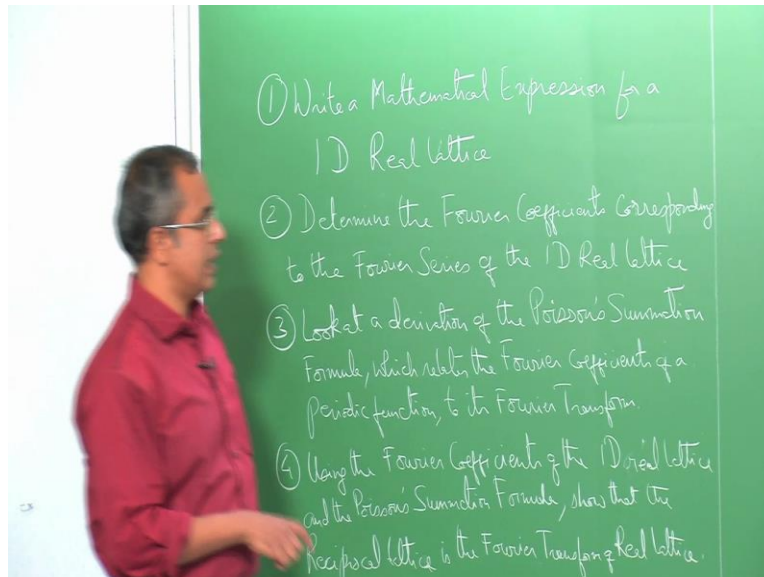


**Introduction to Reciprocal Space**  
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**Lecture10**  
**Reciprocal Lattice as a Fourier**  
**Transform of Real Lattice**

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Hello in today's class we are going to look at the reciprocal space and how it relates to the real space. So far, we have looked at reciprocal space as an independent entity or at least that is how we have focused on it, we have you know had a definition for what this reciprocal space, how it relates to some quantities in real space. And on that basis of the relationship we derived a lot of properties for reciprocal space.

But in general, we looked at that relationship that first set of equations we wrote say you know if you have  $a_1$ ,  $a_2$  and  $a_3$  as the real lattice vectors. Then the relationship between  $b_1$ ,  $b_2$  and  $b_3$  the reciprocal lattice vectors corresponding to those real lattice vectors, we wrote a relationship. That relationship between  $a$  and  $b$  was arbitrary and I did tell you that you know we can select some relationship and then you will see some properties.

But we chose to a particular relationship, so we said you know  $b_1$  is  $a_2 \times a_3$  by the volume of the unit cell etcetera. So, we wrote up some relationship, it did, it was at that point an arbitrary relationship and then we proceeded with it. We got a lot of useful properties for the reciprocal

lattice, corresponding reciprocal lattice. What I am going to show you today is that, that relationship is not really all that arbitrary it has some significance.

The significance is that the real space and the reciprocal space are related as Fourier transforms of each other. The reciprocal space is the Fourier transform of the real space and vice versa. So, we are sort of going to look through some mathematical, you know derivation process that we will go through.

Which will show you that the reciprocal space that we generate, the definition that we give for the reciprocal space that we are typically using for the reciprocal space, is comes about naturally if you treat it as a Fourier transform of the real space. So, this is what we are going to do okay. So, to do this, we are going to take a four-step process and so I am going to put down those four steps.

We are mathematically going to do a bunch of activities related to each of those four steps. When we finish the fourth step you will have this final relationship that the reciprocal space is the Fourier transform of the real space. So, this is what we are going to do. So, we are going to start by first of all, we are going to write an expression, write a mathematical expression for a 1d real lattice. So, we do need a mathematical expression for a 1d real lattice.

Because it is using that mathematical expression only we are going to do further analysis. And then arrive at a mathematical expression for the corresponding reciprocal lattice and then or at least we are going to do something. And we are going to arrive at an expression and then we are going to see that whatever is the reciprocal lattice that comes is a Fourier transform of this lattice that we started out.

So, so we need to write a mathematical expression for the 1d real lattice. Then we need to determine the Fourier coefficient corresponding to the Fourier series of this 1d lattice of the 1d real lattice okay. So, we write a mathematical expression for 1d real lattice. Then we will determine the Fourier coefficient corresponding to the Fourier series of this 1d lattice. Then we will look at a derivation for something that is referred to as the Poisson summation formula.

So, we look at a derivation for something called the Poisson summation formula, which relates the Fourier coefficients of a periodic function to its Fourier transform okay. So, we are going to look at a derivation of the Poisson summation formula, which relates the Fourier coefficients of a periodic function to its Fourier transform and using all of these, using the Fourier coefficients of the 1d real lattice.

Using the Fourier coefficients the 1d real lattice and the Poisson summation formula, we are going to show that the reciprocal lattice is the Fourier transform of the real lattice okay. So, these are the four steps that we are going to do, of course I am doing this in a 1d example is what I am going to do. In principle, similar analysis can be done for 2d and 3d. We will stick to 1d, it is a simpler analysis and it conveys the idea which is all we are interested in.

