Electronic Properties of the Materials: Computational Approach
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Lecture: 08
Numerov Method: Code

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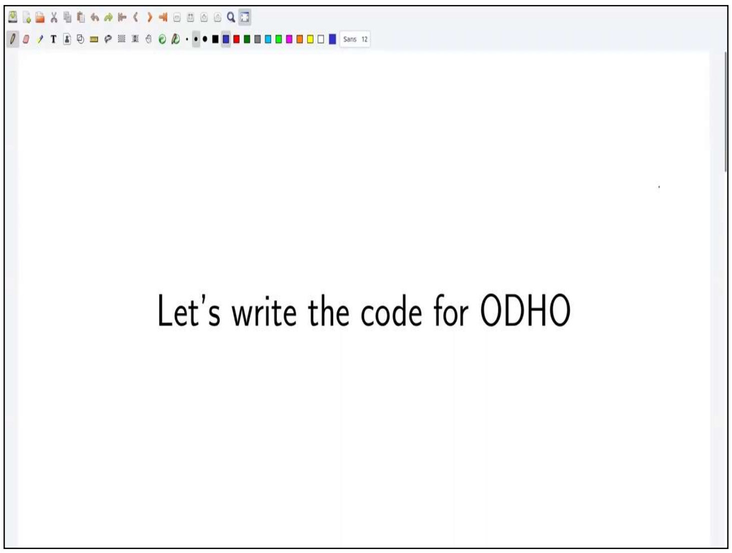

Hello friends in this lecture we are going to learn to write a code to solve energy eigen values and eigen vectors of one dimensional harmonic oscillator. We do a known problem such that we can verify whether the code is correct or not then we can rewrite the code for some unknown potential.

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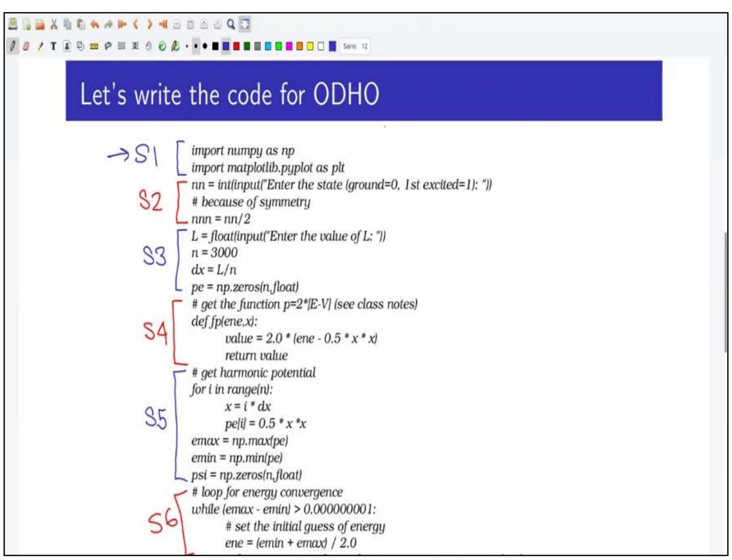

So, first we import the necessary libraries. So, these two lines you see we are importing the libraries. So, we are important two of them one of them is numpy and the second one is matplotlib. So, let us do that just to save some time i am going to just copy paste the relevant portions.

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So, let us import the libraries okay the libraries are important. So, next c step two is to input the number of nodes of the wave function. So, here we are asking the user to input the number of the nodes of the wave function and as mentioned in the class we are solving for a symmetric potential that is why the number of nodes will be half the actual number of loads that means we are only going to solve for psi of x when x is greater than 0 the portion for x less than 0 is automatically known because we are using a symmetric potential.

So, let us copy paste the second portion ok. So, step 3 we define the range of x values for example right we are solving for this wave function psi of x in this section we are defining the range of x and again the user has to input the range of x and then what we do. Now we are defining this entire range in small parts for example if this is the range of x say from 0 to l what we do is we just subdivide this in small values equal to delta x or dx okay.

