Solid State Physics
Lecture 9
Introduction to Brillouin Zone

Hello, we were discussing the reciprocal lattice and the reciprocal lattice vectors in that context let us now discuss a new construction called the Brillouin Zone. (Refer Slide Time: 00:39)

So, Brillouin gave the statement that the diffraction condition the way he casted it in his statement that is the most widely used in the Solid State Physics. A Brillouin zone is like a Wigners-Seitz primitive cell in the reciprocal lattice. So, what is in Wigners Seitz cell? It is dividing the connection between two lattice points into half and constructing a primitive cell that way. So, the Brillouin zone provides a nice geometry a nice geometrical interpretation of the diffraction conditions. So, we have the diffraction condition that $\overrightarrow{k} \cdot \overrightarrow{G} = \overrightarrow{G}^2$. Now what the Brillouin description does is $\overrightarrow{k} \cdot \frac{1}{2}\overrightarrow{G} = \frac{1}{2}\overrightarrow{G}^2$, this is the kind of description that it provides. So, how do we construct a Brillouin zone? We consider a simple example of a square lattice and try to construct few Brillouin zones in that. Let us put the lattice points first. I am drawing few lattice points for the reciprocal lattice. So, these points are reciprocal lattice points and the corresponding real lattice points could be different. So, I have drawn a 5 by 5 square lattice we will imagine its extension in three dimension for our purpose. Now, let us consider the atom at the center sorry, the site at the center not the atom. And we will consider the nearest connecting the shortest connecting vectors and we will half them using a plane. So, if we consider from this one the nearest lattice site is here, here, here and here. So, if we half this vector using a plane that plane will go like this. If we half this vector that will look like this, if we half this vector it will look the plane halfing it would look like this and the plane halfing this one is this. So, what we got? Looking like a square in three dimension it would look like a cube is the first Brillouin zone let us call let us shade it with yellow. So, yellow is the first Brillouin zone. Now, if we consider the next nearest neighbors let us take another color. So, the next nearest neighbor for this site would be this site here and we will half that vector using a plane like this; this is another nearest neighbors neighboring site we will half this with a plane like this. Another G vector for the nearest lattice site would be this one we would half that vector with a plane like this and another is here we will half that with a plane like this. So, now we have the second Brillouin zone that is shaded green like this; this is the second Brillouin zone. Let us consider even further nearest neighbors. So, if we go even further then for this lattice site we will have a nearest neighbor here. Now, we take the red color and we consider a plane halfing this vector this; the reciprocal lattice vector that would go through this. This reciprocal lattice vector if we half it, it will go through this sorry not this it will go through this actually. If we take this lattice vector and half it with a plane that plane will be this one, if we take this lattice vector half it that will be this one. So, the third Brillouin zone here is this region, this region, this region, this region this is the third Brillouin zone. And the area or in three dimension the volume of each Brillouin zone is exactly the same you can show this. Now, you can extend it to fourth, fifth and so on Brillouin zones, but the first Brillouin zone is the most important one the physics that the Brillouin zone captures everything is captured within the first Brillouin zone. And the subsequent Brillouin zones are just translation of that physics nothing new physics is captured in the subsequent Brillouin zones. So, this construction of Brillouin zone is very important for this course. We will also use this outside the concept of crystallography. When we discuss the electronic states the bands we will also make use of this concept of Brillouin zone; Brillouin zone is very important in that case. So, it is important to understand the Brillouin zone very well. Therefore, we will invest some more time on this. We will see the reciprocal lattice for some simple examples and we will try to construct the Brillouin zone for that in the next part of the our discussion. So, we consider a simple cubic lattice. (Refer Slide Time: 09:01)

The primitive translation vectors of a simple cubic lattice that is very simple. The vectors are given as $\overrightarrow{a_1} = a$; that is the lattice constant along x direction $\overrightarrow{a_2}$ is given as $a\hat{y}$ and $\overrightarrow{a_3} = a\hat{z}$. The volume of the cell you can find using scalar triple product. $\overrightarrow{a_1} \cdot (\overrightarrow{a_2} \times \overrightarrow{a_3})$ this scalar triple product you can trivially see will give you a cubed that is the volume of this cell using with a being the lattice constant. Now, if we try to find the primitive translation vectors of the reciprocal lattice then we have to make use of the definition of the axis vectors for reciprocal lattice. We have the definition like $\overrightarrow{b_1} = 2\pi \frac{\overrightarrow{a_2} \times \overrightarrow{a_3}}{\overrightarrow{a_1} \cdot (\overrightarrow{a_2} \times \overrightarrow{a_3})}$; that is the denominator is just the cell volume and the numerator is this and so on. We have $\overrightarrow{b_2}$ and $\overrightarrow{b_3}$ defined in very similar fashion, just for $\overrightarrow{b_1}$ we do not have $\overrightarrow{a_1}$ here for $\overrightarrow{b_2}$ we will not have $\overrightarrow{a_2}$ here and for $\overrightarrow{b_3}$ we will not have $\overrightarrow{a_3}$ here that is all. So, we can after working out this prescription we can write that $\overrightarrow{b_1}$ for simple cubic lattice becomes $\frac{2\pi}{a}\hat{x}$ direction, $\overrightarrow{b_2}$ can be worked out to $\frac{2\pi}{a}\hat{y}$ direction $\overrightarrow{b_3}$ can be worked out to $\frac{2\pi}{a}\hat{x}$ direction. So, these are our reciprocal axis vectors the primitive translation vectors. Here the reciprocal lattice itself is a simple cubic lattice you can simply see. Because of course, the lattice constant of the reciprocal lattice instead of a becomes $2\pi/a$ but it is along the Cartesian direction the axis vectors are along the Cartesian direction. So, you can clearly see that with these axis vectors you will get just a cube nothing else. So, the boundaries of the first Brillouin zone can be obtained by taking normals to the reciprocal lattice vectors. So, if we consider $\pm\overrightarrow{b}_1$, $\pm\overrightarrow{b_2}$ and $\pm\overrightarrow{b}_3$, if we consider these 6 vectors half them by normal intersection using a plane. So, there would be 6 planes and that will cut out a cube and that cube would be the Brillouin zone for this system. So, the Brillouin zone for a simple cubic lattice is also a cube we can clearly see that. So, what would be the volume of the reciprocal unit cells the primitive unit cell in reciprocal. So, the unit cell that we can form using these vectors $\overrightarrow{b}_1$, $\overrightarrow{b_2}$ and $\overrightarrow{b_3}$ that is a primitive unit cell in the reciprocal lattice also the Brillouin zone is a primitive unit cell in the reciprocal lattice. So, these are just two different kind of description of the in primitive unit cell. The Brillouin zone is like the Wigners Seitz cell and this primitive lattice vectors this is like the usual cell that we have in the real space its analogous to those. And you can find out the volume of the reciprocal cell that would be $\frac{2\pi}{a^3}$.