Introduction to Solid State Physics
Prof. Manoj K. Harbola
Prof. Satyajit Banerjee
Department of Physics
Indian Institute of Technology, Kanpur

Lecture – 36
Reciprocal Lattice Vectors Part-I

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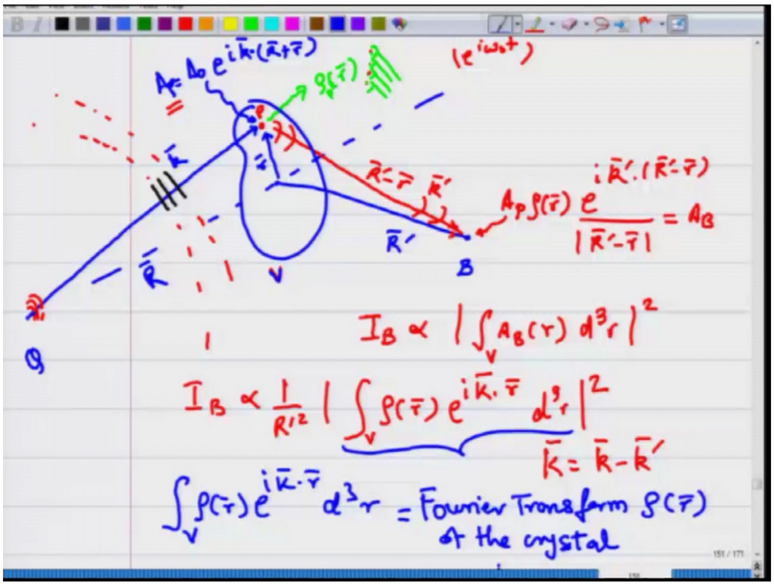

So, in our last lecture, we had begun investigating the scattering of electromagnetic waves from a material. And we had electromagnetic waves which are basically X-rays in this case are impinging on the material, where you have plane wave fronts which are part of spherical waves, but they are very large because this vector the source is far away from your crystal. The way fronts are there for considered to be plane wave fronts. They impinge on a point P on the crystal and the amplitude of the electric field which is reaching point P from the source Q is A naught into a plane wave form e raise to i k dot R plus r. There is also a time dependent part which is given by e raise to i omega naught t which I am not considering.

So, this is the amplitude of the signal or the electromagnetic wave which is reaching point P. Stronger the amplitude more intensity or more electromagnetic wave will get scattered; smaller the amplitude less will be the intensity or the amplitude of the scattered wave. Furthermore, if you have large number of points at this point P, each of these points will act like scatterers, and they will generate the secondary wave which is scattered from point P.

So, if you want to look at the intensity or the amplitude of the wave which is scattered it will not only depend on the amplitude of the incident wave, it will also depend on the density. It will be proportional to the density of particles which are present at point P. More the number of particles at point P, they will act as secondary scatterers, they will assume them to be all in phase and they will scatter more intensity or more light or more electromagnetic point B, it will through more because all of them act as secondary scatterers. If you have one point of course then it will be less, if you have more 10 points at point P, then the effectively each of the 10 points is acting like a scatterer they are generating secondary waves.

So, the amplitude of the wave which reaches point B is dependent on the intensity of the incident wave into the density. And this is the form of the spherical wave which is reaching point P, K prime is the wave vector of the spherical wave front. And then we wrote down the intensity which is proportional to the square of B which is coming from all such caterers like point P which is distributed across your crystal. So, we will integrate this amplitude over the entire crystal to get the net intensity at point B and that will be proportional to this amplitude integrated over the crystal square. And we showed that this intensity, therefore will be will go down as 1 by R square the further you move this point B away from the crystal the intensity will go down as 1 by R square inverse square law.

But it will depend on this quantity rho of r which is the density of the crystal at each point r into e raise to i k bar dot r bar K capital K integrated over the volume and, where K is the difference between the incoming and the outgoing wave vector. This is the intensity of the light which is or the electromagnetic wave which is reaching point P. And we can see that this intensity is proportional to this quality, it depends on this quantity rho of r e raise to i K bar dot r d cube r, which is integrated over the volume of the crystal. If you see this quantity this is nothing else but the Fourier transform of your density rho of r, rho of r of the crystal. So, the intensity directly depends on the Fourier transform of rho of r.

