Solid State Physics
Lecture 11
Fourier Analysis of the Basis and Structure Factor

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After doing this part, we are left with the Fourier Analysis of the Basis. So, our X-ray diffraction or any other wave diffraction that we can consider is going to depend on the electron density that we have in the system. And the electron density is going to depend on the basis of basis that is the group of atoms that we consider at associated with each lattice point, that is going to determine the intensity of the diffracted pattern. So, it is important to perform a Fourier analysis of the basis. (Refer Slide Time: 01:13)

So, when the diffraction condition is given as $\Delta \overrightarrow{k} = \overrightarrow{G}$; when this condition is satisfied, we get some intensity in the diffraction pattern. When this condition is satisfied the scattering amplitude for N cells capital N number of cells. Let us consider that is all we have in the system or that is where we are shining the wave and considering the diffraction. This can be written as, we have this notation F for scattering amplitude and it is a function of $\overrightarrow{G}$ now. So, we are indexing it with $F_{\overrightarrow{G}}$ is given as $N \int_{cell} dV$, the electron density function as the electron density as a function of the position vector $n(\overrightarrow{r})$and $e^{-i(\overrightarrow{G}\cdot\overrightarrow{r})}$. We have worked this out earlier; we are just using it here. This one can be written as $NS_{\overrightarrow{G}}$, where this $S_{\overrightarrow{G}}$ this quantity is called the structure factor, structure factor of the diffraction intensity. It is useful to write the local electron concentration $n(\overrightarrow{r})$ as the superposition of electron concentration functions n_j associated with each atom j. That means, what are we going to do? Consider $\overrightarrow{r_j}$ that is the vector at the center of the j^{th} atom. If we have that, then we can construct a quantity $n(\overrightarrow{r} - \overrightarrow{r_j})$. This quantity defines the contribution of the j^{th} atom to the electron concentration at point r. So, at a given point r, there may be contributions from different atoms in the electron density. So, this quantity here would give us the contribution of j^{th} atom at the position $\overrightarrow{r}$. So, the total electron concentration at $\overrightarrow{r}$ due to all atoms in the unit cell that can be given as $n(\overrightarrow{r})$ this function it would. If we Σ_j, s is the number of atoms in the basis $\Sigma^s{}_{j=1}\overrightarrow{n_j}(\overrightarrow{r} - \overrightarrow{r_j})$. If we perform this, where s is as I said the number of atoms in the basis, ok. So, s is the number of atoms in the basis and if we $\Sigma^s{}_{j=1}$, we will obtain $n(\overrightarrow{r})$. Now, the structure factor $S_{\overrightarrow{G}}$ may be written as $\int s$ number of atoms in the unit cell. So, $S_{\overrightarrow{G}}$ this quantity structure factor is $\Sigma^s{}_j \int dV \overrightarrow{n_j}(\overrightarrow{r} - \overrightarrow{r_j})e^{-i(\overrightarrow{G}\cdot\overrightarrow{r})}$. What are we going to do here? We are going to put $(\overrightarrow{r} - \overrightarrow{r_j})$ kind of terms here and that we will have to compensate somewhere outside. So, we can write this quantity as $\Sigma_j e^{-i(\overrightarrow{G}\cdot\overrightarrow{r_j})}$. If we do this, then inside here we will have $(\overrightarrow{r} - \overrightarrow{r_j})$. So, we write $dV\ n_j$, it is a function of ρ now; we are defining $(\overrightarrow{r} - \overrightarrow{r_j}) = \rho$,$e^{-i(\overrightarrow{G}\cdot\rho)}$. So, ρ is nothing, but $(\overrightarrow{r} - \overrightarrow{r_j})$, we have made this substitution here. (Refer Slide Time: 07:21)

