Time Dependent Quantum Chemistry

Professor Atanu Bhattacharya
Department of Inorganic and Physical Chemistry
Indian Institute of Science, Bengaluru

Module: 03 Lecture: 21

Fourer Transform of a wavefunction

Welcome to python tutorial 3 of the course Time Dependent Quantum Chemistry. In this tutorial, we will go over Fourier transform of our function, if I have a wave function already defined on the screed numerically, then how to get the Fourier transform of that wave function, we need to do this Fourier transform of our function in many occasions particularly while solving while finding out the numerical solution to that TDSE. So, we will go over it.

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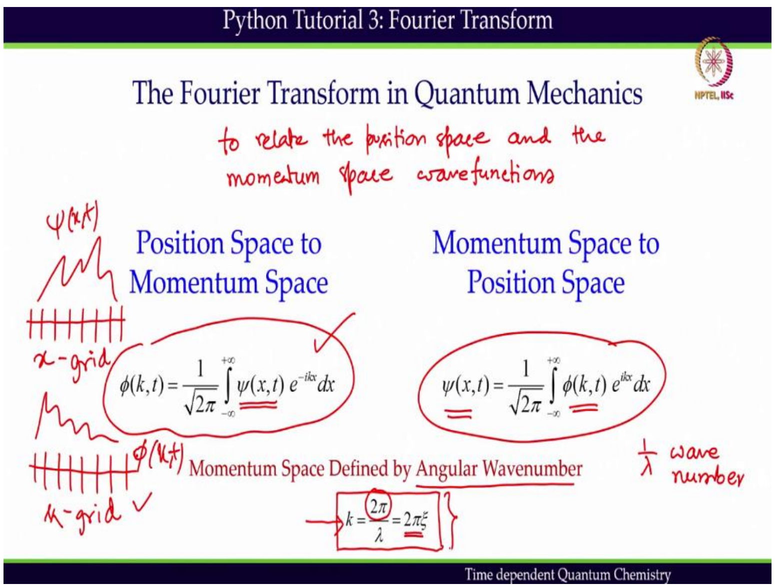

In quantum mechanics, the Fourier transform is used to relate the position space and the momentum space wave function. So, I have to by doing this Fourier transform what we do in quantum mechanics particularly very frequently to relate the position space and the momentum space wave functions.

So, position space so, if we want to convert from position space. So, in the position space, we know that we are expressing the wave function $\psi(x,t)$, and if we want to convert it to momentum space, so, this is the equation which we use

$$\phi(k,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \psi(x,t) e^{-ikx} dx$$

this is the Fourier transform equation we use to for the forward Fourier transform.

On the other hand, and we know that this kind of wave function in position space in the programming language they can be presented in the grid representation. So, we will see how to do that. So, this is your X-Grid in the X-Grid you have an wave function defined that is the $\psi(x,t)$ and if we want to convert it to momentum space.

Which means now in the momentum space, it is going to be the same number of grid window. So, the same grid window which means number of elements should be the same, but now, this is your X-Grid and this is your k-Grid, k-Grid is representing the momentum space and in the momentum space.

We have to find out what would be the representation of the wave function and this is going to be $\phi(k,t)$. So, position to momentum space Fourier transform and then inverse Fourier transform will give me again momentum space to position space. So, one can convert these two representations very easily by doing this Fourier transform.

The position space represents the x-space, which is the coordinate space and momentum space represent the k-space where momentum space this k is defined by $k = \frac{2\pi}{\lambda} = 2\pi\xi$,which will see why the definitions are like that. And we know that $\frac{1}{\lambda}$ is a wave number. And because it is wave number and it is multiplied by 2π .

That is why this k is considered to be the angular wave number. So, angular wave number is presenting the momentum space which is nothing but $2\pi\xi$, ξ , will see that it is the frequency component which we are presenting here. So, the meaning of this equations or representation will be cleared in the next slide.