So, in this case for example we have divided it in 3000 small such parts such that dx is equals to l by 3000 and this is where we are defining some array to hold the values of potential energy. So, let us put this part in our code okay. So, we are done with this next is step four here we are just defining the function you remember that we need a function which is like p of x p of s x is equals to 2m by h cross square and E - V of x what is given to us given to us is V of x and we will assume some value of E.

And then if we do that then we can define this function p of x and what we will do is that we will take m is equals to h cross is equals to 1 such that we just have 2 times E - p that is equal to t. So, this is what we do. So, this is how we define a function. So, we are defining a function the name is f of t and this function will be called with the value of energy and with the value of x and then this function will return this value okay which is equal to 2 into E - and in this case b is 0.5 x square right.

The potential energy for harmonic oscillator V x is equals to 0.5 times x times x right. So, this is like energy and this is the potential energy part okay. And then once we call this function with the value of energy and the value of x the function will return the value of t. So, let us put this part in our code okay. So, this part is done okay next is part 5 here we get the harmonic potential and we are just storing the value of harmonic potential in some array this array was already defined here right we already defined the array here.

So, now we are just putting the values in this. So, you see right potential energy again V of x is given by 0.5 x square this is what is being stored in the array and then you remember that we have to find range correct E min and E max. So, this is like E min and this is E max okay and the actual value of energy must lie within this range. So, the actual value of energy will be somewhere here in this range correct.

So, this is where we define the range of energy. So, how do we do that so E max is taken to be the maximum value of potential energy. So, you see this function this is some in build function which is available in this numpy library right. So, that is what right E max is equals to np dot max. So, max is the function. So, that will find the maximum value of the array and this will find the maximum value of this array E.

So, E max we are assuming to be the maximum value of the potential energy and similarly E mean we are assuming to be the minimum value of the potential energy and again this function min which is available in the numpy library it will find the value of minimum value of the array in p ok. And then we just define here some array which will hold the eigen function okay. So, let us put this part in our code okay.

So, we actually forgot this part also. So, we have to copy this part yes this is what we have to copy. So, getting the harmonic potential as well as setting the minimum and maximum value of the energy range. So, next is we are going to start the loop for example you can take a look at here. So, what we have done is we know the energy range we have set the energy range between E min and E max okay.

And then what we do is we just take the actual value or the guess value of energy the initial guess to be the average of min and max and we start a loop because we know that we need a loop iterative loop to find the value of E. So, this is where we start the loop and then we will just do the iteration as long as the energy value does not converge. So, let us start the loop.

So, this is where we just start the loop and we will come back to this you see that we are starting a while loop we will just come back to this point later but let us see the other parts. So, step seven is we have to set the initial values of psi step seven we set the initial values of okay. So, we know that the odd function right how does the odd function look like if this is x equal to 0 the odd function will start like this.

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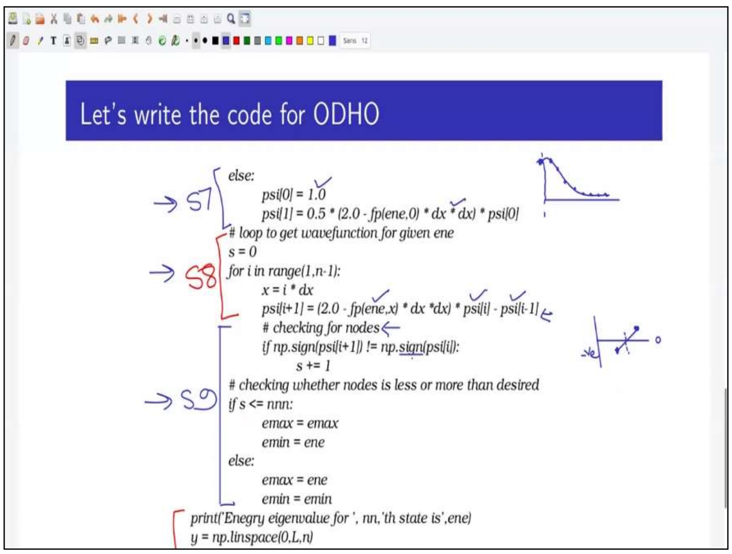

So, this is some odd function correct which has node at x equal to 0. So, that means the odd function will be having a node it will cross this point at x equal to zero. So, that is why here we set the initial values we should set the initial values we need two initial values of the wave function and then we set them the initial values. So, we know that one of the initial values will be zero if we are dealing with some odd function and the second point will be somewhere here correct.