So, at the end of it, so we are going to write a mathematical expression for a 1d real lattice. We are going to determine its Fourier coefficients corresponding to the Fourier series of this 1d real lattice. Independent of this we are going to look at a Poisson summation formula, which will relate the Fourier coefficients of a periodic function to its Fourier transform. So now we have two pieces of information.

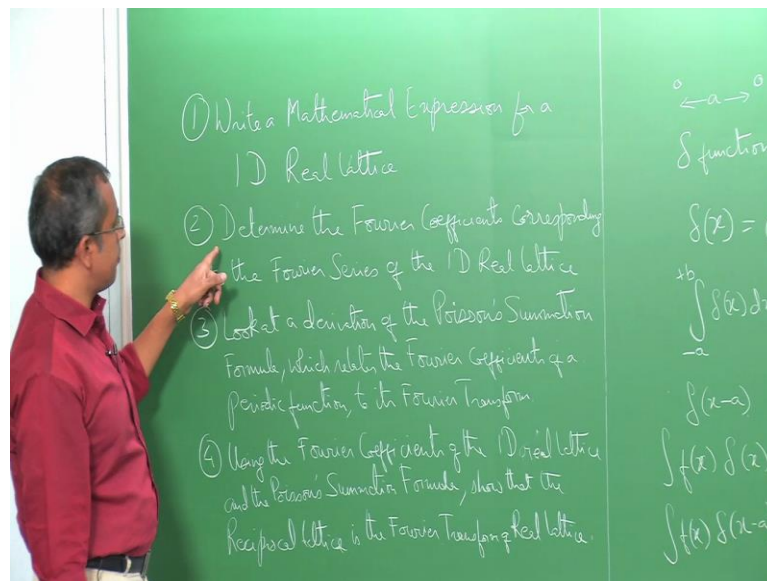
We have the Fourier coefficients for 1d real lattice and we know a way of relating those Fourier coefficients to the Fourier transform of the 1d lattice. So, if you do those two things using the Fourier coefficients of the 1d real lattice and the Poisson summation formula, which will relate these Fourier coefficients to the Fourier transform of the 1d lattice.

We will find that the Fourier transform of the 1d real lattice is the same thing that we would normally use as the definition of that reciprocal lattice okay. So therefore, we will at, when we finish this we will appreciate the fact that the reciprocal lattice is not some totally arbitrary definition but it is actually related to the real lattice through a Fourier transform okay. And recognizing this actually opens up the doors in a big way.

Because mathematically there are various properties that Fourier transforms have and so on. And this kind of relationship knowing that it is, these two are related as the Fourier transform enables you to use all those properties for the real space and reciprocal space okay. So, this is what we

would do. So, let us start with the first step which is writing a mathematical expression for a 1d real lattice.

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So, what is the 1d real lattice, we have a lattice point then we have nothing for some distance, we have another lattice point, nothing in the middle, yet another lattice point and so on. So, we have lattice point, nothing in the middle, lattice points, nothing in the middle, lattice point, nothing in the middle and so on. So, we need a mathematical expression which will simulate this, which basically will represent this.

So, you will need something that is, that has a value only at a specific location. You need a function that has a value only at a specific location does not have a value anywhere else and then that kind of a function we are going to put up periodically. So those are two things that we are going to do. So, a function which enables you to do this is referred to as a delta function. Delta function is a function which is defined such that it has a value only at one location.

It does not have a value anywhere else and so we are going to put up a series of delta functions at various points so that is what we are going to do. The way it is defined is, it has a few aspects to its definition. The one that immediately is relevant to us is that the function delta of  $x=0$ , for all  $x$  not equal to 0. So, as long as this argument  $x$  is not equal to 0, this function will evaluate to 0, it will evaluate to a value only when this  $x=0$ , only at that value of  $x$  is 0.

So, in other words it is defined only at  $x=0$ , it is not defined anywhere else okay. And also in terms of its value, it will work out to, it defined again like this the integral  $-a$  to say  $+b$  such that it goes through the origin of  $\delta x \, dx = 1$ , as long as region of integration includes the origin. So that way I will turn it going from some, minus quantity to a plus quantity it goes through the origin therefore this integral integrates to one evaluates to one okay.

So, this is another property of this delta function and now the way I have; so, this is going to evaluate to zero at all other values except at the origin, at all other values of  $x$ , so at all other locations is going to evaluate to 0. So, it uniquely puts up a value only at one point that is the point of this function. And if you do an integration of this function over this region it will evaluate to one, around this point.

Now this is a function that is now, the way I have written it has a value only at the origin which is  $x=0$ . Supposing you want to put this function at some other location, at say  $x=a$ , so the way you would rewrite this function is simply define it as  $\delta(x-a)$  okay. So now this puts the delta function at the location  $a$ , because this argument evaluates to zero only when  $x=a$  right. So, this is, so similar to this point that we have written here.

