Computational Physics
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Lecture – 42
Differential Equation for Quantum Mechanical Problems: Variational Principle
Part 02

So, what we will do is we will use a discrete basis and our choice will be momentum basis defined in a finite box with periodic boundary condition, that is PBC.

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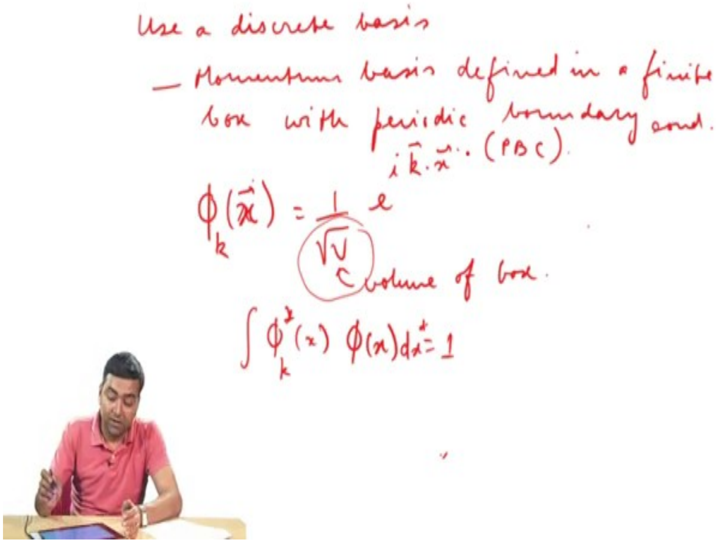

And so, what are the functional forms of this type of basis? So, you can write phi k as a function of x, these are nothing, but my plane waves. So, its e to the power i k dot x and where v is the volume of the, so this v is my volume of the box. And this comes from the normalization constant. So, for example, if I want a normalized value of this phi k here.

So, what I would do is I would take phi squared k x, phi x is constant 1 into integration of d, its d and so if I do that then I will find that my this v, the square root if we see v is the and the square root v that which we get 1 by square root which we get before this e to the power i k x this is just nothing, but the normalization constant. Now, in this basis let us see how the, how our coefficients look like the expansion coefficients C k.

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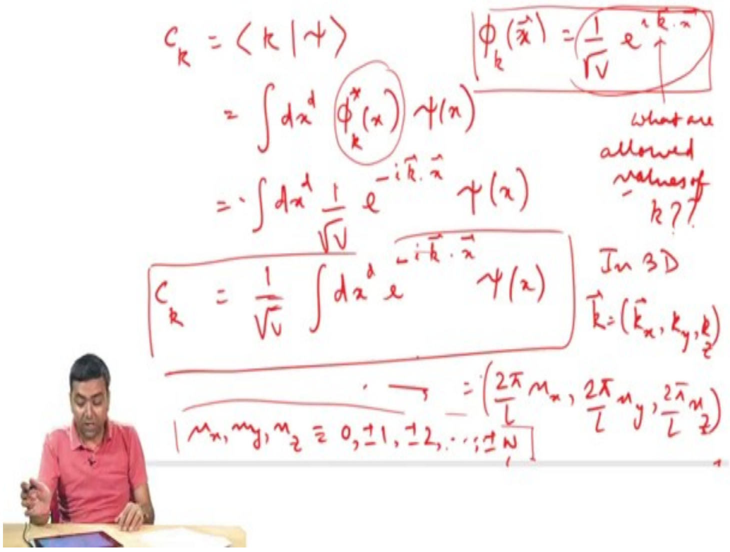

So, what are my C ks? So, if you remember my C ks are given by this function, right. So, what does that mean? That means, is that I need to compute the projection of my wave function on this basis vector k. Now, if you remember my ks are now; so, let me just write down my phi k x is nothing, but 1 by root over v e to the power i k dot x, ok. So, how I compute this? So, this will be, so the k will come as the complex conjugate here. So, it will be phi star k x and then we have psi x, ok.

So, now if I plug in the value of this phi star k x here, so what I will get is the integral over the volume d dimensional volume, 1 by root v e to the power. Now, this is a we have to take the complex conjugate of this particular function. So, that will be to the power minus i k dot x psi x, ok. So, this is written as in this form integration dx d e to the power minus i k dot x psi x. So, this is the value of my coefficient, ok.

