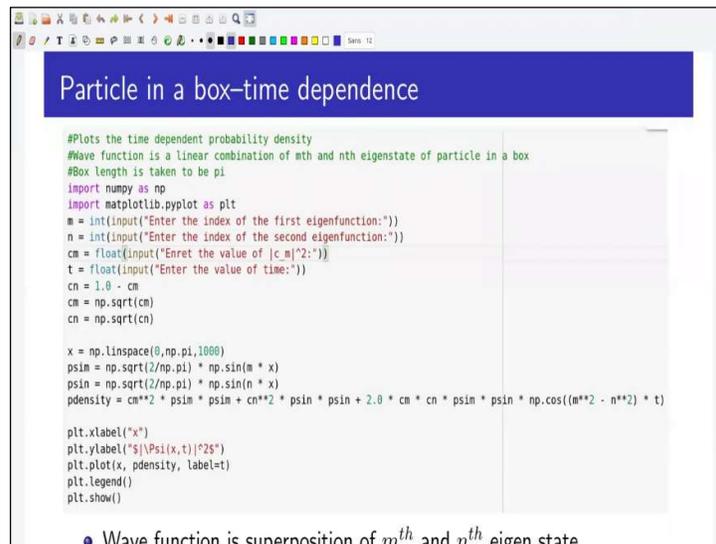**Electronic Properties of the Materials: Computational Approach**
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Lecture: 06
Visualization Using Python (Part 2)

Hello friends in the previous lecture we have worked out some examples of visualization and simple analysis with python. In this lecture we are going to continue on the same topic and solve some more examples.

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So, far we have seen only examples of stationary states let us work out a time dependent problem where the wave function is a linear superposition of mth and nth stationary state. The constants c m and c n satisfies this condition we take the eigen functions of particle in a box with box length l equal to pi. We define frequency omega by dividing energy with h bar. Now the probability density P x t is given by psi star psi and for this given wave function the probability density is this let us try to understand the code.

So, in this code the user has to define the value of m and n here and the user also has to mention the value of c m square the value of c n square is calculated in this step and the user also has to mention the time at which the probability density is going to be plotted. Then we define the

wave functions here and the probability density is defined here finally we plot the probability density here let us look at the code and crq examples.

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So, for example in this region the code will ask the user to input the index of the first and second eigen function and then in this line the code will ask the user to input the value of cm square and the value of cn square is calculated here and the value of time at which the probability density will be plotted ah needs to be mentioned here then we define the mth and nth eigen function here and the probability density is defined here finally we plot the wave function using these commands.

So, let us run the code and generate a few outputs so the code is asking for the index of the first eigen function let us enter 1 then it is asking for the index of the second wave function let us enter 2 that means we are calculating the superposition of the ground state and the first excited state. Now the code is asking for the value of cm square let us enter 0.99. So, cm square corresponds to the first wave function then it is asking for the value of time.

So, let us plot the probability density at initial time that is t equal to 0. So, this is how the probability density looks like let us use some other value again we enter the index of the first wave function as one the second one as 2 and the value of cm square. Now we enter a small value last time we entered 0.99. Now we enter 0.01 and again we plot it at initial time. So, this is how the probability density looks like.

You see that the probability density changes a lot depending on the value of cm square we enter. Next we enter the first eigen function to be equal to 1 the second one is 2 and. Now we use this value 0.5 and initial time that is time t equal to 0 and this is how the probability density looks like. Using the python code we have generated 3 plots of probability density at t equal to 0 let us try to understand in detail.

The probability density is given by this expression. So, if we put time t equal to 0 this term cosine will become equal to 1 and P x 0 is given by this expression we take m equal to 1 and n equal to 2 that is the ground state and the first excited state since c 1 square plus c 2 square is equals to 1 c 1 square equal to 0.99 implies that psi x t is very close to the ground state. On the other hand c 2 square is equals to 0.99 implies that psi x t is very close to the first excited state.

If you look at the probability densities it is indeed very similar to the ground state and similar to the first excited state. On the other hand for c 1 square equal to c 2 square equal to 0.5 the wave function is a 50 50 mixture of the ground that first excited state. Let us run the code to get the probability density at various time. So, we use the ground state and the first excited state and cm square is equal to 0.5.

So, at time t equal to 0 this is how the probability density looks like you see that there is a large peak in the left hand side of the box. Now we use the same wave function that is m equal to 1 and n equal to 2 and c m square is 0.5. Now the time is equal to 1.0472. So, this is how the probability density looks like note that the peak of the probability density has shifted towards the right hand side of the box let us do it for some other time.

So, I keep the wave function same and ah only change the value of the time to 2.0943. Now again you see that the peak of the wave function has come back to the left hand side of the box. We use the code to plot the time dependent probability density for a wave function which is a 50 50 mixture of the down state and the first excited state eigen functions. If we do it for some other set of values this is how the plots will look like let us try to understand the output produced by the code.

