one solve it, but in such a manner that there is self consistency, that solution to anyone will not disturb the solution to the other. And how would you evaluate this, by setting up some conversion criteria, when you say that it should not disturb the other orbitals.

What it means is that if the other orbitals, are turn out to be different from the original one that you are started out with, then let that change between the previous step. And the next step not be any more than some delta, you can set that to be like 10 to the minus 4 in some units, so 10 to the minus 6. So, 10 to the minus 8 that will be the conversion criteria, that is a numerical criterion, that you will impose, and subject to the criterion you will seek self consistency.

I will like to mention that, at the end of our treatment hartree fock formalism, many years ago this was many, many years ago class of this kind once you did not got interested and she said that let me, how do i set up the hartree fock equation I want to it and solve it numerically. So, she wrote a program and got self consistency feel solution, this was a student in a class exactly like this, so each one of you is capable of doing it, she has done it this was a part of herm s e and we have a copy in a lab.

So, your quite welcome to see that report and you want to try it out welcome, so let it be known that it is something with student at your level in this very classroom actually do it. So, thank you all for today if there is any further question, I will be happy to take otherwise, we proceed from this point in our next class.