So, this is what is set here and we know that in case of some even function what we do is there is no node at x equal to zero. So, the even function will look something like this right there is no node at x equal to zero. So, in case of even function the initial value we said to be equal to one and then some other small value okay. So, let us put this part in our code. So, we set the initial values here okay done. Next step eight.

Now finally we apply numerous formula in step eight correct. So, now we have set the initial guess value of energy we have set the initial values of the wave function depending on whether this is like given function or odd function. Now finally we can use the Numerov's formula and starting from these two initial points what we can get is that we can get the all we can get the wave function in all these points right.

And we just have to use the numeral formula for that which has been used here. So, psi i + 1 is equals to 2 - f p E n E x. So, what is this is just we are calling this function we have defined here okay we have defined some function over here yes at this point and we are calling that function from this point in the code and then this is multiplied by d x square star like psi of i - psi of i - 1.

So, this we can start from two initial conditions and so on. So, we use this formula to get the entire wave function. So, let us put this in our code. So, okay look to get the wave function for the given energy come out of this l slope okay. So, this is what is done. Now next is step nine. So, we have solved for the y function correct. Now we have to see whether we are getting the correct wave function or not.

And how do we do that in step nine what we do is that we check for the number of nodes of psi we just obtained if. So, this is where we check for the number of nodes of psi and we use some function called sine. So, if the wave function is changing side correct. So, for example what do we mean by y function is changing sign. So, say I have some node at this point. So, that means left of the point the wave function is negative correct and right of that this point the wave function is positive.

So, that means the wave function is changing sign the wave function is crossing this zero line okay. So, this is how we are going to find whether the there is a node at some point or not. So, you see here we are checking. So, this is some function again that is available in this numpy library that is this function called sine. So, it will just tell you whether it is the sign is positive or negative and then we check the wave function every point of the wave function.

And if the sign of the point at ith point and i + 1 point if the sign is not equal right if the sign is not similar then we know that there is a node. So, we count that node okay and then we count all such nodes as such that we can get the total number of nodes from this portion of the code ok. So, now once we have found the nodes then we have to find whether the number of nodes is less or more than the desired.

Because initially we have set the number of nodes how many nodes we want that has already been set initially. So, now in this portion what we do is that we check for this and then if the number of nodes that the wave function is having if it is less than the desired number of nodes then what do we do that means I have less energy because the number of nodes are less. So, that means in that case for example I started with this E min and d max correct and say the actual energy is here.

And the first guess value was yeah. So, that means the guess energy is less than the actual energy that means I have to increase the energy that means I have to push the immune value up. Similarly if say the actual energy is here and my guess value of energy which is average of mean and d max which is here right. So, in this case we see that we will find the number of nodes to be more than the desired number of nodes.

And in that case what we have to do is that we have to reduce the energy that means we have to push the E max down. So, this is what is being done here if number of nodes is less than the desired then we push E min up and otherwise if it is more then we push E max down. So, let us put this part in our code. So, we check for nodes and then change things accordingly okay. So, we are done with this code. Now let us just check this.

So, we also have put this part which is like the output plotting etcetera. So, now after this step what we do is we go back to this step right because we are running a while loop right. So, from this point what would happen is that we will just go back okay. So, we go back to the start of the loop okay. So, we go back to this point correct and then we have again like reset the value of E min and E max correct.

So, that means we will again have this E max - E min and if the value of E max - E min is greater than this value then this loop will again run okay. So, since this is a while loop this loop will keep on running as long as this condition is being satisfied the moment E max - E min becomes less than this the loop is going to stop automatically we know that for harmonic oscillator the energy is given by E n is equals to n + half h cross omega and we have chosen the units in such a way that this value is equal to 1.