We can say that  $\delta(x-a) = 0$ , for all  $x$  not equal to  $a$ , basically it is defined at 0, so instead of setting  $x$  to be equal to 0, we are setting  $x-a$  to be equal to 0, so  $x-a$  will be 0, whenever  $x=a$ . So, this forces this delta function instead of, this were the origin, you can now by using this kind of a definition, you can force this delta function to show up here and if this spacing is  $a$ , similarly if you want to put it at  $2a$  you will have to put  $x - 2a$  and so on.

So, you can have a series of such point's right. So, this is one aspect of the delta function and incidentally one of the features because of the way it is defined because it shows up as being 0 at all other locations and has a unique value when you integrate it, it integrates to 1, as long as you go through the origin. One of the interesting features that this function provides you is that if you multiply this with any other function okay.

So that function will also, that product will now evaluate to zero at all values other than the origin right. Because at all other values of  $x$  the if you multiply, so if write  $f(x)$  you have  $a$ , you

create a situation that; this is going to evaluate to zero at all values of  $x$  not equal to zero, because this function is equal to zero at all values of  $x$  not equal to zero.

So, it will only have a value of at  $x=0$ , so this will, if you do this integration you will, if and if that region of integration includes the origin, then this evaluates to one around the origin, so this will basically evaluate to 0,  $f$  of 0, this is, so the integral of this  $f$  of  $x$  times delta of  $x$   $dx$  will evaluate to  $f$  of 0.

So similarly if you put in you know the same function at some other location, when you if you create your delta function like this such that it is now positioned at a location  $x=a$  then you can write  $f$  of  $x$  delta of  $x-a$   $dx$ , if you integrate this you know say minus infinity to plus infinity, whatever you integrate it such that it includes the region  $x=a$  primarily it has to include the region  $x=a$ , includes the location  $x=a$ .

This will evaluate to  $f$  of  $a$ , that is all it will evaluate to. So, region of integration should include  $a$ . So, region of integration include  $x=a$ , if you include  $x=a$ , this will evaluate to  $f$  of  $a$ , so this is the function. So now we have some properties for this delta function, we understand that you know by putting this delta function, not all of them are immediately necessary for defining the, I just wanted to put it down.

So that you know what are the properties of the delta function because we are going to use some of these properties. But we are right now at this stage we are simply looking at a function to represent the 1d lattice. And we find that the delta function provides you with some of the important you know features that are necessary for it. So, what we need really is a delta function that is available at each of these locations.

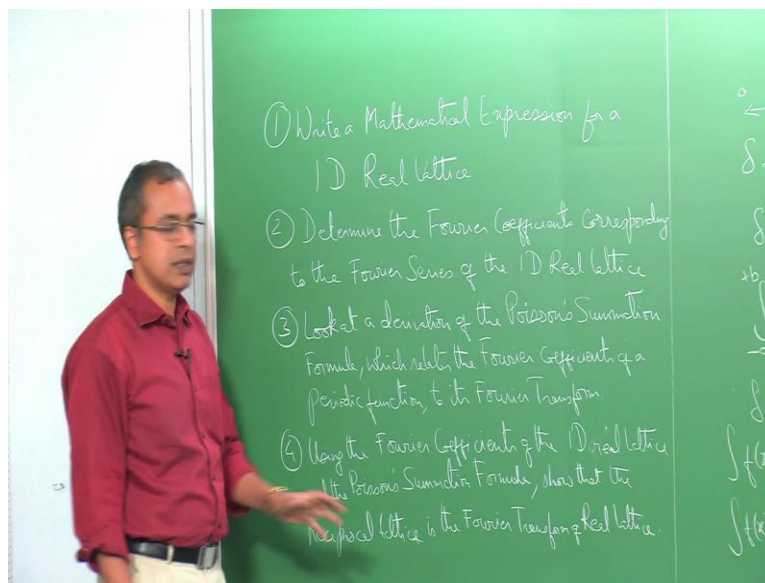
So, what we are simply going to do is, we are going to take a series of delta functions and put a sum, so that you get now a sequence of delta functions. And each term will now create a delta function at each of these points, so that is what we are going to do. So therefore, you can write this, the function  $f$  of  $x$  which will represent this 1d lattice, is basically simply going to be a sum of say  $n$  going from minus infinity to plus infinity of delta of  $x-x_n$  okay.

So, this function  $f$  of  $x$  which is a sum going of  $n$  going from minus infinity to plus infinity for delta function  $x-na$ , creates a situation where you have a delta function at each location because when  $n=1$ , you have  $x-a$ , that will create a function; and this were the origin that would put a delta function at  $x=a$ . If you have  $n=2$ , it will create a delta function that will become valid only at  $x=2a$  because at  $2a-2a$  will give you 0.

So that will create a delta function at this position in the  $2a$ . Similarly, at  $n=3$  you get a delta function here and so on. So, this is a function that now represents your 1d lattice okay. So, we now have a mathematical expression for the 1d lattice which is the; if you come back here the first step that we said we will do, is to come up with a mathematical expression for a 1d real lattice.