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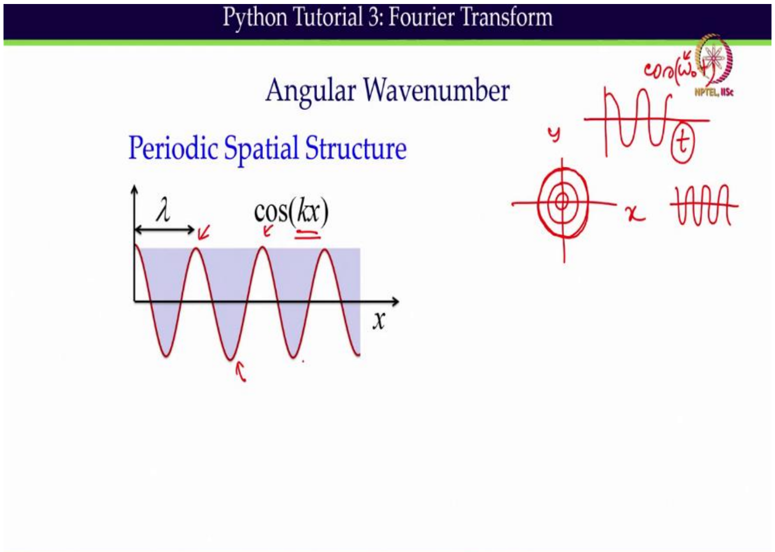

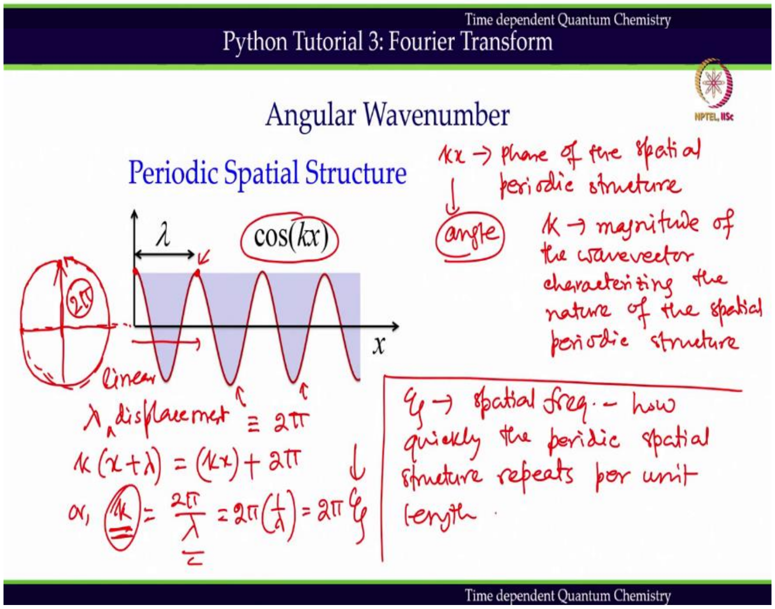

Let us assume that I have a periodic spatial structure we are familiar with plane wave in time and plane wave is represented by $\cos(\omega_0 t)$ like this and we know that this is the angular frequency which is showing part second, how many angular cycles you have. And how quickly it is actually changing the variation in the t-axis.

Similarly, in the spatial structure when you have a spatial structure one can think about, if it is a 2-dimensional spatial structure xy, then one can think of periodic variation. So, where this line positions are actually the higher position it is more like on the x-axis it is now going to be like this.

So, let us say there is an hill and then there is a valley, then there is a hill then there is a valley, this is the wave periodic structure is changing on the space and if I have the change, then the change is controlled by how quickly the change is happening that is controlled by this k value. So, this periodic spatial structure can be represented by this simple cos (kx).

And if we can represent by cos(kx), then (kx) represents the phase of the so, this (kx) is going to be the phase of the spatial periodic structure it is called space and phase is nothing but an angle so, this is representing an angle and this is why k this k is representing the magnitude of the wave vector characterizing the nature of the periodic structure this periodic structure not in time domain it is in the space domain. So, this is a spatial periodic structure. What we can note here is that, if we have a λ linear displacement this is equivalent to 2π phase shift. So, this linear displacement along this direction can be correlated with an angular shift.

So, what we can see here this point this arrow is now making 2π angle once this is making 2π angle I am actually moving from here to here. So, this linear displacement can be conveniently represented with respect to what is term phase advancement I have in terms of angle. So, if it is so, then I will be able to write down $k(x+\lambda) = kx + 2\pi$, 2π phase extra phase I am adding or in other words, I can simplify this equation as $k = \frac{2\pi}{\lambda}$.