Now, since these are discrete basis now the question is what are the allowed values of ks here? So, if you remember, so this function is nothing, but a plane wave, ok. So, now, if I have a plane wave and then I impose periodic boundary condition, so what you can see show is that this case ks you take discrete values and so in 3D the k can take the value of this form k x, k y and k z which is given by twice pi by L n x, twice pi by L n y, twice pi by L n z, where my n x, n y and n z can take values of 0 plus minus 1, plus minus 2 and so on and so forth till plus minus n. So, basically what we have is all possible integers values it can take, the n x, n y and n z.

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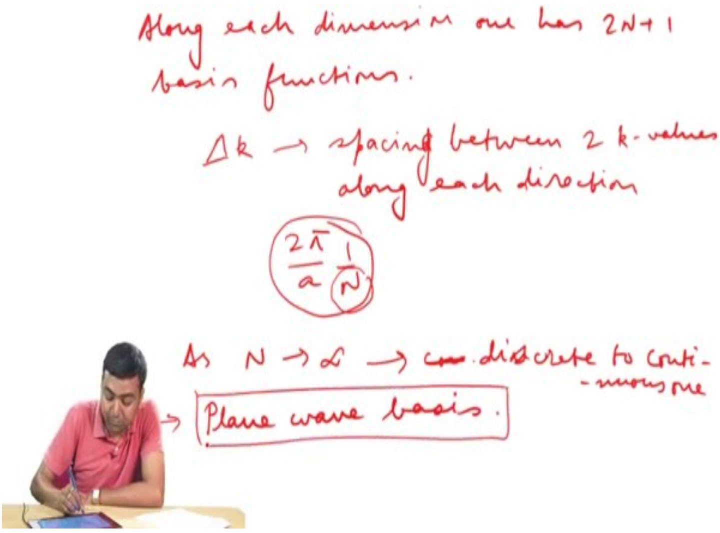

So, what it means is that along each dimension one has twice N plus 1 basis functions. And this also implies, so now the delta, the delta k that is spacing between 2 k values along each direction is given by twice pi by a into 1 by N, right. So, now, you see in this value, so if my N goes to infinity, so that is as N tends to infinity. So, this basis goes from a continuous for sorry from a discrete to continuous one.

And as you might have recalled, so far what we were using is plane waves. So, e to the power i k dot r this is just the functional form of a plane wave. So, this basis is also called a plane wave basis, ok.

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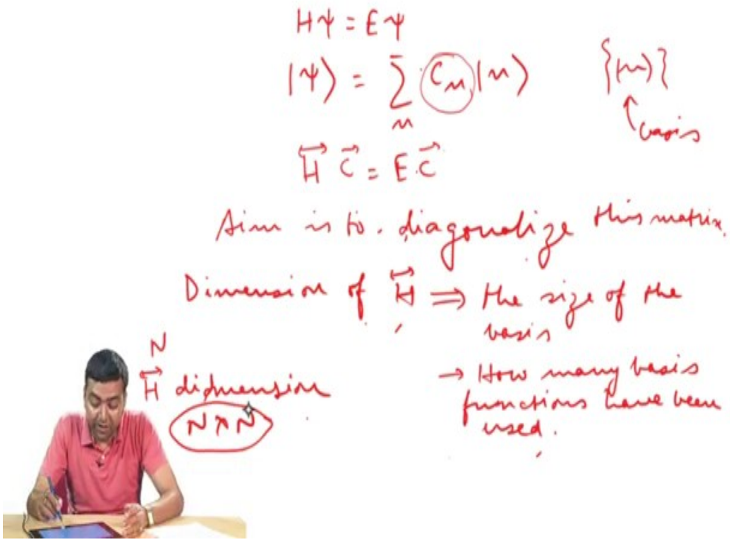

So far what we had seen is we started off with a differential equation which is I mean my Schrodinger equation which is a differential equation and then what we did is we converted it to a N cross N matrix by expanding, by expanding my wave functions psi into a set of into a linear combination of basis functions. So, let me just; let me just summarize what we have done so far.

So, what we had done is we started off with this wave function and then what we did is we expanded my psi as a linear combination of basis functions where my basis is denoted by this one. So, this is my basis and then by taking the projection. So, what we wanted to find was now my unknowns are this C n which are the coefficients. So, if I know the coefficients Cn I can construct my wave function. And to find the coefficients what we did is we projected this Schrodinger equation on to each of the wave each of the basis functions.

As a result what we got is a matrix equation which is of the following form. And now our aim is to diagonalize this matrix. Now, note that the dimension of H this is determined by the size of the basis or in other words what it means is how many basis functions I have used. So, suppose I have used N basis functions then my H has a dimension of N cross N. So, I need to diagonalize this N cross N matrix to find out the (Refer Time: 09:34) eigen values and the coefficients.

