

Introduction to Reciprocal Space
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Lecture –11
Alternate Notation for Reciprocal Space

Hello welcome to this class on which is part of our course on reciprocal space in the past few classes you have seen different aspects of reciprocal space. How it is defined? And how it can be utilized? However most of the classes that you have seen so far are the utility and the description of reciprocal space that you have seen in those classes comes to you more from a material science perspective.

So, that is what you would see in a typical characterization book and also in you know associated with say x-ray diffraction or with electron microscopy and so on. And that is the manner in which it will be utilized in those settings. Of course, reciprocal space is a concept is the same it does not really matter in which context or in which book you read it.

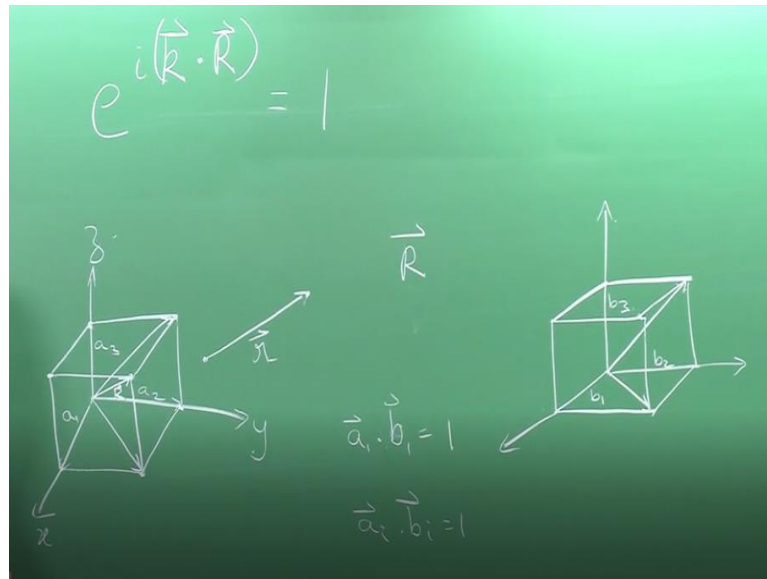
However, I will also point out that based on the book, you pick up the description, up front looks a little different, from based on the discipline in which that book is present. So, for example typical physics books, solid state physics books have a slightly different way in which they represent reciprocal space information. Fundamentally it is the same information; in fact, fundamentally it is being represented also in the same manner.

It is just that when you first look at it, it appears to be different. So specifically, in this class, we are going to look at the manner in which it is described in say a physics book. And work our way through it, look at some try to relate it to things that we are familiar with and then try to see how that is consistent with what you are already familiar with through a material science way of describing it okay.

So that is the basic idea of this class, so we will have an equation, I am going to start by putting down an equation. In most physics books that is the equation they will put up and say that this represents reciprocal space. And then that will look very different from the equations that you have seen so far. And then we will work our way around and towards the end of the class we will

come back to that same equation. And see how it relates to what we have already seen okay. So that is where we are going to go.

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So, let us start now with that equation that you will see and that is simply that the in books you will see this equation $e^{i\vec{k} \cdot \vec{R}} = 1$. So, you will see this equation $e^{i\vec{k} \cdot \vec{R}} = 1$ and in most books in solid state physics they will put up this equation.

And they will say that this represents reciprocal space and I will just tell you a few comments about it very briefly right now. And then we will work our way through a few different things which you are familiar with and we will come back to this equation. So, the point to remember here is the $\vec{k}$ here represents vectors in reciprocal space dimensions. So, L^{-1} dimension is the vector, I mean dimension of the quantities here.

And it is a vector in reciprocal space; $\vec{R}$ is a vector in real space. So, what we have already seen before in terms of real space and reciprocal space vectors, $\vec{R}$ is a vector in real space. And the, they will normally tell you that the collection of $\vec{k}$ vectors corresponding to a collection of $\vec{R}$ vectors, so you already have some real space.

You have a collection of R vectors from that real space corresponding to that collection of R vectors, the collection of k vectors which enables this equation to hold true. That collection of k vectors is then the reciprocal space relative to this relative to real space okay. So, real space is already there and then you find those k vectors with respect to those real space vectors which satisfy this equation.

When that happens, that collection of k vectors is the reciprocal lattice or the reciprocal space description corresponding to this real space lattice okay, so that is what we are going to see. So, we will come back to this right now that still up there we will towards the end, we will come back to this. So, I will begin now by highlighting some subtle things that relate to what is the real space? What is this capital R or uppercase R ? And what is this k ? And then we move from there.

