Introduction to Solid State Physics

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Lecture - 37
Reciprocal Lattice Vectors Part-II

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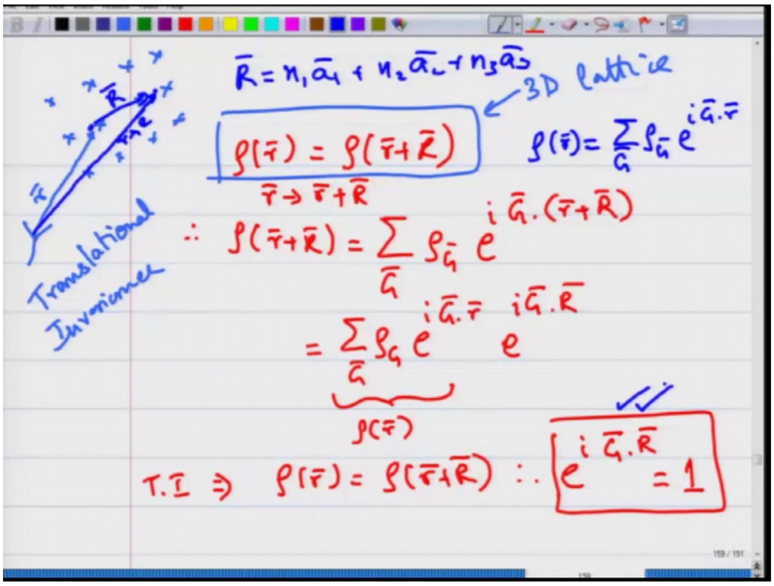

Welcome back to the discussion. And in the last lecture, we had seen that you can take the Fourier transform of a lattice of points whose density at any point is given by this expression. In this is in three dimension, we have done it for one dimension, but this is the general case of a 3D lattice of points. And the requirement rho of r is the number density of points at any point r in the lattice.

So, you have a lattice of points a periodic structure, here I am showing it in two dimension ok. And for any point r in this lattice, the number density at that point is given by rho of r. And the requirement of translation in variance which is an a very important aspect of a Bravais lattice translational invariance requires that if I go from this point r and I translate by an amount which is given by my lattice vector r bar, where this is r plus capital R, then the density at r plus capital R namely at this point should be exactly identical to the density at this point and that is written out here.

And this then satisfies the condition of a Bravais lattice, where this vector R is n 1 a 1 plus n 2 a 2 plus n 3 a 3. This is your translation vector R of the lattice; n 1, n 2, n 3 are the indices of the components along a 1, a 2, a 3, which are the fundamental translation vectors of the lattice. And this translation invariance, so then rho of r you can do a Fourier expansion, rho of r you can write it as summation over some vector G rho G are the Fourier components e raised to i G bar dot r bar where I am taking the Fourier expansion in terms of this vector G. And if I do translation invariance, then the requirement for translation invariance gives me this condition that e raised to G bar dot R bar, R is your lattice translation vector e raised to i G bar dot R bar should be equal to 1.

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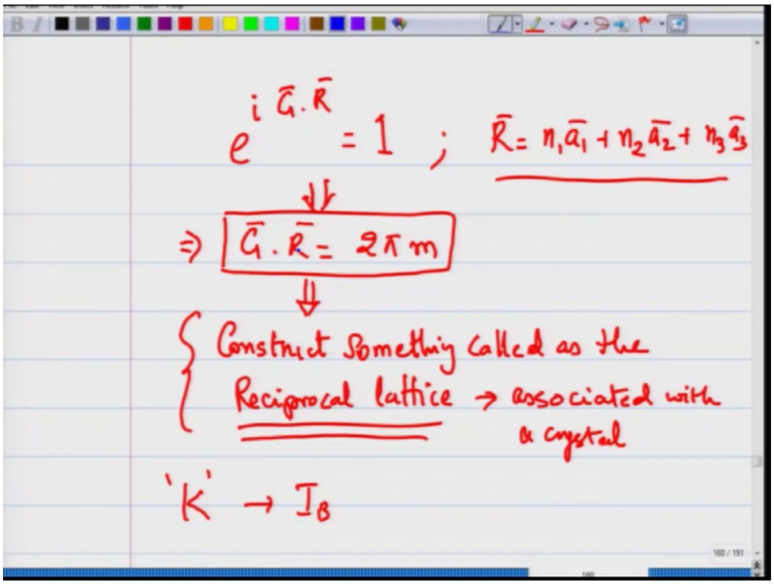

And this suggests that G bar dot R bar is 2 pi m.