So, what we did is we basically converted our problem which was the solution of our differential equation into a linear algebra problem. The reason why one of the advantages of doing it is that we have very efficient matrix diagonalization subroutines which can help you achieve that in a very weaker fashion.

But the drawback of this is that if suppose we are interested in the ground state energy, we will never reach the correct ground state because we always have to truncate our bases at a certain point. And so, our solutions will be closer to the ground state, but we will not we will never reach the exact ground state. Will reach the exact ground state only in the limit the size of my basis goes to infinity. So, then the next question is how does one diagonalize this matrix.

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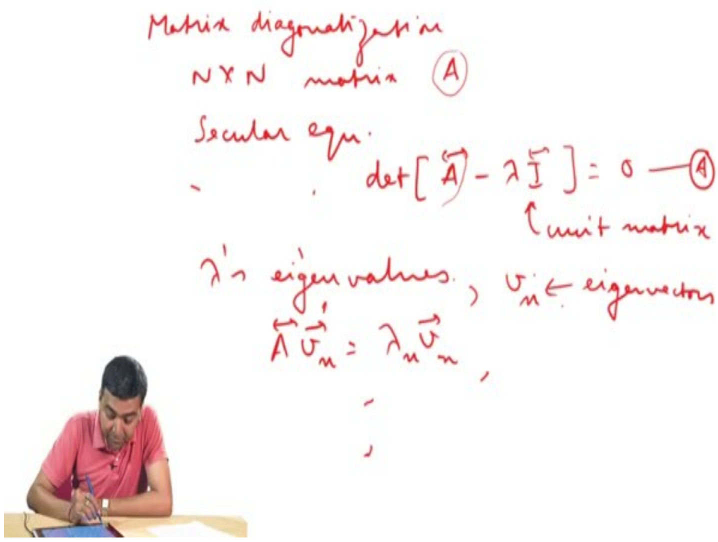

So, we all know that suppose I have a, so matrix diagonalizable, we will talk about matrix diagonalization. So, if I have a N say, I have a N cross N matrix which I am calling as matrix A, ok. So, to diagonalize this what we can do is we can write down the secular equation which is of the form and solve the secular equation, so that is A minus lambda I equals to 0, where my I is the unit matrix and the lambdas are my eigen values.

So, if I denote my eigen vectors as v n, so what I get is. So, basically A v n equals to lambda n v n. So, this I am calling as equation A. Now, usually the dimensions of this matrix A where in our problems, so this matrix has the dimensions of a few million by million of that order, I mean what I mean to say is a very huge matrix and also the matrix elements are quite complicated. If you remember the matrix elements are integral of the product of your Hamiltonian with the where with your basis functions.

So, each of this matrix element of this matrix a here is to evaluate that you need to calculate the integral. So, hence it is a very complex matrix to diagonalize. So, typically what is done is people do not diagonalize the complete matrix. So, rather than what one does is the diagonalization is done in a iterative fashion. So, what I mean by that is the following.

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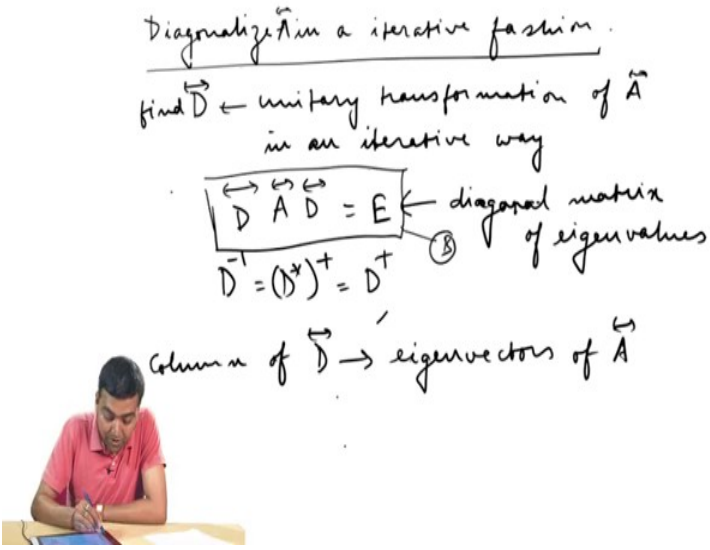

So, what we are going to do is in diagonalize the matrix, diagonalize A in a iterative fashion. So, how this is done is, what you do is instead of diagonalizing the full matrix, so you try to find out a unitary transformation. So, where D is a unitary transformation, what I mean by unitary transformation of A. So, what I, so find D which is a unitary transformation of A in an iterative way. So, what it means is that, so if I write it in this fashion D A D gives me E which is a diagonal matrix of my eigenvalues.