So, if you take a real lattice okay, so I will just draw some cubic lattice, so you have x , y and z coordinates and then let us say we have a cube, so let us say this is the lattice that you have got. So, whatever you know you have a_1 , a_2 , a_3 as the 3-unit vector corresponding to these 3 axes, is the three basis vectors corresponding to this lattice. Now as you can see, any you can always start in, this is real space right.

So, a vector simply has a quantity and a direction right. So, you can actually have any arbitrary vector in this real space. You can have starting from any location here, you can have a vector, which goes that way and it ends at some other location here, so that is the start point and there is an end point. And it is in this space, so this is a vector in this space. So now in general we would designate something like this with a small or lowercase r .

Lowercase r with a indication that it is a vector, so this is lowercase r vector. So, the point here is this is an arbitrary starting point, this is an arbitrary ending point okay, which you have selected. You have selected, or for some other purpose it is relevant. Therefore, this is the starting point and that is an ending point okay. So, under those circumstances we simply called lowercase r or small r with a vector notation on top of it.

On the other hand, if you start at a valid lattice location okay, so this is a valid lattice point, this is a valid lattice point; this is a valid lattice point and so on. So, these are all valid lattice points, so they are a lattice points which form the corners of all these, of this lattice. If you start at this

lattice location and then from here, for example let us say we start at the origin and we come, go through the body diagonal and arrive at this point here.

So, you start at the origin and you arrive at this body diagonal here. So, this, so this is now a vector, which starts at a valid lattice location and it ends at a valid lattice location. So that would then be represented as a capital R or an uppercase R okay. So that would get represented as cap, so here is not much space here to write it but this is that would-be R and that is just one example of an R.

You could start from say the, again from the origin or you can start from here for example and then move to some other lattice location. So as long as you start from a valid lattice location and you end at a valid lattice location those are all valid reciprocal sorry valid real space lattice vectors okay. So, valid real lattice vectors, so a capital R an uppercase R will start at a valid lattice point and end at a valid lattice point.

So, any of these would, so starting at the origin I could draw one which goes up to that point, that would be a capital R. I start at the origin, I could come here, that would be a valid R and so on. So, in general I guess the main point you have to understand is these are specific vectors okay. So, this could be any vector in this space. So naturally this is a subset of this, so you have this is all the possible vectors in real space.

These are only specific vectors which start at lattice points and end at lattice points okay. So, a collection of R, capital R then represents all the lattice points that you can reach starting from a particular origin okay. So, this is what we would refer to as for this capital R. So similarly, we can go to reciprocal space and so let us say for example we have already seen that if you take a cubic lattice and you find its reciprocal lattice.

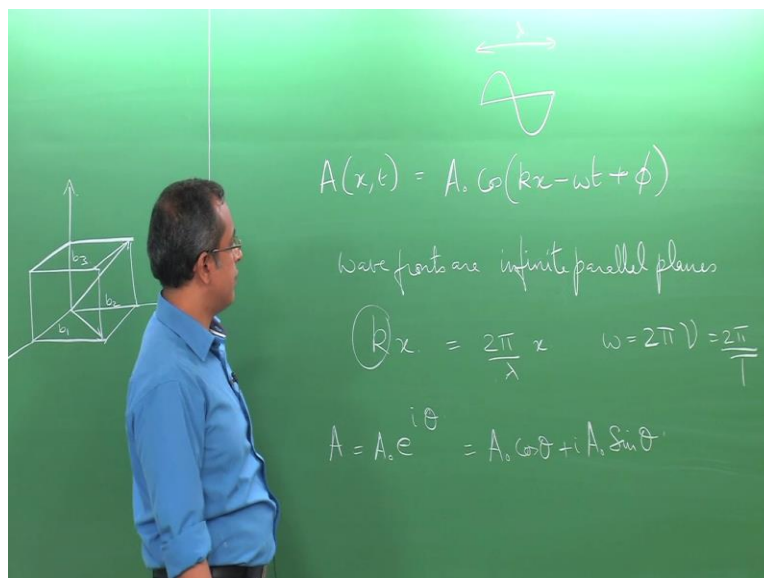
That is also a simple cube, so that is also simple cube and we would simply say this is the b_1 , b_2 and b_3 and here again a valid reciprocal lattice vector would be one, which starts from a reciprocal lattice point and ends at another reciprocal lattice point. So again, I could have all these would be valid reciprocal lattice vectors okay.

So even here you could have a general vector which would not be which would start in some arbitrary location and end at some arbitrary location or it might start at a lattice point but end at an arbitrary location without the lattice point or may be start at a arbitrary location but end at a lattice point. So, if either of the two sides is not defined as a lattice point then it is a general vector in that particular space.