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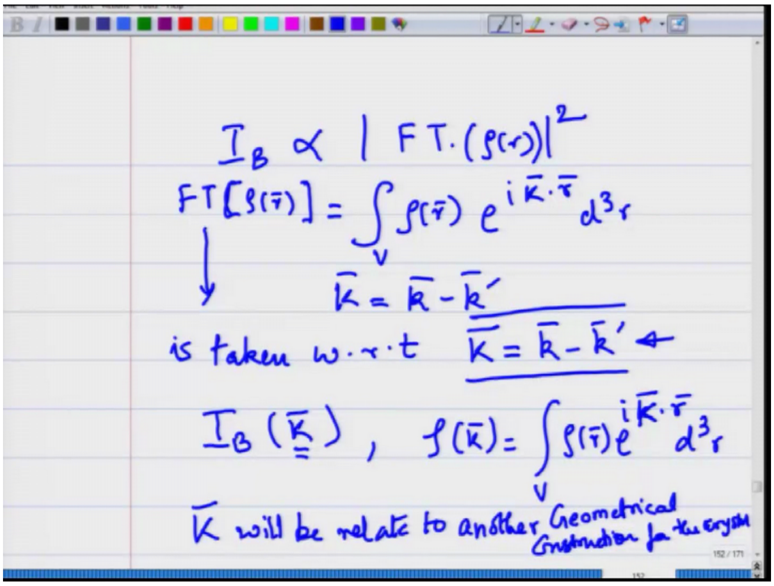

The intensity at point B is related to the Fourier transform of rho of r of the crystal ok, where this Fourier transform of rho of r of the crystal is nothing else but integral rho of r e raise to i K bar dot r d cube r over the volume ok, integral of rho of r e raise to i K bar dot r. And this Fourier transform is taken with respect to this wave vector which is k minus k prime. So, the intensity of the scattered light now depends on the Fourier transform of the density of the crystal.

The density distribution of the crystal the Fourier transform of that density is plays a role in determining the intensity of your scattered light. And therefore, the I of B is a function of this quantity K which is the difference between the incoming wave vector and the outgoing wave vector. And you take a Fourier transform the rho of k is nothing else but the Fourier transform of rho of a r e raise to i K dot r d cube r. So, if you take the Fourier transform of the density of your crystal, then you will get this quantity and I of B is related to square of this quantity.

So, we have an important quantity K out here. And we will see that this K will be related to another geometrical construction for the crystal. So, this K will have important consequences, because it determines the intensity of the scattered light. And we will see that this K will be related to some other geometrical construction associated with the crystal. So, we will leave the point of scattering of electromagnetic waves from the crystal for now, and move on to looking at the Fourier transform of the density of the crystal.

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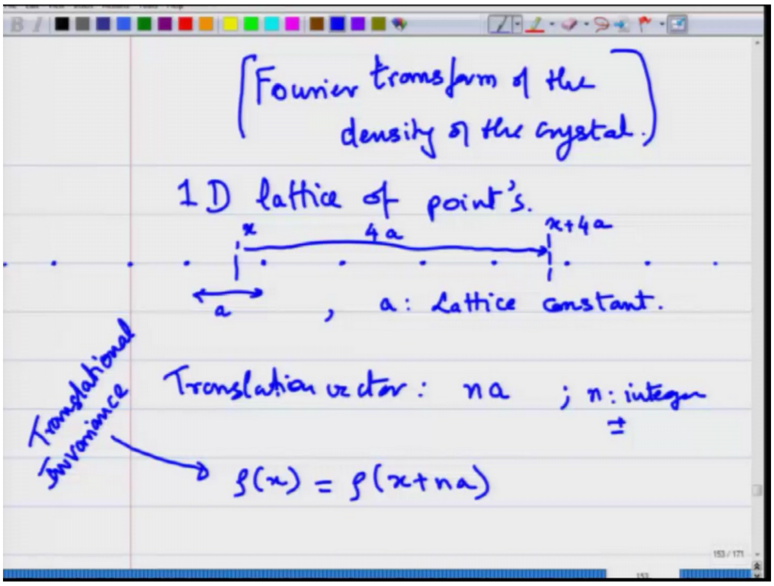

