Computational Physics
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Lecture – 43
Differential Equation for Quantum Mechanical Problems: Variational Principle Part 03

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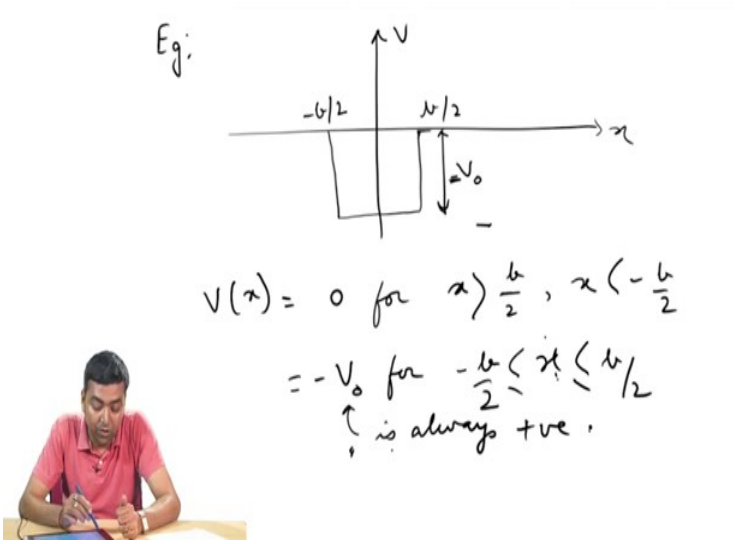

So, let us look into a example. So, what we are trying to solve is suppose we have a so we are trying to find out the solutions to a well known problem which we have seen in our quantum mechanics class. So, we have a potential which is of this form suppose this is my y axis is my potential and this is my x axis. So, we have a potential of this form. So, this is minus b by 2 to plus b by 2. So, from minus b by 2 to plus b by 2 the potential has a form V 0 minus V 0, it is an attractive potential and its 0 at other values of x.

So, what it means is if we write down in general form. So, this means is equal to 0 for x greater than b by 2 and x less than minus b by 2 and is equal to minus V 0 for x lying between minus b by 2 to plus b by 2 ok. Now note that I mean I am talking about an attractive potential. So, I will always. So, my V 0 is always positive. So, this is the potential and I am want to solve the Schrodinger equation for this one dimensional potential using the method using the variational principle.

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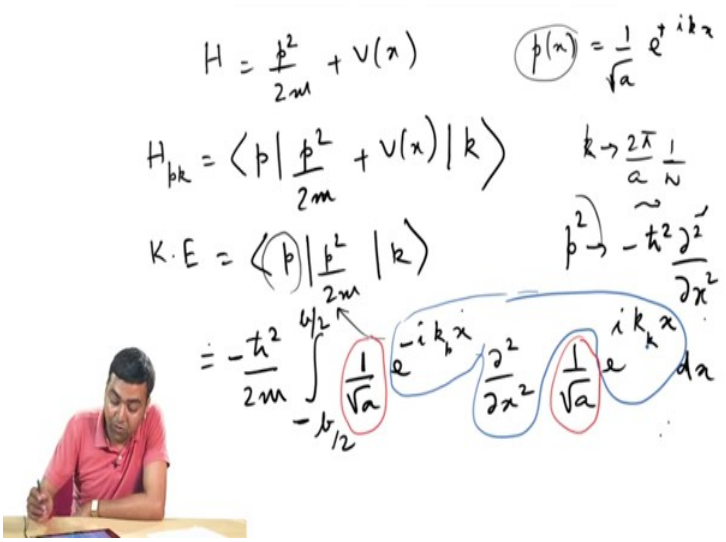

So, what why Hamiltonian is the following. So, why I have my Hamiltonian which is of the following form that is given by p square by twice m plus vx where vx is this potential which is given. Now what I am going to do is I am going to expand my wave functions in a plane wave basis. So, the choice of my basis is I denote my basis function in this fashion. So, I will use a set of plane waves ks where my ks are given by twice pi by a into 1 by n and I will expand my wave function in this plane wave basis.

So, basically what we will do is we need to find out the matrix elements H pk using this basis function. So, what that amounts to is we have to find these terms here these integrals basically. So, this first term here is the kinetic energy. So, let us find the integral this matrix elements for the kinetic energy term. So, that will be p p square by twice m k. Now the kinetic energy operator, so, that is it is a that this p square is given by minus h cut square del, del x 2.

So, if I plug in this p square into this equation here and this form the functional form of p. Here so, I have to evaluate basically the following integral. So, I am taking out the constants outside the integral. So, minus h cut square by twice m is constant and then what I will need to integrate is from the whole length of the box that is minus b by 2 to plus b by 2.