But if it is, if both the starting point as far as the end point are lattice points then it is a valid reciprocal lattice vector. It belongs to that lattice that is the point that you have to understand okay. So that it belongs to the lattice here. And of course, when you have a real lattice and a corresponding reciprocal lattice, we do as we have already seen in our previous classes.

We have if these are the vectors $a_1 \cdot a_2$ sorry, $a_1 \cdot b_1 = 1$ and similarly $a_2 \cdot b_2 = 1$, so $a_i \cdot b_i = 1$ and so this is something that we can utilize okay. So, this is the point that you have to remember with respect to the lattices, so we will use these ideas little later but you have to be aware this. So, starting with this we will now move to a different aspect which will then relate work help us work our way back to this equation.

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Which is the basic idea of how a plane wave is written okay, so we write a plane wave, so it start here, so you have some wave which is there and then you can write it as A, so this is an equation

which describes a plane wave okay. So, this is an equation which describes a plane wave and what do we mean by a plane wave? We simply mean that the wave fronts are a plane of parallel planes or infinite parallel planes okay.

So, wave fronts are infinite parallel planes okay, of constant peak-to-peak amplitude okay. So, of constant peak-to-peak amplitude, infinite parallel wave, planes are the wave fronts right. So now this is, it is sort of written down in a scalar fashion here, we will just see what exactly we have got here. You must understand here that all these terms here inside the parentheses are set up so that they are dimensionless.

So, for example, I mean so basically this is a phase angle ϕ and similarly kx would be set up such that if you look at kx has the dimensions of n , so k will have the dimensions of L^{-1} okay. So that is how you will see it, so typically in fact kx is, if you write it will be 2π by λ times x and this would ensure that every time x increments by the wavelength you are back in phase and that is how the wavelength is defined.

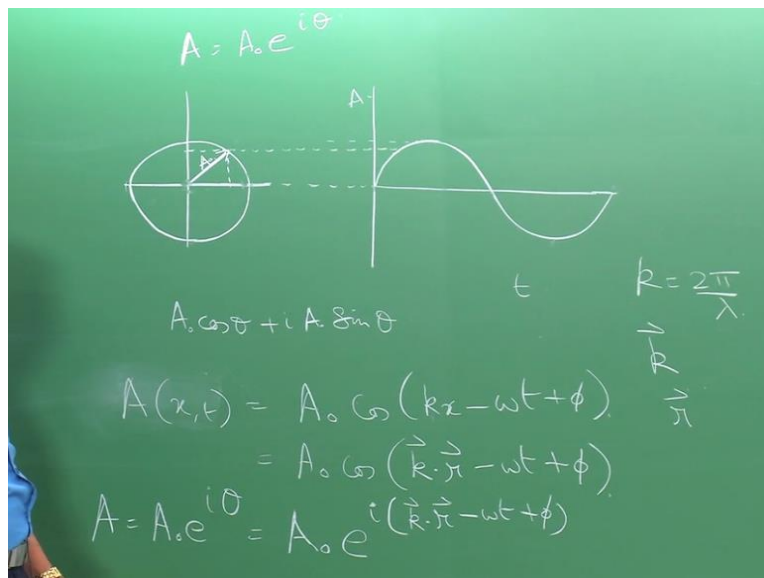
So, we have, by definition when you are, when you draw wave the idea of the wavelength is, if you shift by an entire wavelength, you are back to the same location in that wave in terms of the position right. So therefore, that is the idea of the, so this is λ and therefore when you when x increases by λ you are back in phase with where you started so right, so that is how this is written. So therefore, k typically will have this value of 2π by λ right.

And similarly, Ω for example is $2\pi \nu$ and so that is basically where ν is the frequency and that is also equal to 2π by T , so 2π by T and then and that is how you have ΩT . So, it is a plane wave it means it is a constant frequency wave, it is a constant frequency wave so ν is fixed and then the wave fronts are infinite parallel planes right. So, this is the way we would write a plane wave.

Now any of these waves we basically once you recognize that something is a plane wave. There are different ways in which plane wave is represented mathematically, so this is one way in which we represent it. Another one is the complex notation okay, so using complex notation also you can represent a plane wave. So, for example you could write $A = A_0 e^{i\theta}$ okay.

You can write $A = A_0 e^{i\theta}$, so this will give you $A_0 \cos \theta + i A_0 \sin \theta$ okay. So, this is another way in which you can represent a plane wave. So now for example if you see this notation, what and how let us say this notation represents that wave that you see there, the way to see it would be like this I just draw that wave here, again okay.