Fourier transform of the because we know that the intensity of the scattered light depends on the Fourier transform of the density of points, the number density of points on the crystal, and what is the distribution of that number density. So, let us look at first a 1D lattice of points. So, what is a one-dimensional lattice of points or a one-dimensional crystal, a one-dimensional lattice of points is points which are periodically arranged in one dimension.

So, this is a 1D lattice of points where a is the lattice constant, a is the lattice constant. Now, as you know that for a Bravais lattice if you go from any point to any other point if you translate by the translation vector then your distribution of atoms or the lattice points around you should look identical that is one of the very important aspects of a lattice of a Bravais lattice specifically.

In the 1 D lattice, what is the translation vector, the translation vector is nothing else but n times a, since it is one-dimensional you can only move in 1 D. So, I am not drawing the vector, but it is just an integer where n is an integer it can be plus or minus it. You can move in either direction. You can move by n times a or you can move minus n times a ok. And the requirement is that your distribution of points, when you move by a distance or you move travel by the translation vector the distribution of point should look identical around you.

So, let us start from a position x this is an infinite lattice. So, it goes infinitely in either directions. So, if this is my starting point in the lattice and the distribution of points around x has a density rho of x namely the number density which is present around x, then if I move by say to another position which is say 4 times the lattice parameter this is x plus 4 a. If I move from this point to this point, the distribution of atoms should look exactly identical, then it is of course a Bravais lattice.

And this property of the lattice is called translational invariance. This is a very important property of the lattice that if I move from one point and I translate by using the translation vector, then the distribution of points the number density should look exactly identical. And in one dimension I can write it like this that the density of points at point x, where x is any position in the lattice rho of x should be equal to rho of x plus n a.

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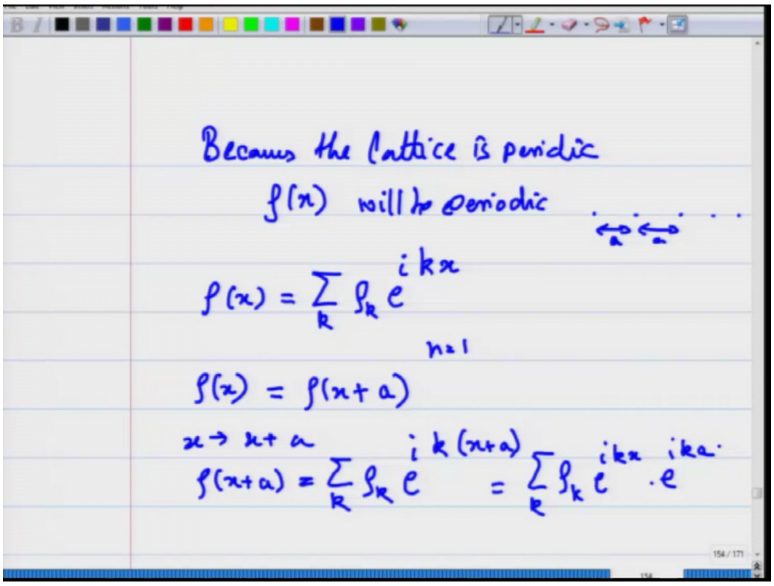

Now, being a periodic lattice, I can take its Fourier transform, because the lattice is periodic, the density rho x will be periodic because I am encountering lattice points after a distance a every time I encounter a distance there is a change in the density ok. So, rho x will be periodic. So, I can write rho x as equal to rho Fourier component e raise to i sum for now let us say k x ok, where I give an index rho k and I take it as a sum overall k ok. So, this is some. So, this is the Fourier transform.