So, we have now gotten mathematical expression for a 1d real lattice. The next step we are going to do is to determine the Fourier coefficients corresponding to the Fourier series of this 1d lattice okay right.

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So, if we have a function  $f$  of  $x$ , so the Fourier series corresponding to this is basically given as 1 by, is basically a sum  $n$  is equal to minus infinity to plus infinity  $C$  of  $n$  to the power  $2\pi i n x$  by  $a$ . So, if you take a periodic function and then you write it as a series of in the terms of a Fourier series then this is how the Fourier series would be written as.

In this class, we are not really looking at the derivation of a Fourier series or of a Fourier transform. So, I am going to assume the definition of a Fourier series and a definition of a Fourier transform. So, if you are not familiar with the definition of a Fourier series or a Fourier transform, so that alone is something you will have to look up. So that definition is simply as I am just going to use it here.

So, this and this is how it would be defined you will have a function  $f$  of  $x$  and we would write it as a it is a periodic function and it is now written as a sum of series of terms and basically an infinite series of terms, which will have the general format a Fourier this  $C_n$  is called a Fourier coefficient and of this Fourier series. So, for each term you will have; for every value of  $n$  you will have a coefficient value.

And corresponding to that, you will have this  $C_n e^{2\pi i n x / a}$  by  $a$  where  $a$ , is the periodicity of that function okay, so this is how we would go about it. And each of the Fourier coefficients itself  $C_n$  would be defined as  $1/a \int_{-a/2}^{+a/2} f(x) e^{-2\pi i n x / a} dx$ , this is an integral, this is how I write, right, so each of the Fourier coefficients written like this.

Now our 1d, so this is by definition sort of, definition of Fourier series, so you can look that up. Now for us for the 1d lattice the  $f$  of  $x$  is basically we have written it as a sum  $n$  going from minus infinity to plus infinity of delta function  $x-na$ . So now if you look at the Fourier coefficients of this 1d lattice, that is simply going to be  $1/a \int_{-a/2}^{+a/2} \delta(x-na) e^{-2\pi i n x / a} dx$ .

We can put the sum here,  $n$  equals minus infinity to plus infinity integral  $-a/2$  to  $+a/2$  delta of  $x-na$   $e^{-2\pi i n x / a}$  over  $a$   $dx$ . So, this is now the Fourier coefficient we are simply substituted the fact that our 1d lattice is represented by this function into this equation. So that is what you have we have got here. Now we also noted one property for the delta function which we will come back here and see.

We noted that when you have a delta function  $f(x)$  times that delta function  $x-a$   $dx$ , if you do the integration, if you include the region, if the region of integration includes that value  $x=a$ , you

will see; it will simply evaluate to  $f(a)$ . So,  $f(x)$  will simply evaluate to  $f(a)$  because of the properties of this delta function.

So, the same property we are now going to utilize. So here we have the delta function, is not simply  $\delta(x-a)$ , So basically you have this delta function and you have a function  $f(x)$  here so this if, as long as it includes this region of  $x=a$ , you will basically you will find that you this will evaluate to  $f(a)$ . And the correspondingly each of these terms will you know it will it will add to those terms in those respective location.

So, this is going to evaluate to  $f(a)$  and in particular in this case you would you are going to see  $e^{i2\pi n x/a}$  by  $a$ , so this simply become  $e^{i2\pi n}$ ,  $e^{i4\pi n}$ , and  $e^{i6\pi n}$  is simply  $\cos \theta + i \sin \theta$ , that is how the  $e$ , exponential function is this function here is being defined by that  $e^{i\theta} = \cos \theta + i \sin \theta$ .

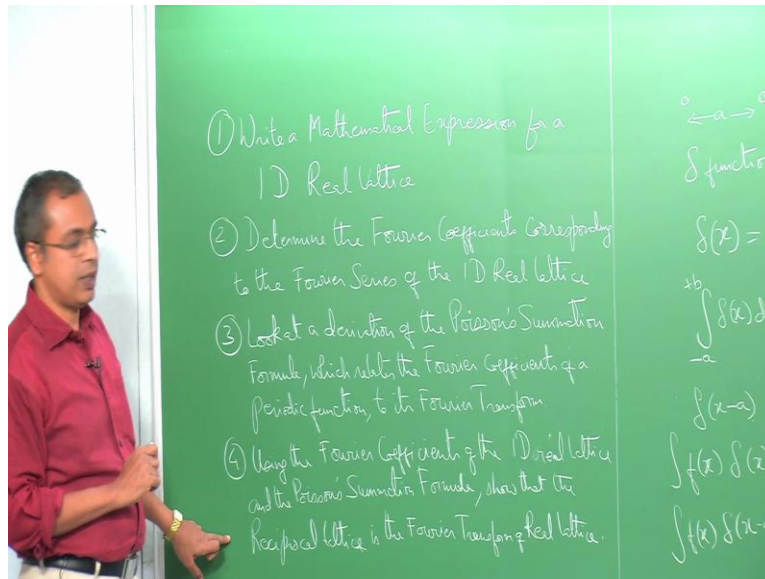
So, when you have  $2\pi n$  as the argument there  $\cos 2\pi n + i \sin 2\pi n$ ,  $\cos 2\pi n$ ,  $i \sin 2\pi n$  will evaluate to zero, this will evaluate to 1. So, we simply basically have one, so therefore this  $f(a)$ , this is basically going to be  $e^{i2\pi n} - e^{-i2\pi n}$  by  $a$  is what we are going to get and therefore this whole integral that is here will always keep evaluating to 1, for all values of  $n$ .