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So, let us say this is time and this is your amplitude. And similarly, you can have, I just circle here and what we are saying is that; you know if you just take this I mean I have just hand drawn it but basically it is a circle. So, this is a vector, you basically you can have this as A , and then you will have the two components $A \cos \theta$ and $A \sin \theta$ right, so $A \cos \theta$ so that would then therefore be that equation $A \cos \theta + i A \sin \theta$ or A_0 .

If you want to call it A_0 , $A_0 \sin \theta$ and this is how it would relate to; so, when this is down you are starting here and then as this goes up there and as it comes down here, you come back here, then it comes back down here, you are here and then it comes back up here, we are here. So that is how this representation relates to this representation and that is how we have this complex notation okay.

So therefore, the point being that you can represent a wave using this equation right. So that is the point that we wish to make. So now our plane wave, we can now represent using a similar notation also keeping in mind that we are actually looking at the wave. In this case we have we have written, so we just write that equation now, we have A , I mean or rather we will have.

We put it down here A of x of t and instead of just using k and x because we are going to use vector notation, we will use $\mathbf{k}$ and $\mathbf{x}$ and we recognize that this $\mathbf{k}$ is in the reciprocal, so $\mathbf{k}$ as I said is in the $2\pi/\lambda$ and $\mathbf{x}$ is a real space for this, this has the dimensions of reciprocal space. So, this is L^{-1} dimension, so this is a quantity in reciprocal space.

So, we can use the wave vector corresponding to this which would then also incorporate the direction of this wave and then instead of simply using x we could also use $\mathbf{r}$. Please note that at this point this $\mathbf{k}$ is in the reciprocal space and it could be, it could have wide range of values. So, it is a general vector in reciprocal space, this is also a general vector in real space. So, we are not putting any constraints on it okay.

So that is why we are using small $\mathbf{r}$ here, so the same thing can be written as $A_0 \cos(\mathbf{k} \cdot \mathbf{r} - \Omega t + \phi)$ right. And now we can use represent the same wave using the complex notation which is simply, where the θ is this now this argument that you have here. So therefore, we can write instead of having okay.

So, $A = A_0 e^{i\theta}$ is the same as $A_0 e^{i(\mathbf{k} \cdot \mathbf{r} - \Omega t + \phi)}$ within brackets or within parenthesis $\mathbf{k} \cdot \mathbf{r} - \Omega t + \phi$ right. So, this is the complex notation we have used to represent the plane waves that we are interested in right. So now what we will do is that we will take this notation, you already see that there is some indications that we are getting closer to the notation that we had at the beginning of the class.

And then we will work on it, so the, what we will now do is we are now interested in waves, we are not interested in the or immediately interested at what is the consequence of the time in it. We are interested in what is happening with respect to space. So, we will assume that it is at constant time okay, it could be some constant time maybe zero time whatever it is we will assume it is constant time.

The phase differential difference is just a constant phase difference, so all of those, these two terms we will treat as constant and so we can remove them from this equation in the sense that we can incorporate or absorb them into the constant in the front right. So, we will simply have this term multiplied by another term which has these two pieces and then they all get incorporated into A_0 . So just to write it down specifically we just write it down there and we will take a look right.

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$$A(x,t) = A_0 \cos(kx - \omega t + \phi)$$

$$A = A_0 e^{i(\vec{k} \cdot \vec{r})} e^{i(-\omega t + \phi)}$$

$$A = A_0 e^{i(\vec{k} \cdot \vec{r})}$$

$$A_0 e^{i(\vec{k} \cdot \vec{r})} = A_0 e^{i(\vec{k} \cdot (\vec{r} + \vec{R}))}$$

$$A_0 e^{i(\vec{k} \cdot \vec{r})} = A_0 e^{i(\vec{k} \cdot \vec{r})} \cdot A_0 e^{i(\vec{k} \cdot \vec{R})}$$

So, what we will do now is, we just write the same equation here right. And these two we are treating as constant, so this whole thing will absorb into here, so and we simply continue to call it A_0 , we are not really concerned about the, that aspect of it as much right now. The exact value of A_0 is not of relevance to us.

If you want you can call it A_0 prime, we will just leave it at A_0 for now, e to the power $i\vec{k} \cdot \vec{r}$ okay. So now we have a plane wave. Plane wave being represented by e to the power $i\vec{k} \cdot \vec{r}$, where $\vec{k}$ is any vector and vector in reciprocal space does not have to be a valid reciprocal lattice vector it can be any vector and a corresponding real lattice vector, which could again be sorry a real space vector.