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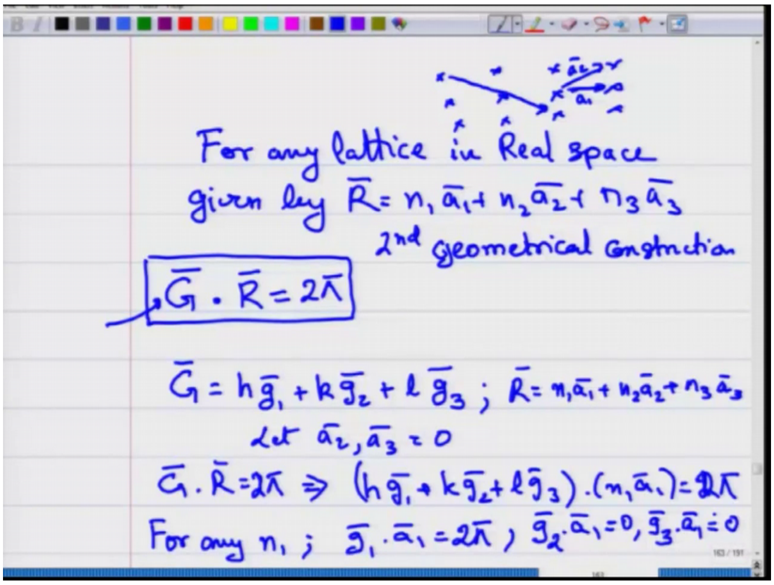

So, for any lattice in real space given by R bar is equal to n 1 a 1 plus n 2 a 2 plus n 3 a 3. For any lattice which is in real space your actual three-dimensional space that we are living in. For any lattice in real space where you can generate the lattice using this translation vector R corresponding to any such lattice you can generate another lattice which is given by this vector G, where G bar dot R bar should be equal to 2 pi. And this vector G is corresponding to taking the Fourier transform of the real lattice. So, corresponding to any lattice in real space which is generated by using this condition namely you have set of points in real space.

So, given a crystalline solid you first make a Bravais lattice using this translation vector, where you can go from any point on the lattice to any other point using this sort of a translation vector. You will have to define your a 1 and a 2 appropriately whatever is your choice that you want to do, and then using this you can generate your lattice points, but you can make another construction. And that second geometrical construction is with these vectors G, where these vectors G satisfy the condition that G bar dot R bar is equal to 1 ok.

Now, we write this vector in terms of we have three components of this vector. We write it has h times g 1 plus k times g 2 plus l times g 3; and R you already know is equal to n 1 a 1 plus n 2 a 2 plus n 3 a 3.

Now, let us say let a 2 and a 3 be equal to 0 ok, then what does this condition mean G bar dot R bar is equal to 1 implies h times g 1 plus k times g 2 plus l times g 3 dot n 1 a 1 is equal to 1, you just satisfy put in this a 2 equal to a 3 and put it back here this is your condition. For any arbitrary value of n 1, this condition can be satisfied by considering g 1 dot a 1 should be equal to 2 pi and so the condition that G bar dot R bar is equal to 2 pi, g 2 dot a 1 should be equal to 0 and g 3 dot a 1 is equal to 0.

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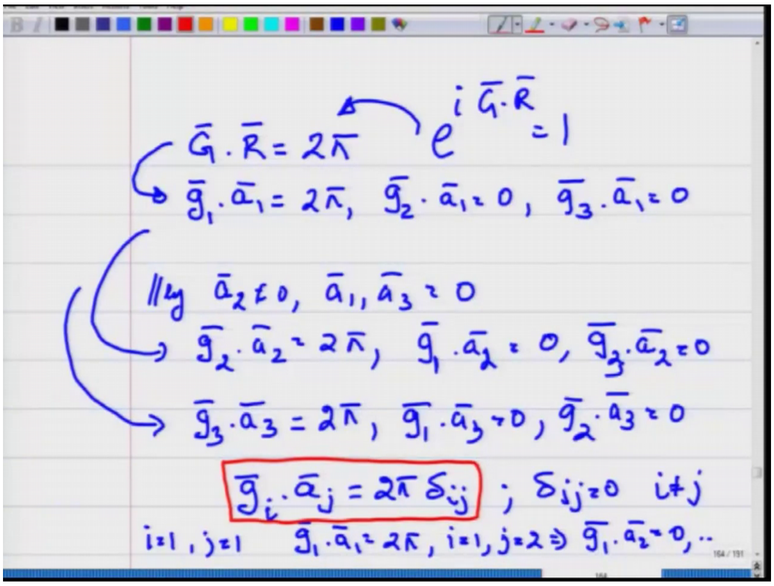

So, the condition that G bar dot R bar is equal to 2 pi gives us our first condition that g 1 dot a 1 should be equal to 2 pi, g 2 dot a 1 should be equal to 0, g 3 dot a 1 should be equal to 0. Similarly, take a 2 not equal to 0, a 1 and a 3 equal to 0. And you will get the condition that g 2 dot a 2 should be equal to 2 pi, g 2 dot a 1 should be equal to 0, and g 3 dot and g 1 dot a 2 should be equal to 0 and g 3 dot a 2 should be equal to 0.