This whole thing will ever wait to 1 because of the property that we see for the delta function times  $t$  is some other function. This happens to be the some other function that is there so it will only have the value of this function at the value of  $a$ , and therefore it will evaluate to 1. Therefore, all the Fourier coefficients will now evaluate to 1 by  $a$ , so you see here  $C_n$ , so this is the Fourier coefficient so it could be  $C_1$ ,  $C_2$ ,  $C_3$  etcetera.

And minus infinity to plus infinity so you have a lot of terms here, all the terms here will evaluate to 1 by  $a$ . So that is the point that we need to know regardless of the value of  $n$ . So, we have now done the second step which of our derivation here. We wrote the mathematical expression for 1d real lattice. We have written the Fourier coefficients corresponding to the Fourier series of the 1d real lattice.

So now we are going to look at the third thing which is look at a derivation of something called the Poisson summation formula which relates the Fourier coefficients of a periodic function to its Fourier transform okay.

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So, this is what we are going to do, so if you take a periodic function  $f$  of  $x$  periodic function and you write it as a Fourier series, so it is written as infinite it is the sum of infinite set of terms all of which have a periodicity  $2\pi$  and so  $2\pi m$ , so basically you can write this as sum of  $n$  is equal to minus infinity to plus infinity  $g$  of  $x + 2\pi m$ , so we will just use  $m$  here  $2\pi m$  okay.

So basically, if you have a periodicity of you know, if you have some periodicity then the function of the value of  $x$  would be the same as the function of the value so  $f$  of, if some periodicity is there if the function at some value  $x$ , will have the same value at  $x$  plus that periodicity, that is the way in which we are defining the periodicity right.

So, a function will have some value at the argument  $x$  and then if you go, increase that value to  $x$  plus the periodicity it will come back to the same value of, whatever is that value of the function. The function keeps getting the same value at that periodicity, so that is the idea of it and therefore if the periodicity says  $2\pi m$  in this case. So,  $g$  of  $x$  will be the same as  $g$  of  $x + 2\pi m$  that is why you end up saying that you know that is the periodicity of that function.

So that is what it is, so you get this, so we can represent this function using a set of infinite terms which have this kind of a periodicity and that is what you are, that is the general way in which you would express this as a Fourier series right. Now if you want to get the Fourier coefficients corresponding to the series.

Then you will have  $C_n$  is basically  $\frac{1}{2\pi} \int_0^{2\pi} f(x) e^{-2\pi i n x} dx$  by a  $dx$  okay. So, this is what your Fourier coefficients are going to look like this  $f(x)$  is this term here, so we just were to put that here, because  $\frac{1}{2\pi} \int_0^{2\pi}$  and there is a sum here so I just put the sum here,  $m$  going from minus infinity to plus infinity of  $g(x + 2m\pi) e^{-2\pi i n x}$  by a  $dx$ .

So, we basically get this so it is  $a_n$ , they are both you know integral, these are integral values of  $n$ , so we can even use the same value here. So now basically if you see here when  $x=0$ , this is basically  $2m\pi$ ,  $g(2m\pi)$  when  $x=\pi$ , this is  $2\pi + 2m\pi$ . So  $2m + 1 \pi$  is what we have right. So, when  $x = 0$ , this would-be  $g(2m\pi)$  right. And when is  $x=2\pi$  this is  $g(2\pi + 2m\pi) = g(2 + 2m \pi)$  right.

So, I can just change the limits of integration to go from  $2m\pi$  to  $2m+1 \pi$  and then this convert this to  $x$ ,  $g(x)$ . We are simply changing the, you know limits of integration and correspondingly adjusting this function, so that the process remains the same. So instead of going from 0 to  $2\pi$  and having this function being  $x + 2m\pi$ , I can go from  $2m\pi$  to  $2m+1 \pi$  and have this simply as  $g(x)$ , so that is all we have we are going to do.

So, I am just going to rewrite this with changing the limits of integration, so this is  $\frac{1}{2\pi} \int$ , we still have this  $m$  is equal to minus infinity to plus infinity, integral  $2m\pi$  to  $2m + 1 \pi$   $g(x) e^{-2\pi i n x}$  by a  $dx$ . So,  $C_n$  is basically this, so  $C_n$  is this function that you see here right. So, I have simply change the limits of integration corresponding, from 0 it as become  $2m\pi$  from  $2\pi$  it has become  $2m+1 \pi$ .