So, in real space is $\mathbf{r}$ it does not have to be a real space a valid real space vector okay, so this is what we have. Now, so these are all sorts of plane waves that can that are possible, we are interested, so we choose now, we make a choice now, which is what leads us to the specific reciprocal lattice.

Because please understand you have a real space lattice and we are making some conditions based on which we select the reciprocal lattice corresponding to that real space lattice right. So, in this description, the condition that we are using is that we would say, we would like to select plane waves such that they have the same amplitude when they are shifted by a real lattice vector okay.

So, whatever is the value of this; so, if you have a real lattice, so I just draw some points here, so this is the origin, you have a point here, you have a point here. So, on this plane there are some lattice points okay, so there are some lattice points on this plane. So now what we are interested in are the set of planes sorry the set of the plane waves which relate to the real lattice.

In such a way that the value of the amplitude of that plane wave, when it is at some lattice point, is the same value that it attains when it comes to the next lattice point, the same value when it attains when it comes to the next lattice point and so on. So, or at any point you take a valid very real lattice vector and if you shift simply shift we move to a location further down in the lattice where you have shifted by a valid lattice vector.

You want the plane wave to have the same amplitude okay. So, this is the rule we are imposing, so you could say I mean what is the purpose in it but that is the, that is how we are defining the reciprocal space corresponding to it. So, the idea is that we are looking we are interested in plane waves which give you the same value of amplitude, when you move in real space through valid lattice vectors.

So, in other words we are moving by valid values of $\mathbf{R}$, upper case $\mathbf{R}$ okay. So, you shift the wave by a valid uppercase $\mathbf{R}$, which means it could be anything, it could be starting from here, this is the valid uppercase $\mathbf{R}$, this is a valid upon case $\mathbf{R}$ and so on okay. So, you it does not matter where the wave is you add an uppercase $\mathbf{R}$ to it, you shift, shifted by a valid real lattice vector.

And you could even, I mean you can even start in from some place here and then shift it by that R , okay. So that that is the point we wish to make. The shift is the, is a valid value right, so that is what we are interested. And when you do that the amplitude should work out to be exactly the same okay. So that is the point that we want to do. So, we are interested in those plane waves okay.

So, what is the significance of it mathematically given that your wave is being represented by this equation? So, it means that you have at a given location R , some so let us say you start at origin you arrive at a location R , the amplitude of this wave is simply $A_0 e^{i\mathbf{k} \cdot \mathbf{r}}$, at this location $\mathbf{r}$. Now from this location $\mathbf{r}$, we are moving a capital R , which means a valid or uppercase R which means a valid lattice displacement.

We are making from here starting equivalent of a lattice point to a lattice point that much displacement we are making. So, you add that to this, so you will now have the amplitude being given as $A e^{i\mathbf{k} \cdot \mathbf{r} + \mathbf{k} \cdot \mathbf{R}}$ okay. So, this is a, what we have done is you are originally at $\mathbf{r}$ you have moved by further, you know lattice displacement which is this R , capital R here.

And so therefore you have $\mathbf{k} \cdot \mathbf{R}$ instead of what was originally simply $\mathbf{k} \cdot \mathbf{r}$ is now $\mathbf{k} \cdot \mathbf{r} + \mathbf{k} \cdot \mathbf{R}$ okay. So that is what we have done here and so these two amplitudes are now; we have said that we are interested in waves, which have this situation with respect to a real lattice that we have selected okay, so we have originally selected a real lattice and for that we are interested in a set of waves.

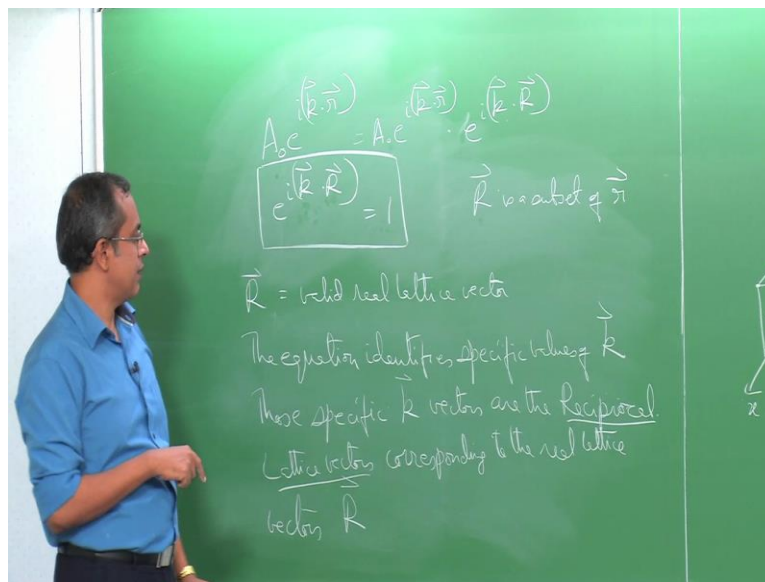
Which relate to that real axis, to the real lattice, such that this relationship holds? That we move that move the wave by, move by and no real lattice vector and then the amplitude is the same okay. So, the two things that we have selected are that first of all that there is a real lattice that we have selected and for that we have applied this particular constraint that we will arrive at this behaviour.