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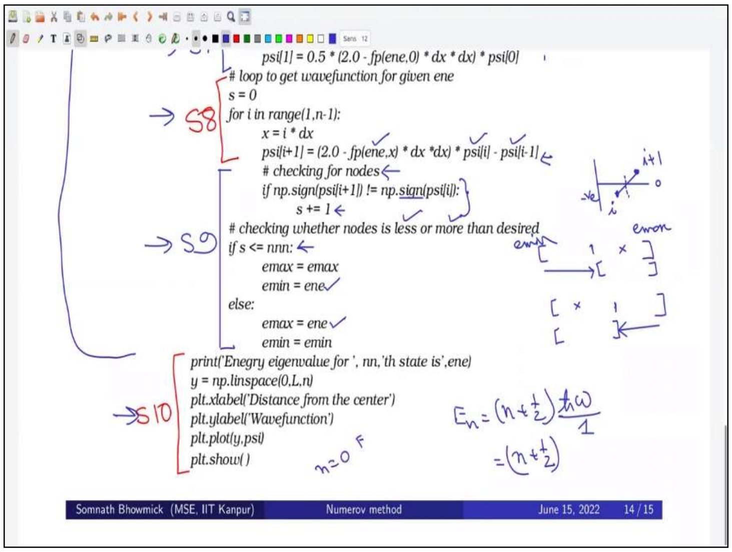

So, that means energy will be just n + half and if we put n equal to 0 then. So, you put n equal to 0 you get is this is the ground state the ground state energy is 0.5 you put n equal to 1 E is 1.5 n equal to 2 equal to 2.5 and so on. Now let us run the code and check whether we are getting the correct energy eigen values or not. So, it is asking for the number of nodes of the wave function for ground state we enter 0 and then it is asking for the value of l.

So, let us enter 4 and. Now the ground state energy eigenvalue is 0.5 which is matching with the analytical result and the blue curve is the probability density for the ground state next let us run it for the first excited state. So, we enter one for the first excited state and the value of l we enter four the energy eigenvalue for first excited state is 1.5 which is again matching with the analytical result and the blue curve is the probability density of the first excited state.

N ext we enter the number of nodes and now we are going to do it for the second excited state that means we have to enter 2 and the value of l we enter 4 and finally we find that the energy eigen value is 2.5 which is matching with the analytical result and the blue curve is the probability density for the second eigen state.

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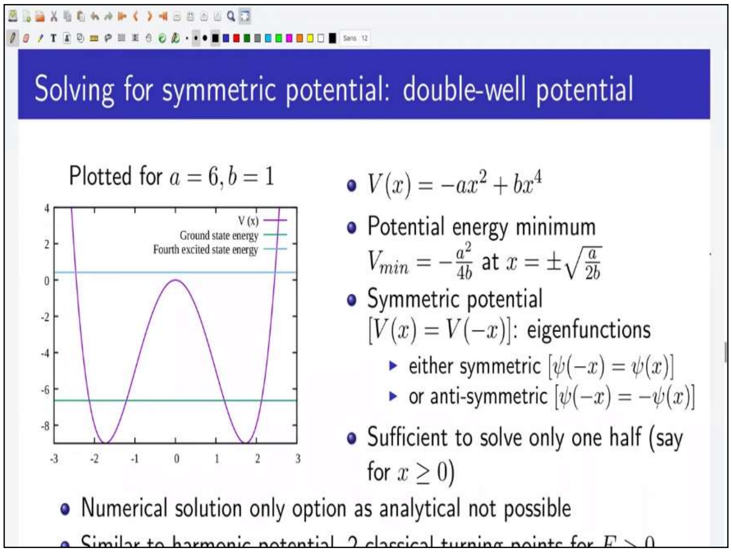

Thus we have written a code and verified that the numerical results are matching with the analytical values for harmonic oscillator. Now we are going to write a code for double well potential for which analytical solution is not available. The potential energy is given by V of x is equals to - ax square + b x to the power 4 we are going to use a value of a equal to 6 and b equal to 1 in our code.

Most of the code remains as it is the only changes we have to make is to account for the change of the potential energy function. So, we take a equal to 6 and b equal to 1. Now we redefine the function p because now the potential energy has changed. So, now we enter the correct potential energy a star x to the power 2 - d star x to the power 4. Next we also have to define the potential energy. So, - a star x to the power 2 + b star x to the power 4 rest of the code remains as it is.