And therefore, correspondingly this function has changed from  $x + 2m\pi$  to simply  $x$ . So, when it is  $x$  it is, when it, so you can correspondingly see, we just saw here how they are equivalent. Now the interesting thing to notice is you are now summing from minus infinity to plus infinity

and you are integrating from  $2m\pi$  to  $2(m+1)\pi$ , so essentially  $m$  is changing from minus infinity to plus infinity.

And in at the same time you are integrating from  $2m\pi$  to  $2(m+1)\pi$ , it is the same as saying that you are integrating from minus infinity to plus infinity right. You are doing two things here you are doing as sum and an integration which are you know together. And in the process, you are going from minus infinity to plus infinity, so it, this is also effectively an integral from minus infinity to plus infinity.

So, this whole thing can be combined into any single integral going minus infinity to plus infinity. So mathematically this can simply be written as  $\frac{1}{2\pi} \int_{-\infty}^{\infty} g(x) e^{-2\pi i m x} dx$  okay. So, what we have done is we have written our formula for the Fourier series corresponding to a function.

And we have recognized that it has a certain periodicity and that is why it is written in a certain way and then we wrote the Fourier coefficient, the expression for the Fourier coefficients corresponding to a function. We have introduced that function here and so that is the expression for the Fourier coefficients corresponding to that function.

We notice that there is a sum, we then change the limits of integration because that is works out convenient for our understanding here. So, from 0 to  $2\pi$  we change to  $2m\pi$  to  $2(m+1)\pi$ , correspondingly change the function so that the form is still being maintained. And then we recognize that since we are doing with respect to  $m$ .

We are doing sum from minus infinity to plus infinity and an integration from  $2m\pi$  to  $2(m+1)\pi$  is the same as integrating from minus infinity to plus infinity that is basically what it is because at minus infinity this would be minus infinity  $-2\pi$  and this would be  $+2\pi$ , so that is why it is the same as going from minus infinity to plus infinity.

So,  $\frac{1}{2\pi} \int_{-\infty}^{\infty} g(x) e^{2\pi i m x} dx$ , I mean  $x$  by a  $dx$ , so this is the expression. Interestingly again I am going to use a

definition, which is therefore for Fourier transforms now, so that definition again we are not deriving here so Fourier transform definition is something that you would have to look up.

But this is basically the Fourier transform of your original function  $f$  of  $x$ , this expression that is written here this, integral that you have written here, that is written here is the expression for the Fourier transform of the function, so this is nothing but  $1$  over  $2\pi$  okay. So, this is  $1$  over  $2\pi$   $f$  tilde  $k$ , so this is the Fourier transform of the function okay.

So, we started with the function  $f$  of  $x$ , the Fourier transform of it is typically represented with this  $f$  with this tilde mark on top of it with a new variable  $k$ , such that the  $k$  and  $x$  are conjugate variables they relate to each other through Fourier transform. And this is the expression you are getting. So now this is the expression also which is the Fourier coefficient of the function okay.

And in our case the function that we are if you take the, so this is in general right, in general you have a Fourier series, you have a function, you have it has a certain periodicity and when you evaluate the function you look at its Fourier coefficients and what those Fourier coefficients represent, you find that for the function which if it has a certain set of Fourier coefficients then those Fourier coefficients can be related to the Fourier transform like this okay.

So, this  $C$  of  $n=1$  by  $2\pi$  or  $1$  over  $2\pi$   $f$  tilde  $k$ , this is basically what we have done here is we have sort of looked at one derivation for the Poisson summation formula, which relate the Fourier coefficients of a periodic function to its Fourier transform okay, so this is the Poisson summation formula and please note this is  $C$  of  $C$  subscript  $n$ . So, it can take several values  $C_1$ ,  $C_2$ ,  $C_3$  etcetera, it can have several values okay.

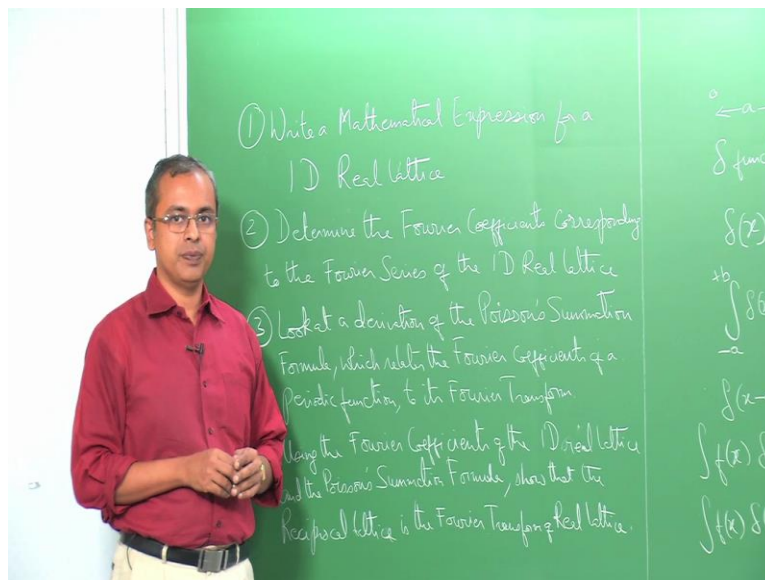
So, we have got specific things done, we have basically got a few important relationships here we have of course first of all written the mathematical expression for a 1d real lattice. We have arrived at the Fourier coefficients corresponding to the 1d real lattice. And we have also independently seen that the Fourier coefficients of a function can be related to the Fourier transform of the function right.