So, this says the above conditions g 1 dot a 1 equal to 2 pi, and g 2 and g 3 dot a 1 is equal to 0 suggest that g 2 and g 3 are perpendicular to a 1. So, this directly gives us way to construct g 1, g 2 and g 3. Similarly, g 2 is having some component along a 2, but g 1 and g 3 are perpendicular to a 2 ok. And you can write down the same thing g 3 dot a 3 is equal to 2 pi, and g 1 dot a 3 should be equal to 0, and g 2 dot a 3 should be equal to 0.

So, the condition that G bar dot R bar which is coming from the condition that G bar dot R bar is equal to 1 this gives us this condition gives us a way to construct these vectors g 1, g 2 and g 3. In general I can rewrite the all these conditions as g i dot a j is 2 pi delta i j where delta i j is equal to 0 for i not equal to j. So, you put i equal to 1, and j equal to 1, then g 1 dot a 1 is equal to 2 pi; i equal to 1 and j equal to 2 implies g 1 dot a 2 is equal to 0 and so on. So, this is a condition that one uses to find out these vectors g 1, g 2 and g 3.

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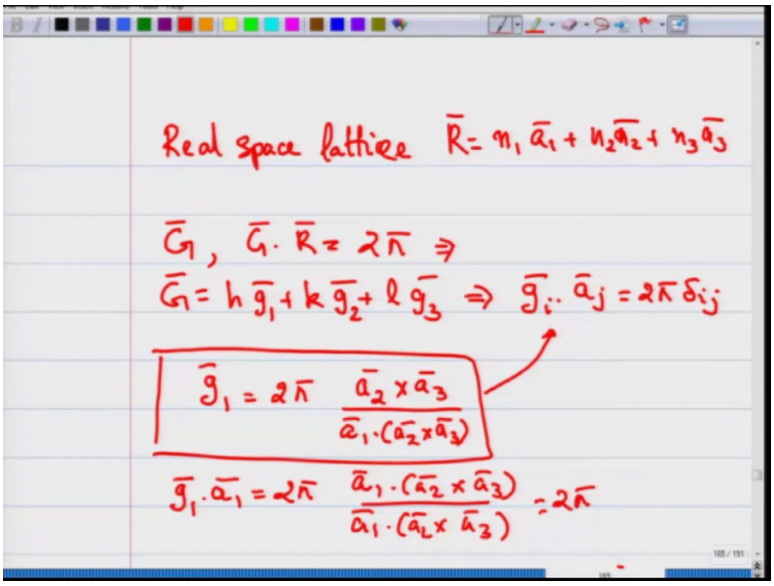

So, corresponding to any real space lattice, real space lattice which is generated by the translation vector n 1 a 1 plus n 2 a 2 plus n 3 a 3, one can find another lattice where G bar dot R bar is equal to 2 pi. And this gives the condition and this G is written as h times g 1 plus k times g 2 plus [vocalize-noise] using the above condition if you know a 1, a 2, a 3, one can construct g 1, g 2, g 3 by using the conditions g i dot a j is equal to 2 pi delta i j.

Now, how can we write, is there a simple way to write this down? There is of course, a simple way to write this down g 1 can be written as 2 pi a 2 cross a 3 divided by a 1 dot a 2 cross a 3, one expression which actually satisfies this condition is writing g 1 like this. And one can easily check g 1 dot a 1 is 2 pi a 1 dot a 2 cross a 3 divided by a 1 dot a 2 cross a 3, this is nothing else but 2 pi.