So, this will be the complex conjugate of this function that is 1 by root over a e to the power i, sorry this will be a plus here it is a plane wave e to the power minus i k for that

the basis p x then del 2 del x 2 then 1 by root over a e to the power i k for the k x then d x. So, if I do these integrals, so, if I now if I try to simplify the things what I will get is now this 2 are constants. So, this does not depend on x.

So, I can bring out these two outside the integral. So, what I am left with is the following thing marked with blue. So, I have this function here which depends on x then i have this operator here and then I have this function here. So, if you first operate this grad square operator on this function. So, what we get is the following.

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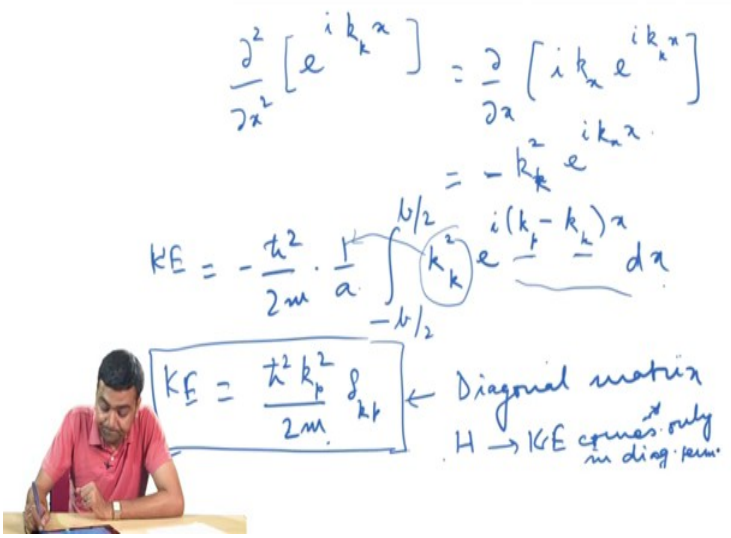

So, I have del 2 del x 2 e to the power i k k x. So, if I do this as operation for the first time what I will get is del del x i k x then again then e to the power i k k x ok and if I do it again on this so, I will get another minus i k x here. So, I will get basically minus k x square then e to the power i k x x.

So, now, if I plug this in my kinetic energy a matrix element for the kinetic energy, so, what I will get is minus h cut square by twice m into 1 by a into minus b by 2 to plus b by 2 k square sorry this will be k k square k e to the power i k p minus k k x d x. So, this integral, so, this again I can bring out of the integral here and this term will give me a nonzero value only if k p is equal to k k because this is integral of a periodic function. And so at the end of the day if i do the algebra what i will get is the following.

So, this is my kinetic energy matrix element here. So, now, if you look at this so, the matrix corresponding to the kinetic operator is a diagonal matrix or in other words in my Hamiltonian the kinetic energy operator the kinetic energy comes only in diagonal terms. Now what happens to the potential energy term? Let us look into that.

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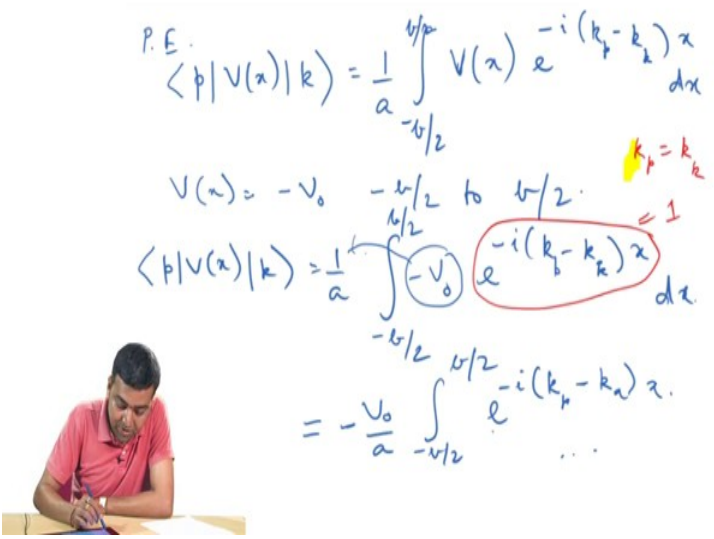

So, the potential energy I can do it in a similar way. So, my potential energy is given by this following matrix elements p V x k. So, I am writing it 1 by a, this comes from the normalization constants under of the plane waves p and k which is each of which is 1 by root a minus b by 2 to b by 2 p x e to the power minus i k p minus k k x d x this is the integral. Now if you remember, so, my V x is equal to minus V 0 for minus b by 2 to plus b by 2. So, I just plug the value of v x here.

So, what I get is p V x k this will be equal to 1 by a integration minus b by 2 to b by 2 minus V 0 e to the power minus i k p minus k k x d x ok. So, this term is a constant. So, this I can bring out here. So, what I will have is this is equal to minus V 0 by a integration of e to the minus b by 2 to b by 2 e to the power minus i k p minus k x x.