So, what we are seeing is that k is the magnitude of k is related to $k = \frac{2\pi}{\lambda}$ which is nothing but 1 by lambda this is 2π this ξ notation to represent this spatial frequency. So, this ξ is called spatial frequency which is representing how quickly the periodic spatial structure repeats per unit length we remember that in the time domain we have used ν as the frequency.

But here in the spatial domain we are using ξ as a spatial frequency. So, if we have that then what we see is that this k is related to these spatial frequencies ξ and how to get the spatial frequency we will over it. So, and this k is representing the momentum space in quantum mechanics.

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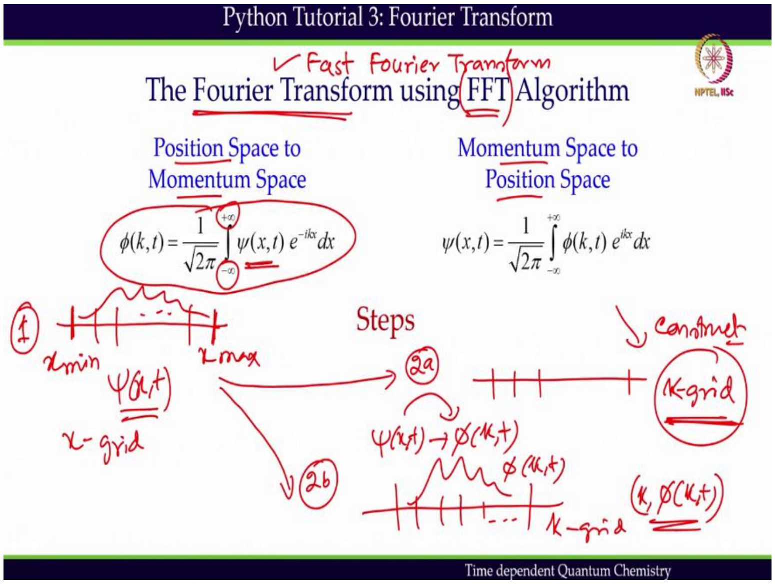

So, what will do here in order to convert this from position space to momentum space and momentum space to position space which is the inverse Fourier transform, we will make use of an efficient algorithm it is called Fast Fourier transform algorithm this is called so, numerical implementation of Fourier transform through Discrete Fourier Transform it is called Fast Fourier Transform.

So, this is the algorithm which we use FFT algorithm to transfer this function. So, basic idea is that this is an analytical expression and one cannot use this kind of analytical expression, we have to define we cannot use this minus infinity to plus infinity limit, we have to always think about finite limit.

So, in the finite domain, we will say that x has a minimum value and x has a maximum value. And this is the grid which we create first and, on this grid, will represent $\psi(x,t)$ and we know that how to represent this $\psi(x,t)$, once we present that $\psi(x,t)$ in the position space, so, this is the space step number 1.

How we are going to do perform this Fourier transform with the help of Fast Fourier Transform algorithm. So, first we have to represent the wave function in a finite grid and we know how to select those finite grid in when you are selecting the finite grid, we have to make sure that the at the boundary of the grid the wave function should go to 0.

And because we cannot use minus infinity to plus infinity limit in the finite grid in that numerical method. Now, once we have represented the wave function in the X-Grid, then all we need to do is that there are two things we have to find out there are two points we have to take care. First point is going to be we have to now create the k-Grid and on this k-Grid will be representing the wave function Fourier transform Wave function.

So, we have to construct the k grid that is the second step and another step we have to consider is the Fourier transform that wave function and then present it. So, I have to Fourier transform, so, $\psi(x,t)$ has to be converted to $\phi(k,t)$ this has to be converted and this on this constructed k-Grid, we have to now represent this $\phi(k,t)$.

And when we are constructing this k-Grid, we cannot just randomly construct the k-grid, there is a particular protocol or particular restrictions we have for the Fourier transform of the grid and that we will go for very soon. But, the bottom line is that we have to follow two different steps first we have to convert the X-Grid to k-Grid.