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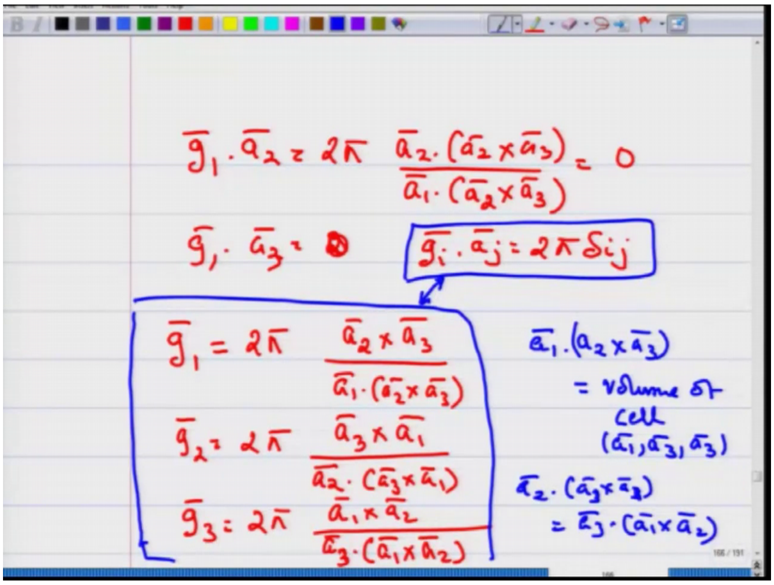

And you can show similarly that g 1 dot a 2 will be 2 pi a 2 dot a 2 cross a 3 is equal to a 1 dot a 3 this is 0, because a 2 is along the plane a 2 is perpendicular to a 2 cross a 3. So, this dot product has to be 0. And similarly g 1 dot a 2 is equal to 0, a g 1 a 3 is equal to 0. So, g i dot a j which is equal to 2 pi delta i j can be generated using the g i which actually satisfy this condition is given as 2 pi a 2 cross a 3 divided by a 1 dot a 2 cross a 3, g 2 which is 2 pi a 3 cross a 1 divided by a 2 dot a 3 cross a 1, and g 3 is 2 pi a 1 cross a 2 divided by a 3 dot a 1 cross a 2.

One can show that if you use g 1, g 2, g 3 of this form they will satisfy this condition. So, from a 1, a 2, a 3, you can generate another set of vectors g 1, g 2, g 3 which can be expressed in terms of a 1, a 2, a 3, but they satisfy a very fundamental condition that g i dot a j is equal to 2 pi delta i j, this is a very necessary condition.

Now, a few words about this denominator a 1 dot a 2 cross a 3 is nothing else but the volume of the cell which is defined by these vectors a 1, a 2, a 3. And a 1 dot a 2 cross a 3 is equal to a 2 dot a 1 cross a 3 which is also equal to a 3 dot a 1 cross a 2. So, at the denominator, all of this is nothing else but the volume of the real space, this is the volume of the cell in real space which is defined by your fundamental translation vectors a 1, a 2 and a 3.

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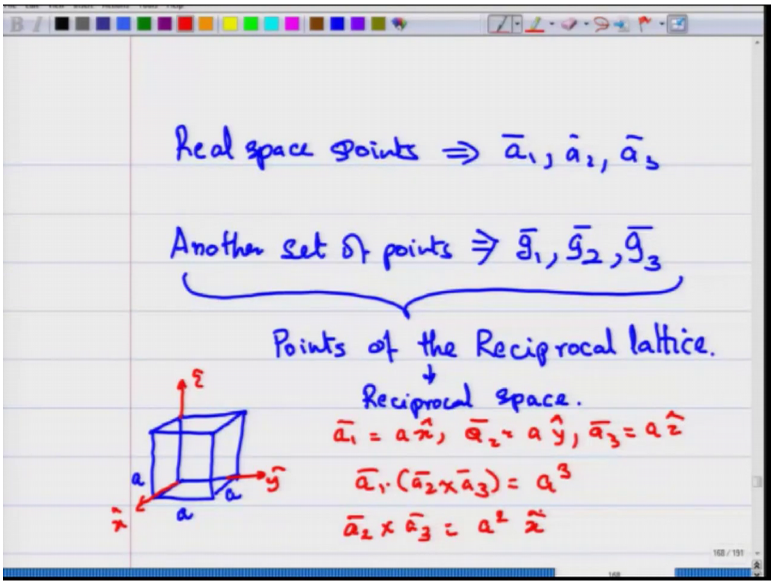

The points which are generated so I have said that you have a set of real space points which are generated with a 1, a 2 and a 3 and you have another you can generate another set of points which are g 1, g 2 and g 3. The points which are generated using this are called the points of the reciprocal lattice. This is a very important concept that corresponding to every crystal, you have a real space lattice. And corresponding to every crystal you can also do another geometric construction where you can define the reciprocal space lattice g 1, g 2 and g 3.