So, if we walk out the algebra. So, we will get the following thing.

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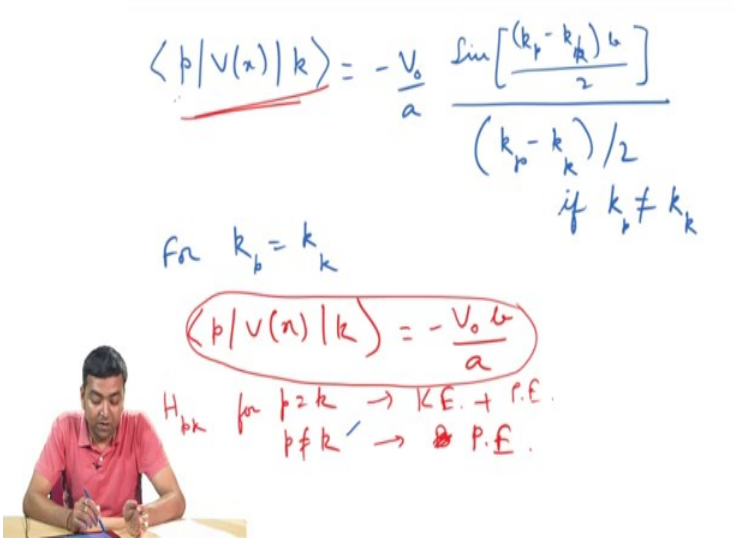

So, we will get. So, note here we will get 2 different terms from the diagonal and for the off diagonal term. So, this, so, if we evaluate the integral. So, what we will get is k p minus k v sorry k k by into p by 2 into k p minus k k by 2. Now this is valid if my k p is not equal to k k. Now if my k p is equal to k k so, for that is basically the two wave vectors corresponding to these two are so, we need to evaluate it in a slightly different way. So, if these 2 are same what happens will that this term here.

So, let me highlight it, so, if my not highlight sorry if we use a different color. So, if my k p equals to k k, so, this term will be equal to 1. So, if i do the integral, so, what I will get is the following; p x k this will just be minus V 0 b by a ok. So, for the matrix elements so, if I have, so, for example, h p k this matrix element for p equals to k will have a contribution from the kinetic energy term plus this term of the potential energy. While for p not equal to k the matrix elements will have only contributions from the potential energy. That is from this particular term here.

So, what we will do is we will now write a program to solve these things.

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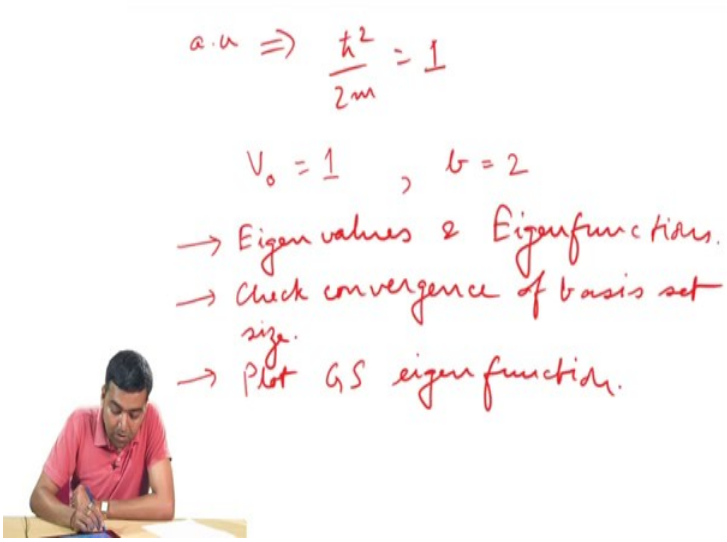

So, in order to just simplify our life so, what we will do is we will use atomic units which what I mean by atomic units is I will assume there is h cut square by twice m equals to 1 ok. So, we I will just use some numerical values of the potential. So, I will use my v 0 to be 1 I will use my b to be equal to 2 and what I will see is so, we need to find Eigen values and the Eigen functions. Now see if I told you that if we increase the size of the basis set in a systematic way then my total energy should always go down.

So, we should check the convergence of basis set size also and we will plot the ground state Eigen functions.