So, the matrix has the following property that is the inverse of this matrix is also happens to be the transpose of the complex conjugate of the D matrix, ok. Then what one can do is one can show that columns of D is basically the eigenvectors of A. So, columns of D contains the eigen vectors of A. So, now, what we are going to do is we are going to show that in a minute stream. So, this equation; this equation I am calling as equation B.

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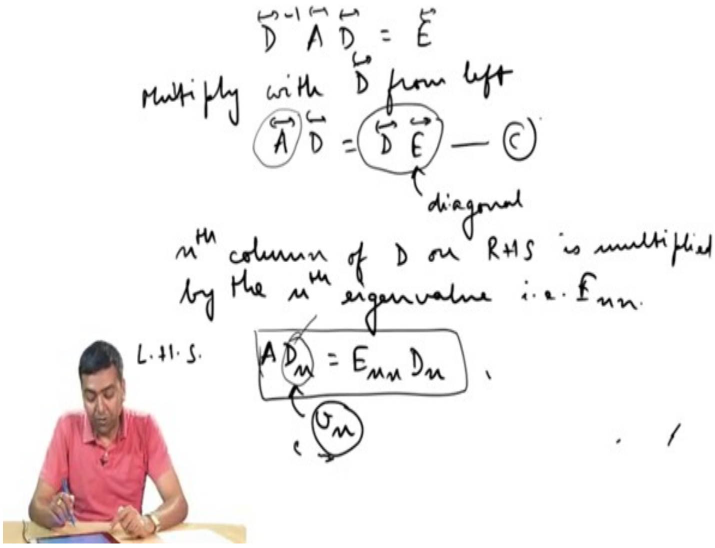

So, I let me start with the equation B. So, what I have is, so my equation B I have. So, let me start with this equation. So, I have D inverse A D this gives me E. So, E is also on entering matrix. Now, if I multiply with D from left, so what I will be getting is A D equals to D E. So, this I am calling as my equation C.

Now, remember this E is my E E E is a diagonal matrix. So, my E you should remember is diagonal because this is my eigen value matrix. So, what it implies is that, what it implies is that the nth column of D on right hand side of this above equation that is on this side is multiplied by the nth eigen value that is E n n. On the left hand side, what do we have on the left hand side?

In the left hand side, the multiplication by A with the nth column of D, so that means, so we have on the left hand side is A D n. So, this is equal to E n n D n. So, or in other words what does this mean? This means that these are my eigen vectors v n, the nth eigen vector v n. So, that is what the point I am just is trying to make is that basically the each column of my matrix D n this corresponds to one eigen vector of the matrix A because now you see we have the this is multiplied by and this has this will become and on the right hand side, ok.

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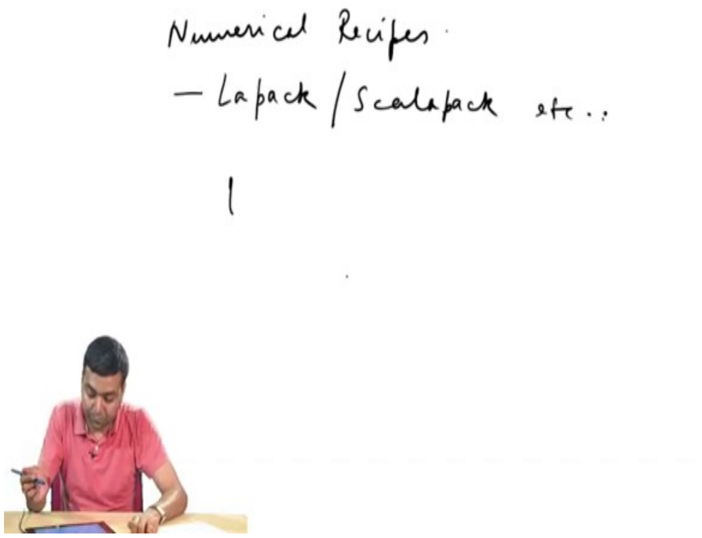

So, now what we need to do is we need to use diagonalization subroutines and to diagonalize that and typically if you look into the numerical recipes book there are lot of subroutines there are for example there is, also there is this lapack, then there is scalar pack which are efficient subroutines which can do the diagonalization problem. So, we will see how to use that with an example now.