Now let us run the code and find out the energy eigen values and eigen functions the code is asking for the number of nodes of the wave function for ground state we under 0. Now it is asking for the value of l and let us enter 3.5. So, the energy eigen value of the ground state is -6.642 and this is how the probability density of the eigen function looks like let us run it for the first excited state.

So, in this case the number of nodes is equals to 1 and we again enter the value of l to be equal to 3.5 and the energy eigenvalue is -6.6406 and the blue curve is showing the probability density of the eigen function. Let us run for second excited step and again enter the value of l to be equal to 3.5 and we find that the energy eigen value for the second excited state is -2.4511 and the blue curve shows the probability density of the energy eigen function.

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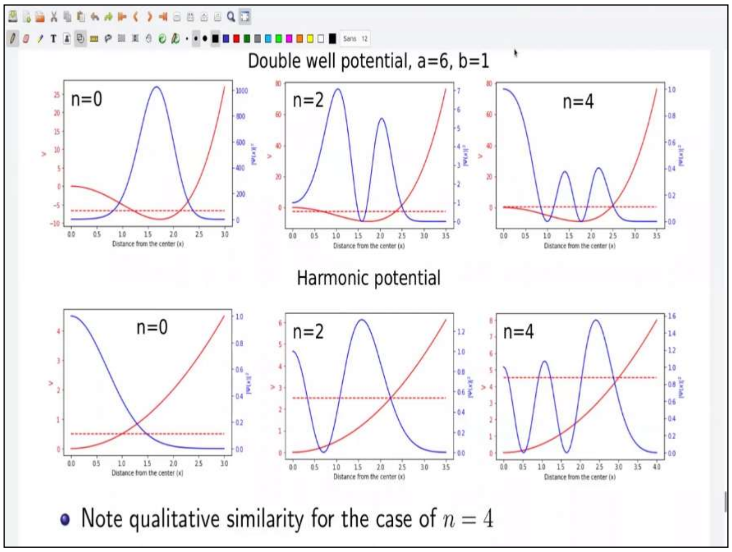

Let us compare the results obtained for double well potential and harmonic potential. The first row shows the plots for double well potential and the second row shows the plot for the harmonic potential the solid red line is the potential the dashed red line is the energy eigen value the blue line is the probability density of the eigen functions. Note that qualitative similarities for n equal to 4.

The eigen function has two nodes one here one here and similarly for the harmonic potential the eigen function has two nodes one here and one here. So, there are two more nodes for x less than 0 which is not shown here. At x equal to 0 the probability density is comparable for both the double well potential and the harmonic potential for n equal to 2 both the eigen functions have a node for x greater than 0.

The node for the double well potential is here and the node for the harmonic potential is located here there is one more node for x less than 0 which is not shown here. However the probability density at x equal to 0 is significantly less in case of double well potential than compared to the harmonic potential similar trend is observed in case of the ground state wave function probability density at x equal to 0 is significantly less in case of the double well potential than compared to the harmonic potential.

To understand the difference let us find the number of classical turning points in both the cases. For n equal to four both double well potential and harmonic potential has one classical turning point. The classical turning point is the point where the energy shown by the dashed line becomes smaller than the potential energy shown by the solid red line in case of double well potential this is the classical turning point.

And in case of harmonic potential this is the classical turning point. Classically a particle cannot go beyond the classical turning point and it turns back quantum mechanically a particle can penetrate in classically forbidden region provided the potential is finite. But the wave function decays exponentially in the classically forbidden region. In case of n equal to 0 and n equal to 2 harmonic potential is still having only one classical turning point.

For example in case of n equal to 2 this is the classical turning point and in case of n equal to 0 this is the classical turning point. However double well potential has one more classical turning point than that of harmonic potential. For example double o l potential for n equal to 2 has a classical turning point close to the center and another classical turning point which is away from the center.

Similarly for n equal to 0 double well potential has one classical turning point close to the center and another classical turning point away from the center. Since the wave function has to decay exponentially in the classically forbidden region it looks different in case of double well potential near x equal to 0o because there is a classical turning point near x equal to 0 in case of double well potential which is not there in case of harmonic potential.

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