So, this is what we have got, so we now have only the fine, if you go back to what we started out with if you come here we will take a look so we finish the step one, we have finished step two,

we have still finished step three we are now going to in the last step we are simply going to relate the parameters that we have obtained.

We have we have the Fourier coefficients of the 1d real lattice and we also know how in general the Fourier coefficients relate to the Fourier transform okay. So, using then we are going to look at how the 1d real lattice, the reciprocal of, the Fourier transform of the 1d real lattice represents the reciprocal lattice okay.

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So, we see that as part of the through the Poisson's summation formula that the Fourier coefficient of the periodic function have this form  $C_n$  is given as  $\frac{1}{a} \int_{-\infty}^{+\infty} g(x) e^{-2\pi i n x / a} dx$ . So, this  $a$ , is the periodicity of that function, so that is how we get that  $a$  and then  $n$  is the an integral number is an integer.

So now if you look at this the what, the term that you have here within this integral is the, is mathematically the Fourier transform of the function  $g$  of  $x$ . So, we are not deriving the Fourier transform formula but this is the form you will arrive at if you did a Fourier transform. And you take a function  $g$  of  $x$  and you did the Fourier transform this is the form that you will get and this gets represented as  $\tilde{f}(k)$ .

Please not now we were working with a variable  $x$ , we have shifted to a variable  $k$  and this  $\tilde{f}(k)$  is the Fourier transform of  $g$  of  $x$ . So, these are two different variables in a moment I will tell

you something about the general, you know relationship between them but this is  $\tilde{f}(k)$ . And so, this whole thing works out to be the Fourier transform of this function  $g(x)$  represented by  $\tilde{f}(k)$ .

Therefore, you can write now  $C_n = \frac{1}{2\pi} \tilde{f}(k)$ , so this is the Fourier coefficients of the series that corresponds to a periodic function  $g(x)$  and they are now related to the Fourier transform of that function and that was the whole purpose of the Poisson summation formula. To relate to the Fourier coefficients of a function to the Fourier transform of that function okay.

Now we also saw that for our periodic function which is the lattice, a one-dimensional lattice, we found that we  $C_n = \frac{1}{a}$  for all values of  $n$ , so for all values of  $n$  it could keep evaluating to  $\frac{1}{a}$ . And therefore, if you equate these two for our linear lattice one dimensional lattice, if you equate the, what the result that you get through the Poisson summation formula.

With the actual Fourier coefficients that we are getting for the one-dimensional lattice, basically this means this is  $\frac{1}{2\pi} \tilde{f}(k)$ . Therefore, you have  $\tilde{f}(k) = \frac{2\pi}{a}$ , for all values of  $n$ , so that is the general result that we are getting. I also said that you know we have shifted from  $x$  being the variable we to  $k$  being the variable.

And that is typically what happens you will have a pair of variables when you do a Fourier transform you will go from you know sort of one space to another space. In general, these variables will be inversely related, so in general in as part of the Fourier transform process you will have  $k$  to be inversely related to the value to the variable  $x$ .

And therefore, typically we will write  $k = \frac{2\pi}{x}$ ,  $\frac{2\pi n}{x}$ ,  $\frac{n2\pi}{x}$  is the general form of the relationship between  $k$  and  $k$  and  $x$ . And that is  $y$  so for example if you have time as the variable, you will get frequency  $\frac{2\pi}{\text{time}}$  is what you will get, if time is the variable  $x$  then the  $k$  variable will work out to be the angular frequency  $\frac{2\pi}{t}$ .

And similarly, if you have a wavelength as the  $x$  you will get wave number something like that you so you will sort of have inverse relationship between these variables in this relationship. So now we also see that for our linear lattice, we are not looking at all right values of  $x$ , we are only

looking at the specific values of  $x$  equal to a specific values of  $a$ . So  $x$  is equal to  $a$  in steps of  $a$  is what we are looking at, so in general  $k$  will have the form  $2\pi n$  over  $a$  or  $2n\pi$  over  $a$  okay.

So, this is the typical form you will have. So now we have two things here, we have the Fourier transform which works out to a value of  $2\pi$  over  $a$  and the variable itself has this general form to  $2\pi n$  over  $a$ , where  $a$  is the periodicity of that function. So, if you take these two together we find that essentially if you look at our original one-dimensional lattice, we basically said that it only has values at specific values of  $a$ , the rest of the place it does not have a value.