This is a discrete, because it is a discrete lattice, it is not a continuous lattice, I write the rho x as a Fourier transform where I am doing the Fourier transform on a discrete lattice. So, rho of x is written in terms of Fourier components k e raise to i k x, where k are the labels for the Fourier component.

Now, if I want my lattice to be transnationally invariant rho of x should be equal to rho of x plus a ok, where n is equal to 1. So, even if I move by one lattice point, rho of x should be equal to rho of x plus a ok. Then if I take x to x plus a, what is my Fourier transform of rho x plus a, rho of x plus a is summation over k, rho k e raise to i k into x plus a which is nothing else but rho k e raise to i k x into e raise to i k a.

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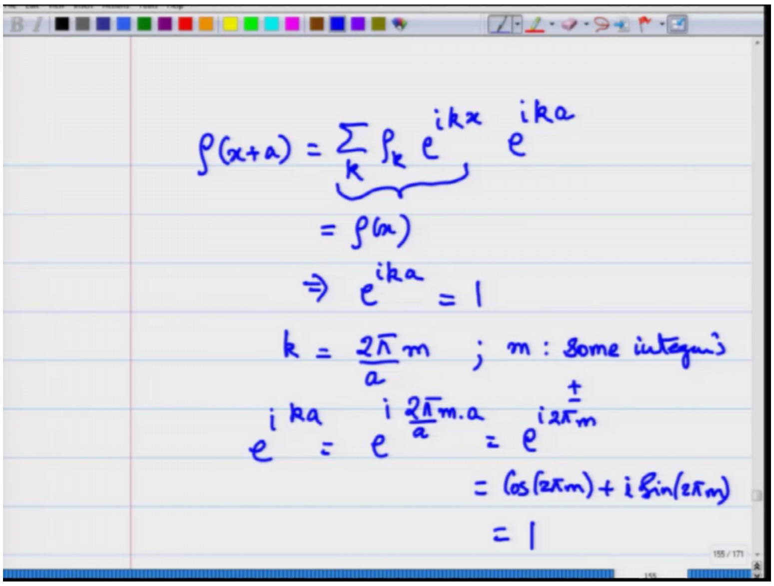

So, rho x plus a is equal to summation over k rho k e raise to i k x into e raise to i k a. Now, for translation invariance this should be equal to rho x. And rho x is essentially this part, which implies e raise to i k a should be equal to 1. And this puts a condition on k as they should be 2 pi by a times m, where m is some integers which can be both positive and negative.

It can be 0; it can be 1; plus minus 1; it can be plus minus 2. But when you put this integer e raise to i k a becomes equal to e raise to i 2 pi by a m into a e raise to i 2 pi m. This is cos 2 pi m plus i sin 2 pi m, where m are positive negative integers this has to be equal to 1. So, the requirement of translational invariance puts a condition on this k that you obtain when you take a Fourier transform of the lattice.

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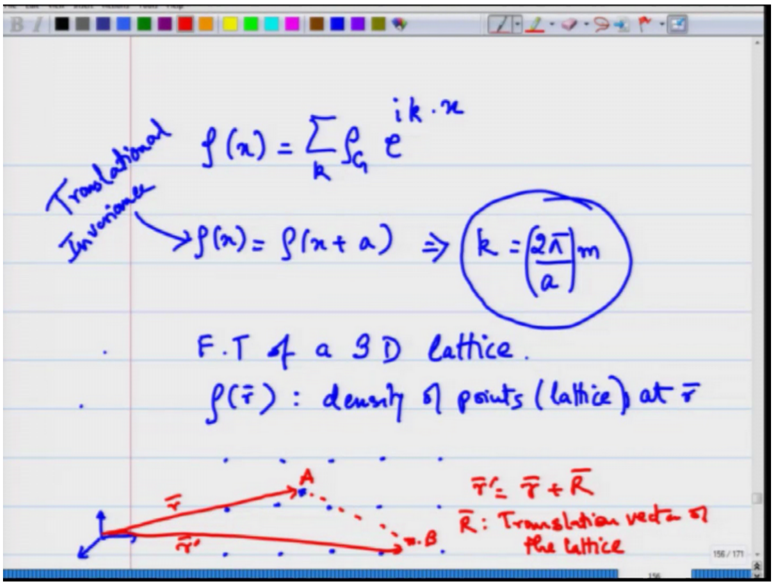