So, we know that for c1 square equal to 0.99 the wave function is similar to the ground state. So, in this case the peak of the probability density is located just left of the center of the box at P equal to 0. Now at t equal to pi by 3 the peak moves to just right of the center of the box and again at t equal to 2 pi by 3 the peak moves back to the initial position. For the first excited state like wave function there are 2 peaks initially the left one is higher than the right one at time t equal to 0.

At time t equal to pi by 3 the higher peak moves to the right hand side of the box and then it comes back to its initial position at time t equal to 2 pi by 3. For the 50-50 mixture there is a large peak in the left hand side of the box which moves to the right hand side at time t equal to pi by 3 and then it moves back to its initial position at time p equal to 2 pi by 3. Let us try to understand why does the wave function come back to initial position at P equal to 2 pi by 3 the time dependent term in probability density is cos 3 omega 1t.

Let us take omega 1 is equals to 1 in that case at t equal to 0 cos 3t is equals to 1. Similarly at t equal to 2 pi by 3 cos 3t is equals to 1. Thus it takes P equal to 2 pi by 3 to complete a cycle and come back to the initial state. Since probability density is a function of time position expectation value should also be a function of time let us investigate that. For a given probability density the position expectation value is calculating by evaluating the integral numerically let me explain the code.

The user has to insert the values of m and n here the user also has to insert the value of cm square and the value of cn square is calculated in the next step. A function is written here which defines the eigen states calculates the probability density and finally calculates the integral to get the position expectation value at some particular time. Then we divide the total time in 1000 steps and run a for loop to get position expectation value at every time step.

The function to calculate the position expectation value is called 1000 times using the volume finally we plot the probability densities. Let us run the code and see some output this is how the code looks like these are the input variables this is the user defined function that will calculate the integral to get the position expectation value and this is the for loop which calculates the position expectation value at different time and this is where we plot the position expectation value let us run the code.

So, we take the same wave function that is the ground state and first excited state. So, first we run it for our value where c1 square is equals to 0.99. So, this is how the plot looks like the black line is the position expectation value for the stationary state and the blue line is the position expectation value where the wave function is given by the superposition of 2 stationary states. Next we run it for a value where c1 square is equals to 0.01.

And this is how the position expectation value changes as a function of time finally we run for a value of cm square is equals to 0.5 and then the blue line shows how the position expectation value is changing as a function of time. We have generated the position expectation value for 3 different wave functions using a form let us try to understand the plots. The first plot is for a wave function somewhat similar to the ground state because c1 square is equals to 0.99.

The blue line shows the time dependent position expectation value the black line shows the position expectation value for a stationary state for particle in a box position expectation value

is given by x n is equals to l by 2 for any n. Since the wave function is very close to a stationary state function the blue line does not deviate from the black line which represents the stationary state. Similarly the third plot is for a wave function similar to a stationary state in this case the first excited state note that it is exactly same as the first plot.

Because the position expectation value is same for any stationary state it does not matter whether this is a ground state or first excited state. In the second plot the wave function is a 50-50 mixture of the 2 eigen states in this case the blue line deviates significantly from the black line which represents the stationary state. If we define position uncertainty as the difference between the maximum and minimum value of position expectation value that is delta x is equals to x max minus x mean.

For example in this case the x mean is here and x max is here and in the second case the x mean is here and x max is here thus we see that delta x in case 2 is higher than that of case 1 and case 3. So, in this case delta x is low in this case delta x is high and in the third case delta x is similar to the first case and delta x is low. Let us now discuss about harmonic potential. Consider a particle rolling up and down in a harmonic potential the blue line represents the potential energy which is minimum at x equal to 0.

As the particle moves away from the minimum potential energy increases quadratically from the minimum classically the particle turns back and slide downward from the point where the potential energy exceeds the total energy this is known as the classical turning point. We can get the classical turning point from the energy eigen values. For example take n equal to 0 such that E of n is equals to half thus the particle has to turn back when potential energy is more than half.

Now the potential energy is given by half x tilde square. So, if we equate these 2 half x tilde square is equals to total energy for the ground set is equals to half and then from this equation we see that the classical turning point is plus minus 1. Similarly we can get the classically allowed region for excited states. For example for n equal to 1 the classically allowed region is from minus of square root 3 to plus square root of 3 and for n equal to 2 the classically allowed region is from minus square root of 5 to plus square root of 5.

So, if we think classically then the particle cannot go beyond these points. However quantum particle go in classically forbidden region. Let us find this out using a counter. Let us divide the probability density in 2 regions one in the classically allowed region and let us call it P of A and then the second one is the probability density in the classically forbidden region and let us denote it by P of f and P of f is equals to 1 minus P of A.

To calculate the probability density within the classically allowed region we have to evaluate this integral where xcl is the classical turning point. We know that x l is equals to 1 for ground state that is n equals to 0 this is equal to square root of 3 for the first excited state and this is equal to square root of 5 for the second excited state. Let us try to understand the code first we define the wave function.

And then we check that whether it is normalized or not by calculating the integral of probability density all over the space this should give you a number equal to 1. Next we calculate the integrated probability density within the classical limit and then we plot the wave function to show the classically allowed and classically forbidden region let us run the code and see some output.