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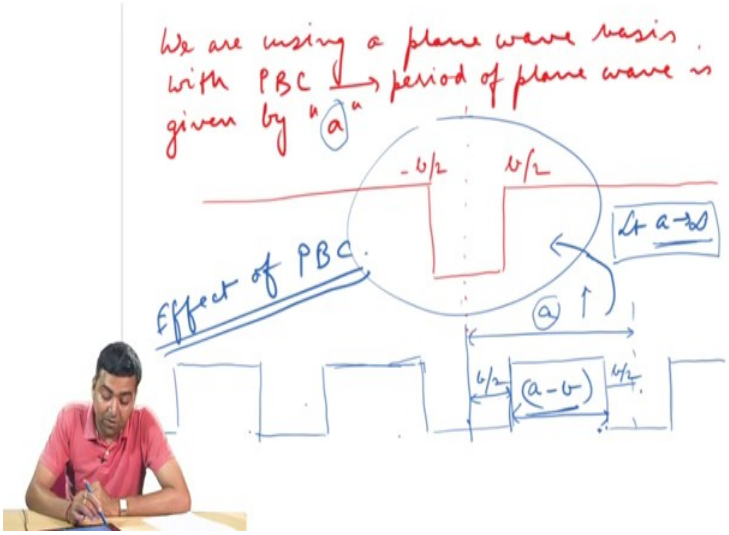

Also another thing here 1 should notice we are using. So, we are using here a plane wave basis with periodic boundary condition whose the period of plane wave is given by a. So, what does this mean to our problem? So, our original in our original problem, so, what I had is a potential which is of this form, this is my minus b by 2 plus b by 2. Now I am using this periodic boundary condition.

So, what it means is that now my potential is getting repeated. So, in my original potential, so, at values of x at any values of x less than minus b by 2 the potential is always 0 and similarly at any values of x when which is greater than b by 2 the potential is 0, but now this is not true anymore. So, what is happening now is I have something like this and so on and so forth ok. So, this distance is my e. So, now, I have a potential which is repeating now this is effect of periodic boundary condition here.

So, for this particular problem this effect is solved this periodic boundary condition imparts a spurious interaction between say this potential here which is present here with its periodic imager. So, we need to also take into a count of this same fact and of this fact.

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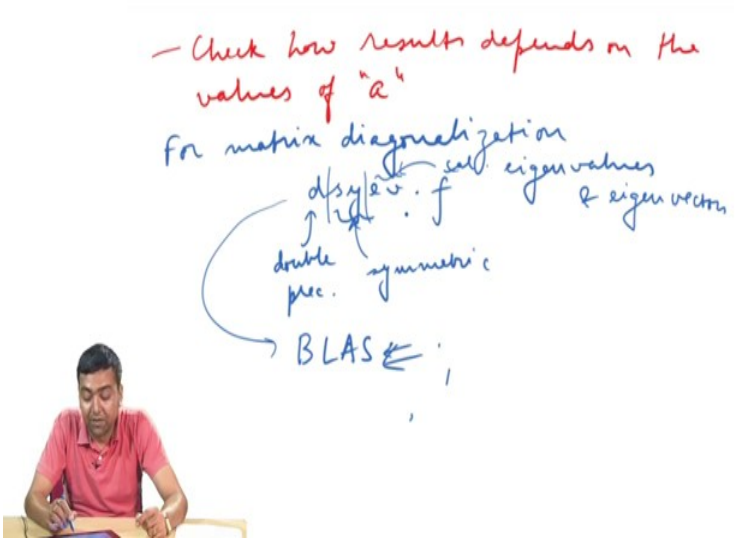

So, in addition to the different things which we need to check here we also need to check how results depends on the values of a. The reason it is important to do is to get the correct physical picture of the problem that is the correct solutions to this particular wave function to this particular potential what we should do is we should start with a value of a and then gradually increase a and in the limit a tends to infinity only this will go to this particular to my actual solution.

So, we should choose I mean that this it is not practically possible to achieve this limit. So, what instead one needs to do is one needs to systematically increase the value of a such that it is large enough that the distance between these 2 periodic images so that is what it basically means is that this was my say b by 2 this is also b by 2.

Then this distance, so, you should choose a such that this a minus b this distance is large enough. So, that the potential here do nots feel the effect of the potential which is generated because of the periodic boundary condition. So, this is something also one needs to be careful of using plane waves as a basis set, but another advantage of the plane waves as a basis set is that, if you look at the function.

So, I can very easily systematically add the I increase the size of the basis set by just increasing the values of the k in my expansion. Now in order to do this thing do the matrix diagonalization you will be needing a subroutine. So, for matrix diagonalization you would be using this subroutine d s y e v dot f. So, this what it means is so, this is a

routine you can find from the LAPACK subroutine. So, d stands for double precision, s y so, this s y stands for symmetric and e v this stands for calculate eigen values and eigen vectors. So, this subroutine also depends on a particle few particular subroutines which is supplied by this BLAS library. So, you need to install BLAS in this in your machine also. And then you can use this subroutine to diagonalize it. So, reason we have chosen to diagonalize a symmetric subroutine with diagonal is the symmetric matrix is because if you look at your matrix your matrix is a for this particular problem your matrix turns to be a symmetric one.