So, for this equation to hold true, we simply have this is A_0 , so this for this relationship to hold true, we simply have okay, so you will have this, so we have $\mathbf{k} \cdot \mathbf{r} + \mathbf{k} \cdot \mathbf{R}$. So, product of these two and this is equal to, at this original value that you have here right. So, $A_0 e^{i\mathbf{k} \cdot \mathbf{r}}$

small r or lowercase r is A am sorry not A_0 the power i same term shows up at both places multiplied by a second term.

Which is $A_0 e^{i\mathbf{k} \cdot \mathbf{r}}$ dot uppercase $\mathbf{R}$. So, the direct implication of this equation is that this term here, so these two will cancel out so this becomes 1 and therefore you have $A_0 e^{i\mathbf{k} \cdot \mathbf{r}}$ dot $\mathbf{R} = 1$, so we, which is what we will write down here.

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I just rewrite that equation here, I am sorry there is no second A_0 here there is simply e to the power $i\mathbf{k} \cdot \mathbf{R}$ okay. So, there is no second A_0 here, that is A_0 is not here, I can remove it right. So, you have, so this is the equation we have $A_0 e^{i\mathbf{k} \cdot \mathbf{r}} = A_0 e^{i\mathbf{k} \cdot \mathbf{r}}$ times $e^{i\mathbf{k} \cdot \mathbf{R}}$, so the two terms show up here right. So therefore, this implies that $e^{i\mathbf{k} \cdot \mathbf{r}} = 1$ okay.

And this is the equation we started with okay, so we have arrived at that equation. So now still we have explained a few things and arrived at this equation. Let us just reconsider what we have done here and understand the significance of what we have arrived at. So, we basically had a real lattice, so that or something that we selected with which we were working, we also had and which when these r values were defined.

We also took a plane wave, which could be any wave and that the r , even though a quantity r exists and it is a vector in real space. That vector would be any vector, so that was the small r , lowercase r that we had. And then we also had k which is a reciprocal lattice vector but it could be any vector in reciprocal space, I am sorry not reciprocal, any vector in reciprocal space.

And therefore, we had this, we had we wrote down the equation for the plane wave, we then wrote, wrote it down in complex notation and then we applied this restriction that the wave should be such that the amplitude of the wave works out to be the same when you move by a real lattice vector and then you arrive at this value. So now in this equation the manner in which we have arrived is such that this is this is now a valid real lattice vector.

So, R is real lattice vector, so this means, the R cannot take arbitrary values okay. So, it cannot take arbitrary values, it has only specific values that are allowed okay. So now if you look at this equation, therefore since there are only specific values allowed for R . For this equation to hold, the k values that enable this equation to hold, will also be specific values of k okay.

So originally if you see the dimension wise this is simply a quantity in reciprocal space. So, in principle you can have any value in reciprocal space but this equation is holding true, but it is not holding true in all conditions, it holds so true only under those conditions, where this is a valid real space lattice vector.

And therefore, those are only a small subset of the all possible R that you have. So, R is a subset of r okay, so it is a subset of r and therefore this could have taken any value, whereas this can only take specific values right. So therefore, this is only holding specific values corresponding to that this can only hold specific values, such that this equation holds.

Therefore, this equation implies that there are particular values of k for which corresponding to each value of R for which this equation and hold. So, this equation identifies okay, so this equation identifies specific values of k all right. So, it identifies specific values of k and those correspond to specific values of R , such that this equation becomes one, those specific values of R are from the real lattice vectors selection of real lattice vectors.

And this then therefore forms a specific set of k values corresponding to that. Those specific set of k values, so this but this iden, the specific values of k that you are selected, those specific k values or k vector, are the reciprocal lattice vector corresponding to the real lattice vectors R okay.