And so, we wrote this as  $f(x) = \sum_{n=-\infty}^{+\infty} \delta(x - na)$ , this ensure that whenever  $x$  has integral values of  $a$ , this function has a value, otherwise it is undefined. And then that is how we, so this by the way since it ensures that there is a function only at specific locations it is a basically a spike at specific locations, it is effectively as a function that sort of looks like that and so on.

So, this is it looks like a comb, so it is referred to as a Dirac comb, is the term that is used for it. Now we have a similar situation for  $f(k)$ ,  $\tilde{f}(k)$ . We see that it has to have values of we see come back here, we see that it has to have values of  $2\pi$  over  $a$ , but it can have these values only at specific values, so we are only, I mean these are defined only, these are defined for all values of  $n$  it is going to be  $2\pi$  over  $a$  values of  $n$ .

And the  $k$  itself has this formal, this particular value, so it is also defined only at values of  $a$ ,  $k$  itself gets defined it values of  $a$  and the, you have the function itself being defined as  $2\pi$  by  $a$  at all values of, at all values of  $n$ , which corresponds to this expression that we have here. So, at all values of  $n$  this variable will be, this will evaluate like this and that those values of  $n$  this variable should always evaluate to this.

Fourier transform should always evaluate to  $2\pi$  over  $a$ , so it should be at  $2\pi$  over  $a$ , at integral values of  $n$  with this being the variable. So therefore, in a very similar fashion we can write that here as  $2\pi$  over  $a$  sum of  $n$  equals minus infinity to plus infinity delta function again this time the variable we are looking at this  $k - 2n\pi$  over  $a$  okay.

So, what we see is the Fourier transform will get the value of  $2\pi$  over  $a$ , at integral values of  $n$  and this is  $2\pi$  over  $a$ ,  $2n\pi$  over  $a$ , so this will keep evaluating to 0 at integral values of  $n$  and then this will basically give you the delta function. So, only under those conditions it will evaluate to  $2\pi$  over  $a$ .

So therefore, so just the way you get this  $f(x)$  as a Dirac comb, you get the Fourier transform of the function also as a Dirac comb except that it is an inverted notation, so you have  $2\pi$  over  $a$ , where you originally had  $a$ , so where you had  $a$  you now have  $2\pi$  over  $a$  or  $2\pi$  over  $a$  is what you are getting. So, a real lattice, real one-dimensional lattice gets represented as a Dirac comb and has you know a linear dimensions of  $a$ .

It is represented Fourier transform of it comes out to, also to be a Dirac comb, so that is also it also means, that it is also a spot pattern of similar to you know a specific set of spots that you see here or specific locations that you see here, this will also work out to specific points. So, what is  $a$  here will now become  $2\pi$  over  $a$  here and so this is the result that we are getting from the mathematical part of it.

Where we have just taken a function, which represents the real lattice, we have found out the Fourier transform of it using the Poisson summation formula. With the help of Poisson summation formula and then we find that the Fourier transform of it, is also a set of, discrete set of points except that the spacing between them is  $2\pi$  over  $a$ . So, a Dirac comb was facing  $a$ , the Fourier transform is a Dirac comb of spacing  $2\pi$  over  $a$ .

And as you can see this form, is the form that we have seen through our earlier classes as the reciprocal spacing off so this spacing here. So therefore, we see that the reciprocal spacing, so this is basically reciprocal space, so we have seen here that we take the real space, you do the Fourier transform and you arrive at the reciprocal space.

So therefore, the real space or reciprocal space, so therefore we are able to see that the reciprocal space is the Fourier transform of the real space, reciprocal space is the Fourier transform of the real space and so this was the exercise that we wanted to do today, you can see that all the mathematics that we have done has shown us that this is the case.

Previously we had been defining this independently and looking at properties between the real space in the reciprocal space, now we see that mathematically we are able to go from you know writing down an expression for the real space, writing down the Fourier transform of it, going through the Poisson summation formula to understand the relationship between the Fourier transform and the Fourier series and the Fourier transform.

And then seeing that the Fourier transform actually implies that you have arrived at the reciprocal space. So just to sum up we started by first writing a mathematical expression for a 1d real lattice. Then we determined the Fourier coefficients corresponding to the Fourier series of this 1d real lattice. So, we had the Fourier coefficients.

Independent of that we looked at something called a Poisson summation formula which related Fourier coefficients of a periodic function to the Fourier transform of that function. Now taking point three and point two together we related the Fourier coefficients of the 1d real lattice to the Fourier transform of the 1d real lattice.

And then in that process we realized that the Fourier coefficients of the 1d real lattice and the Poisson summation formula create the situation that the reciprocal lattice is essentially the Fourier transform of the real lattice or we are able to recognize that the reciprocal lattice the Fourier transform of the real lattice.

So, this is the process that we have done and it shows you how a real lattice and reciprocal lattice are related as a mathematical entity okay. So, with that we will conclude the discussion and hopefully you will find this, I mean realizations of this relationship are useful in many of the things that you are trying to do okay. So, with that we will halt. Thank you.