So, if rho of x is written as a Fourier transform this is rho of g e raise to i k x this is a one-dimensional lattice, then by translational invariance requirement this is the requirement of translational invariance suggests that this vector k with respect to which we take the Fourier transform or this k with which we take the Fourier transform with respect to which we take the Fourier transform has to be in integral multiples of this 2 pi by a. We looked at the Fourier transform of a one-dimensional lattice. And we got a condition on your wave vector with respect to which you taking the Fourier transform.

Now, we will look at the Fourier transform of a three-dimensional lattice. So, rho of r is the density of points lattice points at r in the lattice. So, you have lattice points here for just simplicity sake I am drawing a two-dimensional lattice. And the condition so, with respect to some origin you have a point in the lattice which is located by r. Now, translational invariance says that if you move from this point to another point in the lattice from this point in the lattice you move to another point in the lattice r prime, where r prime is equal to r plus capital R, where capital R is the translation vector of the lattice then the distribution of points or the density around these two points A and B have to be identical.

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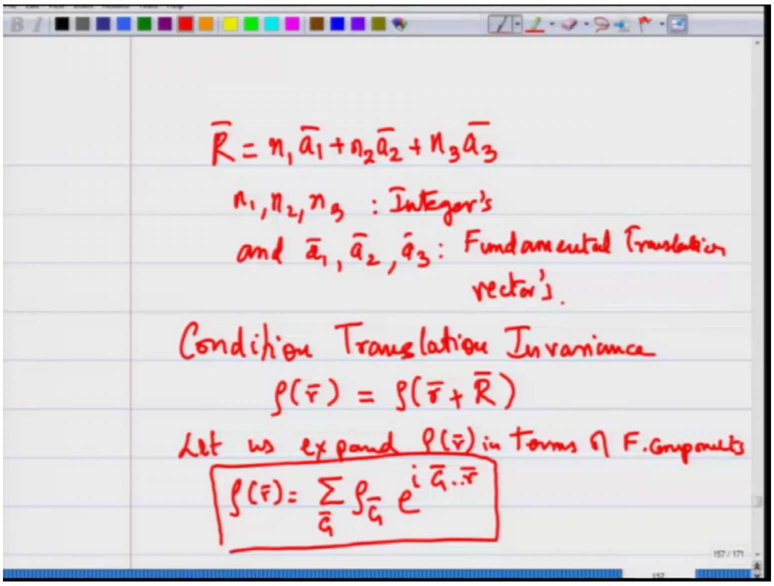

And what is the translation vector, the translation vector is n 1 a 1 plus n 2 a 2 plus n 2 a 2. Where n 1, n 2, n 3 are integers, and a 1, a 2, a 3 are the fundamental translation vectors. These are the fundamental translation vectors of the lattice. So, your condition for translation invariance which is an essential requirement to get a Bravais lattice to describe a crystal structure requires that the density at r point r in the crystal should be equal to the density at point r plus capital R.

Let us expand rho of r in terms of Fourier components. So, rho of r is summation over a vector G with respect to which we are taking the Fourier transform. So, these are the Fourier components rho of G e raise to i G bar dot r bar. This is how I expand my density in the three-dimensional lattice, where I expand it in terms of these Fourier components g is the vector with respect to which we are taking the Fourier components Fourier transform ok, and e raise to G bar dot r.