So, this equation identify specific values of k and those specific k vectors that are being identified this, by this equation are the reciprocal are the ones that we are referring to as reciprocal lattice vectors, are the reciprocal lattice vectors not arbitrary reciprocal lattice vectors they are reciprocal lattice vectors corresponding to the real lattice vectors that you have selected which is this capital R okay.

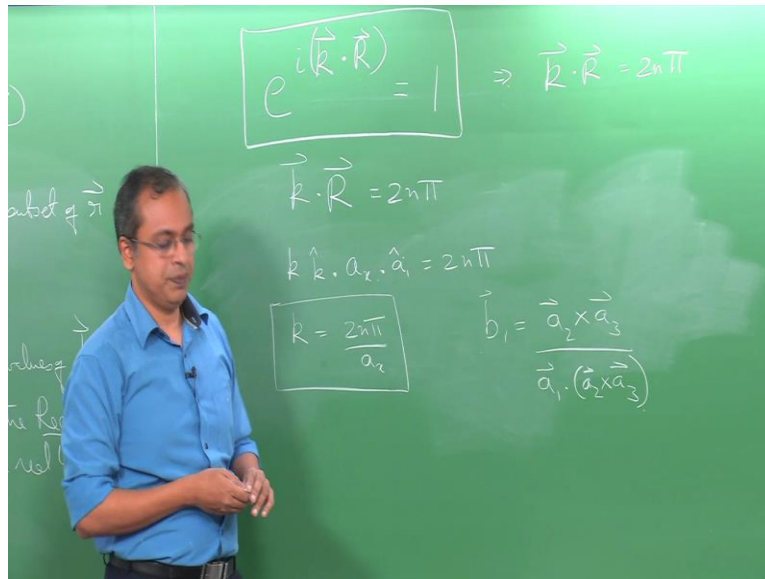
So, you could select the simple cubic lattice in which case you will have a collection of R vectors corresponding to the simple cubic lattice. And if you use this equation the k vectors that you will get out of it will help you create the reciprocal lattice corresponding to the simple cubic lattice okay. Similarly, you could have a Body Centered Cubic lattice, so then you have a specific collection of R values corresponding to the Body Centered Cubic lattice.

Then you apply this equation you will get a set of k back, k vectors which would then be the reciprocal lattice corresponding to that Body Centered Cubic lattice, similarly Face Centered Cubic lattice. So, like this you can continue doing, so therefore this equation by the nature of how it has come about helps you identify those particular set of k vectors which enable this, the amplitude of that plane wave to be the same when you move by those values okay.

So that so that is how you get to the reciprocal lattice or corresponding to that real lattice right. So, the points are the key points are that when you finally arrive at this equation, you started out with general values of r and general values of k . You did not have any control on them, by the time you arrived here you have specific values of r and therefore corresponding to that specific values of k and therefore this helps you identify a particular set right.

And therefore descriptively, I mean this shows you how you are creating a set of quantities or you identifying a set of quantities in reciprocal space corresponding to the real lattice quantities okay. We will explore this thing a little bit more, just to understand what we are dealing with here right. So now we will come back here.

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We have $e^{i\vec{k} \cdot \vec{R}} = 1$, so this implies should be equal to $2n\pi$ okay. If that is true then your $\cos \theta + i \sin \theta$, will enable you to get you a 1 right. So that is because that is the θ value that you have there, right. So, we can write this as a value k , so we will just, I will just clear the board here, so we have $\vec{k} \cdot \vec{R} = 2n\pi$, so let us assume that you know this is, we are looking at just relate to something that we are familiar with.

We will assume that this is the $\vec{a}_1$ vector that we are looking at, so you will have a value k and say a unit vector $\hat{k}$ dot the value a_x , which is the modulus of the vector in the a direction times a_1 . So, this is what we will have and we already said $\vec{a}_1$ dot, the if it were in the same direction this is this would-be b for example and therefore those two would become 1 and therefore dimensionally you can see how this would-be $k = 2n\pi$ by a_x .

So, in principle you can at least see, I mean this is for a specific selection that we have done, I mean so it does not have to come to exactly this, I am making a selection that this is $\vec{a}_1$ and for this to hold then this would be $\vec{b}_1$ and then only this equation would hold. Then $\vec{a}_1$ dot $\vec{b}_1$ as we said this one and therefore k will be equal to $2n\pi$ by a_x . And this equation that we arrive at is consistent with the equations that we have derived in our previous classes' right.

Where we did it in a very material science approach so to speak, where we simply said that you define a real vect in real space by a_1, a_2, a_3 and you define reciprocal space by b_1, b_2, b_3 . And then we see, we had all those definitions that you know, you will have b_1 given by $a_2 \times a_3$ by b . So b_1 , so when you do these kinds of definitions they do relate to each other right.