So, corresponding to every real space point which is defined by linear combinations of a 1, a 2 and a 3, you can generate another set of geometrical points both are geometrical constructions for a crystal you can generate a real space lattice using linear combinations of a 1, a 2, a 3. There is another set of points which you can generate not in the real space ok. There is another set of points which you can generate with these vectors g 1, g 2 and g 3. Those are the points which are generated which are called as the points belonging to a reciprocal lattice and they are in a space called as the reciprocal space.

Simply put let us take a cubic lattice with lattice constant as a. And these are your x, y and z. For this cell, you can define a 1 as a x cap, a 2 as a y cap, a 3 as a z cap. a 1 dot a 2 cross a 3 will be the volume a cube, a 2 cross a 3 will be equal to a square y cap cross z cap which is x cap.

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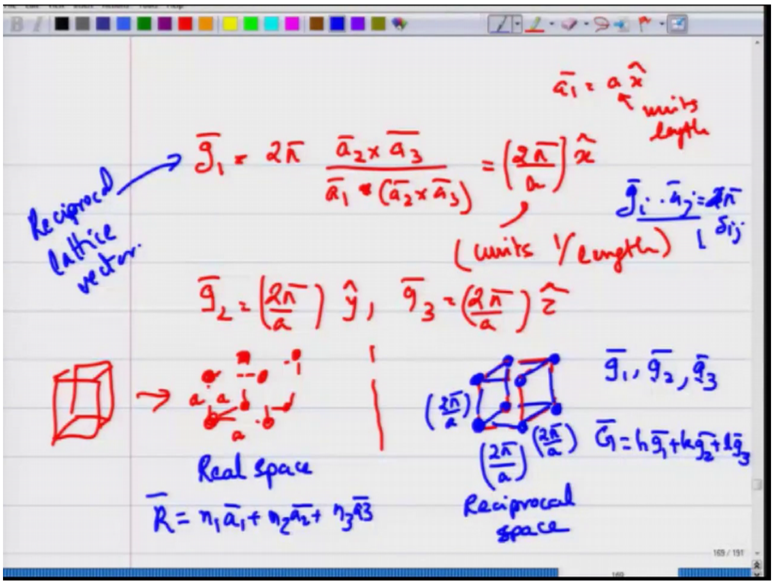

So, g 1 which is 2 pi a 2 cross a 3 divided by a 1 dot a 2 cross a 3 will be equal to 2 pi by a x cap. So, g 1 is along the a 1 direction, if you recall a 1 is a x cap, so g 1 is along the a 1 direction, but whereas in the real space a 1 is a the reciprocal space vector has units of 1 over length. The real space has units of length, the reciprocal space has units of 1 over length. Similarly, g 2 will be 2 pi by a y cap and g 3 will be 2 pi by a z cap.

So, corresponding to a crystal which is cubic, you can in real space generate cubic set of points these are your cubic lattice points in real space whose spacings are a. And you can define your lattice vectors a 1, a 2, a 3. And using those lattice vector a 1, a 2, a 3, you can generate the full space of lattice points, but you can also generate using g 1, g 2, g 3, which is also a square lattice another set of points. Let me draw it in blue.

So, corresponding to this crystal with real space, you can also generate equivalently another set of points which is governed by g 1, g 2, g 3 as given here, which also happens to be a square lattice, but now the lattice constants here are 2 pi by a rather than units of length they are units of inverse of length. So, this is in real space, this is in reciprocal space, reciprocal because they are inverse of length ok.

So, corresponding to every real lattice, you can generate another lattice using your reciprocal lattice vectors. These vectors are called as reciprocal lattice vectors. And your here you have a translation vector r which is written as linear combination of n 1 a 1 plus n 2 a 2 plus n 3 a 3, here your vector which is your translation vector in reciprocal space is h times g 1 plus k times g 2 plus l times g 3.

So, you have for every lattice you can do two types of geometrical constructions, one is the real space which your familiar with a 1, a 2, a 3, linear combinations of a 1, a 2, a 3. And corresponding to the same lattice in reciprocal space, you can generate another set of points with these vectors g 1, g 2, g 3 which you can calculate explicitly using the condition that g i dot a j is equal to 2 pi into delta i j. This condition gave us these expressions which help us to calculate your reciprocal lattice points and the reciprocal lattice is inverse of length. And as you see for the cubic lattice it is 2 pi by a; a is the lattice constant of your cubic lattice.

So, this is a very important concept of a reciprocal lattice corresponding to every real lattice you have also a reciprocal lattice. And it is very useful for understanding the properties of the crystal. By using the reciprocal lattice for a given lattice, you can understand various properties like diffraction of waves through the crystal which we will do next in our coming lecture.