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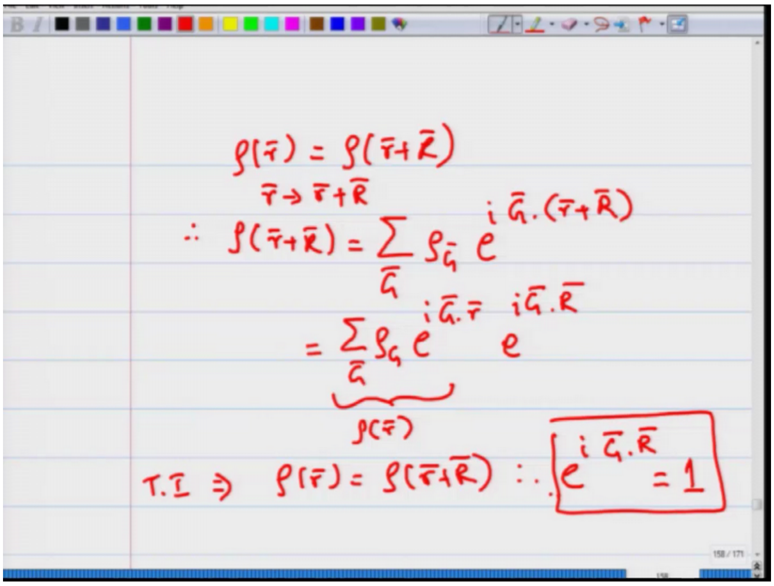

Rho of r should be equal to rho of r plus capital R. So, therefore, if I take r going to r plus capital R, then my density at r plus capital R becomes which is equal to summation of G rho g e raise to i G bar dot r bar into e raise to i G bar dot capital R. This is nothing else but rho of r and translational invariance implies rho of r should be equal to rho of r plus capital R, therefore, e raise to i G bar dot r bar should be equal to 1.

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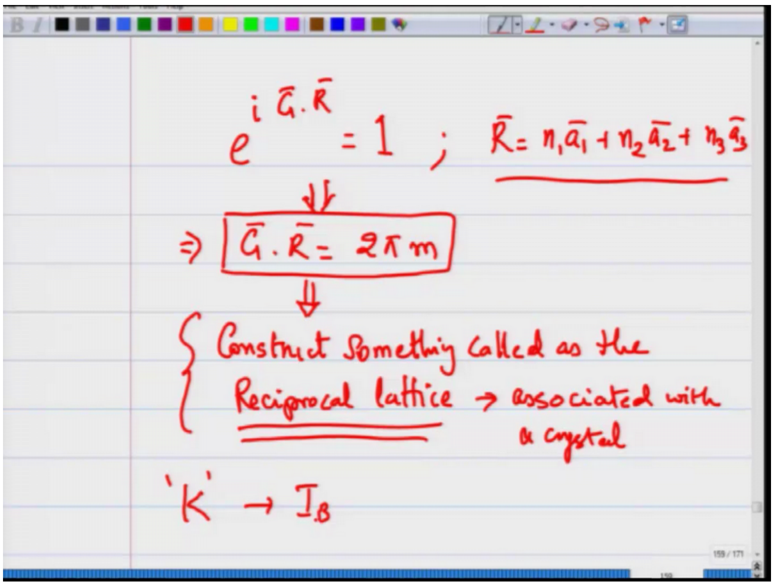

This sets a condition the condition from translational invariance is that G bar dot R bar should be equal to 1, where R is equal to n 1 a 1 plus n 2 a 2 plus n 3 a 3. And this condition that G bar dot e raise to i G bar dot R bar should be equal to 1 implies that G bar dot R bar should be equal 2 pi times some integer. If you take G bar dot R bar is equal 2 pi times some integer, then this will satisfy this condition, the above is satisfied by this condition. And now through this we will be able to construct something called as the reciprocal lattice, which is associated with a crystal.

So, we will be able to do a geometrical construction using this expression to construct something called as the reciprocal lattice, a very important aspect of crystals using this vector G, we have got a condition on this vector G, R is the translation vector which is written in terms of the fundamental translation vectors of the lattice. And using this expression, we will construct something called as a reciprocal lattice which will satisfy this expression. And it will be important for describing various properties of the crystal. We will find that this reciprocal lattice will be related to the capital K that we had found in the scattering intensity of the electromagnetic wave.