And then we have to convert the function which is the Fourier transform to the k-grid and then we can plot this as x and y. So, it is going to be now k versus your function is k t. This is what we can plot. So, this is the basic idea behind this entire procedure of Fast Fourier transform algorithm.

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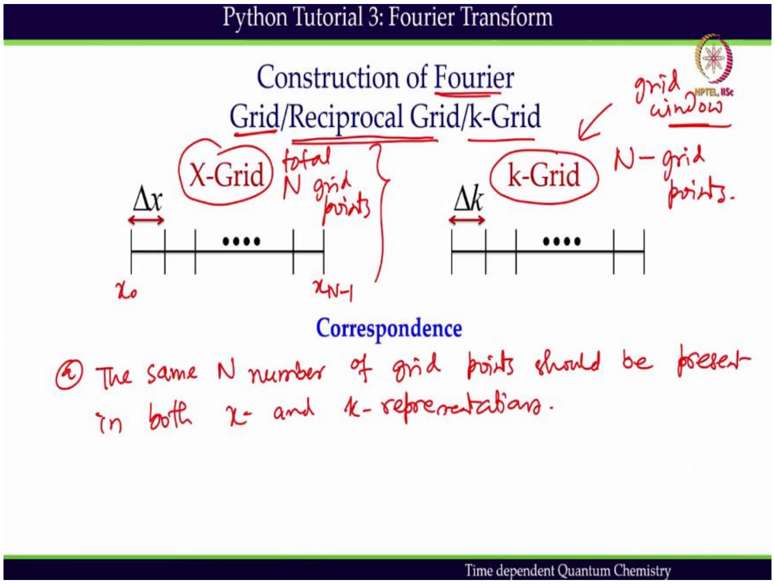

So, let us look at the construction of the fourier grid or reciprocal grid or k-Grid, they are synonymous and often we use reciprocal grid to represent the k-Grid or fourier grid. So, what we while constructing this, the k-Grid first we will first note down and interesting correspondence between the x-domain and k-domain.

So, this is your x-domain, which we have to create and we know how to create x-domain with the help of arange functionality of scipy. And, while we are constructing the k-Grid, we have to follow a particular procedure. So, what are the correspondence we have between this X-Grid and k-Grid the first correspondence is that the same N number of grid points should be present in both x and k representations.

So, in the X-Grid when you have presented the X-Grid, let us say this is starting from x0 and this is going to x N-1 which means that I have N number, N total N grid points we have in the X- Grid. In that case, when will be constructing the k- Grid, I should have the same grid window it is called grid window which means that the same number of grid elements we should have. So, this is going to be N number of grid points. So, that is the first correspondence, we have understood when we are converting X-Grid to k-Grid.

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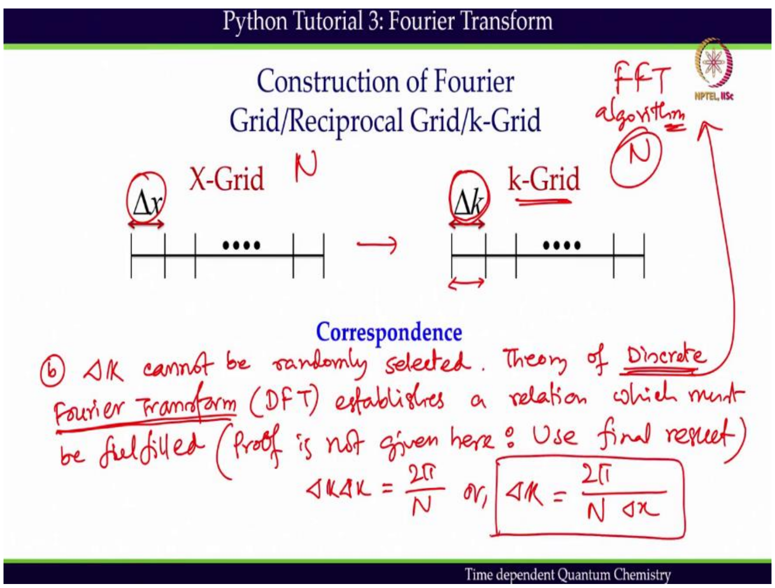

Second thing that when you are selecting, so, here I have N number here I have N number, but when you are selecting this Δk, I cannot select delta k randomly. So, second correspondence is that this Δk which is defining the spacing between two adjacent grid points in the k-Grid. In the k-Grid, this is the spacing between two grid points adjacent grid points Δk cannot be randomly selected. In fact, theory of discrete Fourier Transform abbreviated as DFT Discrete Fourier Transform establishes a relation which must be must be fulfilled while type transforming this X-Grid to k-Grid.