So, this is how the code looks like this is where we check the normalization and then this is where we calculate the integrated probability density within the classically allowed and classically forbidden region and this is where we plot the wave function. So, let us run it. So, first we are running it for the ground state and then you see this is the wave function the probability density for the ground state wave function.

And these red vertical lines these are the classical limit thus the probability density outside the classical limit for the ground state is 0.157. Next we run it for the first excited state and you see that the integrated probability density outside the classical limit is 0.1 this is less than the ground state value. Similarly if we run it for the second excited state this is what we get the probability density outside the classically allowed region decreases further.

Let us try to compare the plots for ground state and few excited states some of the way functions are listed here in case of ground state area under the curve in the classically forbidden region is 0.1573 this is equal to the area marked here. Similarly the area under the curve in the

classically forbidden region for the first excited state is 0 point triple 16 and for the second excited state this is equal to 0.0915.

Thus probability density in classically forbidden region decreases with increasing value of n thus one can conclude that the particle becomes more classical at higher energy. We already have learned that plane waves are eigen functions of free particles. If we combine several plane waves then we get a wave packet. Let us try to understand the consequences of adding many waves.

For example we take many cosine waves and combine them to get some wave packet given by psi of x is equals to sum over n cos kn of x.

We take n equal to 20 that is we are going to calculate psi of x is equals to cos k 1 x + cos k 2 x + cos k 20 x we shall vary the range of k values that is delta k from 0.1 to 1 to 10. This implies that k values will lie between 1 and 1.1 in the case of delta k equal to 0.1 it will lie between 1 and 2 in the case of delta k equal to 1 and it will lie between 1 and 11 in the case of delta k is equals to m.

Let us try to understand the code. The user has to insert the value of n max that is the number of waves we are going to add and the value of delta k the range of k values then we have one user defined function which will return the value of cos kx for a given value of k and the given value of x. Finally using a for loop we calculate the sum of all the cosine waves and we plot psi of x here.

This is how the code looks like we have to input the number of waves and the range of k here and then we have some user defined function that returns the value of cos kx for a given k and x. Then we have a for loop to calculate the sum of cos k n x for a range of n and finally we plot the wave function here let us run the code for some values. So, it is asking for the number of waves.

So, we enter 20 and range of k we enter 0.1. So, this is how the wave packet looks like. Now we again enter the number of waves to be equal to 20 and the range of k is equal to 1 and this is how the wave packet looks like. Number of waves equal to 20 and the range of k equal to 10

and this is how the wave packet looks like. Analyzing the output we find that psi of x for small delta k is wavelength.

For example see the plot of psi x for delta k equal to 0.1. On the other hand psi x becomes particle like for larger values of delta k for example the plot of psi x for delta k is equals to 10. For a particle like psi x the position is localized in space that is the position of uncertainty delta x is very small. However small delta x comes with large delta k thus we can write that delta x is inversely proportional to delta k.

This is similar to the Heisenberg uncertainty principle. We can plot the of packet in real space and k space. We know that energy of a particle is a function of 2 variables position and momentum. Real space is related to the position variable similarly k space is related to the momentum variable the wave function in real and k space can be written in these forms. Thus if we know psi of x we can evaluate phi of k and vice versa.

We can switch back and forth between real and k space by a Fourier transform if we take a Gaussian wave packet psi of x then the k space is also a Gaussian function for example this is how the wave packet looks like in real space this is a Gaussian function. Now we can use this equation to find phi of k and if we do that then we find that phi of k is also a Gaussian function. The spread of the packet in real and k space is given by delta x and delta k and they follow this equation delta x delta k is equals to half.

Let us write a code where we vary delta x and delta k and see how does the wave packet look like in real and a space. So, this is how the code looks like the user has to insert the value of delta x and then in the next line we calculate the value of delta k and then we define the functions in real space and in k space and then we plot them. This is how the code looks like the user has to insert the value of delta x in this step and then we calculate the value of delta k in this step.

Here the Gaussian wave packet is defined in the real space and the Gaussian wave packet is defined in the k space in this step finally we plot both the wave packets. Let us run the code for some values of delta x and delta q. So, it is asking for the value of delta x and we enter 0.5 and then this is how the wave packet looks like the blue one is in the real space and the orange one is in the k space. Note that the x scale and y scale is arbitrary in this plot.

Let us run for some other value of delta x let us enter 1 and then this is how the wave packets look like in real space and in k space. Now let us enter the value of delta x to be equal to 2 and then this is how the wave packets look like the blue one is in the real space and the orange one is in the k space. Comparing the plots we can conclude that when delta x is small the wave packet is localized in the l space but spread out in the k space.

For example look at this figure the value of delta x is equals to 0.5. So, the wave function is relatively localized in the real space and it is spread out in the k space. On the other hand when delta x is large the off packet is spread out in the real space but localized in the k space. For example look at figure 3 in this case delta x is 2 and then we see that the wave function in real space is really spread out and the wave function in the k space is somewhat localized. Thus more precise is the position of a wave packet less precise would be its momentum and vice versa this is related to the Heisenberg uncertainty principle.

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