So that is the point that we want to highlight, I will also point out that invariably because we are dealing with the lattice and waves going through the lattice and so on. That is how this 2π comes in from the perspective of the phase and so on of the waves. The, which you do not sometimes see in the material science the description of reciprocal space. But otherwise they are actually consistent with respect to each other okay.

So that is how these quantities relate and that is how the reciprocal space which we define in material science context relates to how we define in the physics context. So, in physics books you only see this equation and they will tell you $e^{i\mathbf{k} \cdot \mathbf{R}} = 1$, defines the set of lattice vectors in reciprocal space, which are the reciprocal lattice corresponding to the set of $\mathbf{R}$ vectors in real space okay.

So, I will just briefly summarize the discussion we have done in this class and with that we will halt. So, we started out by saying that this is the equation that physics books show you, for reciprocal space. Then we discussed the fact that in both in real space as well as reciprocal space, we can have vectors which are you know random in the sense that they could start or they need or they need not necessarily start at a lattice point.

They need not necessarily end at the lattice point, so in both these spaces, where the reciprocal space as well as real space you can have a general vectors, which do not have to necessary start or end at all at this point. You can also have specific vectors which do start, which do, which are required to then start at a lattice point and end at a lattice point right. So that would be the difference between those two.

I highlighted at that point that in this equation the $\mathbf{R}$ then represents those specific vectors which start at the lattice point and end at a lattice point, so this is a subset of all the possible vectors that

are available to you in real space. Then we looked at the, we came here, we looked at a plane wave we wrote down what a plane wave is.

And the fact that this simply means it is the constant frequency wave, it is something that has you know the wave fronts or planes of are infinitely parallel planes of constant peak to peak amplitude. And then we also said that you know this is one way of representing a wave and that is how it would be and these quantities are written such that this has a reciprocal space dimension that has a real space dimension.

And also that we are interested in the space aspect of this equation, we are not so much interested in the time aspect and in as far as this definition goes, derivation goes. And then we then saw that you know the same equation can now be written in terms of a complex wave notation and therefore you have $A = A_0 e^{i\mathbf{k} \cdot \mathbf{R}}$. And then you also have this additional term here which is present out here.

And we basically absorbed that into this A_0 , so that is what we got here as this equation. And then we said that you know, so this is a way and we said that in we are interested, so this has real space quantities it has reciprocal space quantities. We said that, we are interested in those plane waves, which have this behaviour that the amplitude will work out to be the same, when you move by real lattice vectors with respect to specific real lattice.

So that implied mathematically you require $A_0 e^{i\mathbf{k} \cdot \mathbf{R}}$, should be equal to $A_0 e^{i\mathbf{k} \cdot \mathbf{r} + \mathbf{R}}$. So, which therefore mathematically implied that $A_0 e^{i\mathbf{k} \cdot \mathbf{R}}$ would be equal $A_0 e^{i\mathbf{k} \cdot \mathbf{r}}$ times $e^{i\mathbf{k} \cdot \mathbf{R}}$. And when you go through this equation you arrive at this you come back to this equation $e^{i\mathbf{k} \cdot \mathbf{R}} = 1$, because the other terms cancel out right.

And then I also highlighted again that this is the this is a specific collection of real lattice vectors, so whereas originally, we had all possible $\mathbf{k}$ values allowed for us in that in the general equation of a plane wave. We have restricted ourselves to specific values which are for this particular value of $\mathbf{R}$ and therefore corresponding to that there are only specific values of $\mathbf{k}$ that can be looked at.

And then which would then still enable you to reach this value of one right. And we also saw that this simply means that $\mathbf{k} \cdot \mathbf{R} = 2n\pi$, and then if you assume that a_1 and these a_1 and b_1 axis then you will arrive at $2n\pi$. And therefore, $\mathbf{k}$ equals this particular dimension right. So that is the discussion we wanted to, I wanted to convey to you in this class.

In and to see how the physics description of reciprocal space corresponds to the material science description of material reciprocal space which we had already seen in our previous classes right, so with this we will halt for today, there ahead we do still have a couple more points to discuss which are interesting. We are going to look at how the reciprocal space is the Fourier transform of real space.

So, they are related in some ways the connection is sometimes not apparent to begin with. So, we look at it you know, we arbitrarily say that reciprocal space is defined in a certain way. We use these definitions and proceed but we are going to see that actually they are mathematically related. And that the reciprocal space is a Fourier transform of the real space.

And then I think the significance of the relationship becomes deeper and that is something that we would look at okay. So, with that we would halt for today. Thank you.