So, when I am transforming this, this Δk and Δx they are related and how they are related the proof is not be given here just use the final result. And the proof comes from the Discrete Fourier Transform methodology. This Discrete Fourier Transform methodology is implemented through this FFT algorithm.

So, the algorithm which we are going to use FFT algorithm this FFT algorithm is based on the Discrete Fourier Transform Theory. And it shows that

$$\Delta k \Delta x = \frac{2\pi}{N}$$

N is the number of grid points we have or in other words, this Δk when I am selecting Δk that has to be

$$\Delta k = \frac{2\pi}{N \Delta x}$$

That an restriction of the Fourier Transform. So, we have to remember this two. This restriction, while we are transforming the X-Grid to k-Grid.

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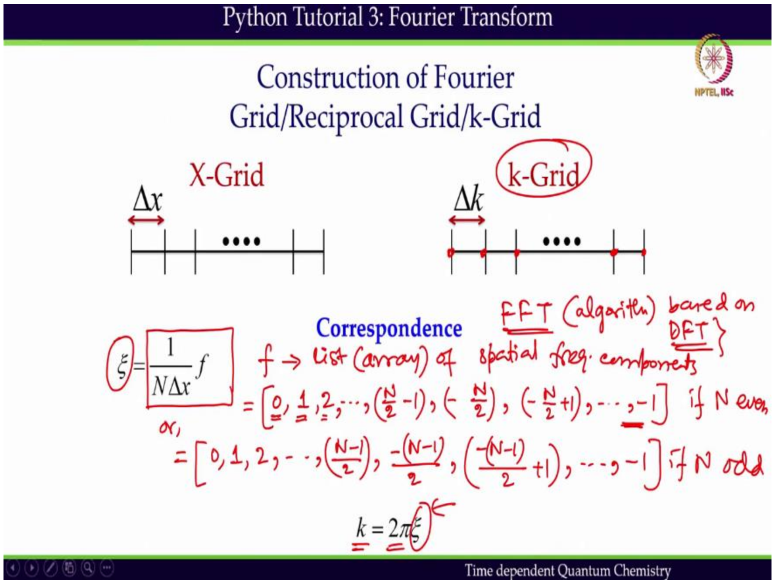

Finally, this is the final step. So, based on this restriction, we have been able to create this k-Grid and once we have got the k-Grid, we have to specify it how to get this k-Grid. The Fast Fourier Transform algorithm the FFT algorithm.

This is the computer algorithm based on Discrete Fourier Transform Theory it will allow us to sample the spatial frequencies spatial frequency is defined by this and that spatial frequency will be defined by this expression where f represents, this f represents our list or we can call it an array of spatial frequency components which is given by this.

It is going to be 0 1 2 then N/2-1 then, -N/2 then, -N/2+1 up to -1. If N is even or if it is odd then I have to use it is going to be 0 1 2 then (N-1)/2 then, -(N-1)/2, -(N-1)/2+1 upto -1. If N is odd.

And so, this is the way FFT will create the frequency components and once we know the frequency components we know how to get the k-Grid points. So, k-Grid points will be just multiplied by the, this frequency component needs to be multiplied by 2π. So, then we can get the k-Grid points here. That is the way we are going to construct.

So, what we see that FFT algorithm or DFT this Discrete Fourier Transforms will actually create the frequency components which is first is 0, then is going to be 1 2 and so on. And we have also negative components as well because negative components comes from the fact that in the Fourier Transform.

It is a complex notation and once complex notation is converted, we get the negative frequencies as well. In practical purpose we can neglect those negative frequencies but for the completeness of the theory, negative components should be there. We will continue this session in the next class.