After doing this, now we can define the atomic form factor f_j; that is the contribution from each atom as for i^{th} atom, it is $\int dV n_j(\overrightarrow{\rho}) \exp(-i\overrightarrow{G}\cdot\overrightarrow{\rho})$. So, this integral part is called the atomic form factor and the part outside integral is that of summing over the contribution from every atom. So, this one has to be integrated over all space. And if n_j is an atomic property, then the atomic form factor f_i is also an atomic property. But this assumption that n_j would be an atomic property is not really confirmed, because in a solid there would be overlap of electrons. So, this assumption has some restrictions although by and large it is valid. But, so when we consider X-ray diffraction it is the majority of the electrons that are going to matter. So, those that participate in bonding or minority, those are associated with nuclei that is majority. So, this one, this assumption that we made is not true; but still it would be useful. With that understanding, we can combine the above equations that we have constructed so far to obtain the structure factor for the basis $S_{\overrightarrow{G}}$ with the help of the previous equations; we can write that it is $\Sigma_j f_j$, ok. Let it let us write it f_j, because we have function

of j here, not i. So, it is $\Sigma_j f_j \exp(-i\vec{G} \cdot \vec{r_j})$. Now, for an atom j, we can write its position vector $\vec{r_j} = x_j\vec{a_1} + y_j\vec{a_2} + z_j\vec{a_3}$; x_j, y_j, z_j. These have values ranging from 0 to 1 as we have discussed earlier. With this we have $\vec{G} \cdot \vec{r_j}$, this quantity going to $(v_1\vec{b_1} + v_2\vec{b_2} + v_3\vec{b_3}) \cdot (x_j\vec{a_1} + y_j\vec{a_2} + z_j\vec{a_3})$. By putting the forms of $\vec{b_1}, \vec{b_2} and \vec{b_3}$ that we have obtained for different kind of lattices; we can find exactly what this is going to be. Well, we have the relationship between $\vec{b_1}$, the dot product of $\vec{b_1}$ and $\vec{a_1}$, $\vec{b_1} \cdot \vec{a_2}$ and all that; it is $2\pi\delta_{ij}$, $\vec{b_i} \cdot \vec{a_j} = 2\pi\delta_{ij}$. With that we can already write that this dot product is going to give us $2\pi(v_1\vec{x_j} + v_2\vec{y_j} + v_3\vec{z_j})$; the other components of the product will vanish. And with this we can write $S_{\vec{G}}$ equals. So, $S_{\vec{G}}$ is now a function of these indices $v_1,\ v_2,\ v_3$; this becomes $\Sigma_j f_j \exp[-i2\pi(v_1\vec{x_j} + v_2\vec{y_j} + v_3\vec{z_j})]$, this is what we have for the structure factor. The structure factor does not need to be a real number it can be a complex number in general. When we take the diffraction intensity, it would be square of the structure factor, so that would become a real number anyway. So, structure factor being complex does not require any physical quantity to be complex; amplitude is not really a physical quantity, it is the intensity that is the physical quantity. So, the physical quantity would still be real. Now, let us consider an example of the bcc lattice, structure factor for the bcc lattice we are going to find out. (Refer Slide Time: 13:033)

The bcc lattice can be referred to with a cubic lattice, that is cubic the axis vectors corresponding to a simple cubic lattice and we can have identical atoms located at the origin and another point that is the body center, the coordinate $(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$. With these two identical atoms at these two coordinates using the simple cubic translation vectors, primitive translation vectors, we can represent a bcc lattice that you have already worked out in one of the homework's. So, we can write $S(v_1v_2v_3) = f$ that is the atomic form factor times $[1 + \exp[-i\pi(v_1 + v_2 + v_3)]]$. So, where did we get this 1? If we put $(v_1 + v_2 + v_3)$ sorry $(\vec{x_j}, \vec{y_j}, \vec{z_j})$ everything equals 0; we will get $\exp 0$ that is 1. And for the other thing, $\exp -i2\pi(v_1\vec{x_j} + v_2\vec{y_j} + v_3\vec{z_j})$ that is going to give us this quantity here. So, with this the f is the atomic form factor, so that we are yet to calculate. But we can already see that if this quantity, exponential is the value is minus 1; then S will be 0. So, when would be with it be minus 1? If we have $(v_1 + v_2 + v_3)$, if this quantity is an odd integer and S would be 2f. If this becomes $(v_1 + v_2 + v_3)$ becomes even integer; then this quantity exponential of this would be 1 and 1 plus 1 we will have 2 from this curly bracket. So, this condition is $(v_1 + v_2 + v_3)$is even integer for S being 2f. So, obvious homework here for you would be, to find the structure factor corresponding to an FCC lattice, ok. Now, let us deliberate on the atomic form factor.