Solid State Physics
Lecture 6
Fourier Analysis of Diffraction

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So, why do we go for Fourier Analysis or rather what allows us to go for Fourier analysis? We need to so, a crystal is invariant under any translation of the form T is given as $u_1\overrightarrow{a_1} + u_2\overrightarrow{a_2} + u_3\overrightarrow{a_3}$. So, every crystal subject to its axis vectors that is primitive translation vectors $\overrightarrow{a_1}$, $\overrightarrow{a_2}$ and $\overrightarrow{a_3}$ is invariant under this kind of a translation where u_1, u_2, u_3 these are integers. We have discussed this earlier. We have defined the lattice in terms of this, therefore, this is true. And when this is true then all physical properties like charge density, magnetic moment any other physical property that we can consider for a crystal must be invariant under this kind of a translation. There is no exception in that. There cannot be any exception in that means; we have a periodic system, a perfect periodic system that is ideal to be described using Fourier analysis. Therefore, first we consider an arbitrary function $n(x)$ in 1 dimension for simplicity. So, we want. So, $n(x)$ is a periodic function and it has a periodicity of a. So, we want to represent this function in a Fourier series comprising sine and cosine functions. So, $n(x)$ in a Fourier series can be written as $n_0 + \Sigma_{p>0}[C_p \cos\frac{2\pi px}{a} + S_p \sin\frac{2\pi px}{a}]$. Here we have considered p to be positive integer, C_p and S_p are real. So, C_p and S_p these are called the Fourier coefficients corresponding to this Fourier series and we have a factor of $\frac{2\pi}{a}$. So, this $\frac{2\pi}{a}$ this factor ensures the periodicity. Cosine and sine functions are periodic in with the period 2π. And if we put $\frac{2\pi}{a}$ in the argument of cosine and sine functions the periodicity becomes that is the period becomes a. Let us test it. (Refer Slide Time: 05:00)

So, if we calculate $n(x) + a$, what do we obtain? We obtain nothing but $n_0 + \Sigma_p[C_p \cos(\frac{2\pi px}{a} + 2\pi p) + S_p \sin(\frac{2\pi px}{a} + 2\pi p)]$ this is what we obtained. So, cosine of twice so, this part will go away if we consider the periodicity of cosine and sine functions because p is a positive integer, p is any integer is fine. So, this becomes nothing but $n_0 + \Sigma_p[C_p \cos\frac{2\pi px}{a} + S_p \sin\frac{2\pi px}{a}]$ and this is nothing but $n(x)$. So, we have verified that this function $n(x)$ the way we have constructed and represented it in terms of a Fourier series is indeed periodic with the period a. Once we have that then after confirming this we can say that $(\frac{2\pi p}{a})$, this is a point in the reciprocal lattice of the Fourier space of the crystal. That means, we are performing a Fourier transform on the real space to get another space and that is a reciprocal space and in that reciprocal space $\frac{2\pi p}{a}$ is a lattice point. It is a point of the reciprocal lattice that is the idea. So, we have introduced the idea of reciprocal lattice in 1 dimension. Now, these reciprocal lattice points suggest us the allowed terms in the Fourier series. So, we have written a generic Fourier series here and depending on the periodicity of the crystal some of the terms would be allowed and some of the terms forbidden and these lattice points suggest us the allowed terms. A term is allowed only if it is consistent with the inherent periodicity of the crystal. Now, the Fourier series may be written in a compact exponential form allowing for complex numbers. (Refer Slide Time: 08:24)

We can write $n(x) = \Sigma_p n_p \exp{(i\frac{2\pi px}{a})}$. So, what have we done now? We have allowed p to be any integer, be it positive, negative or 0 and now the coefficients n_p are no longer real numbers. The n_p are in general complex numbers, but we have to ensure that $n(x)$ remains to be a real function. How do we do that? We would require for that ${n_{-p}}^* = n_p$. This will ensure that $n(x)$ is a real function. Let us verify this. Now, if we put for simplicity of writing $\frac{2\pi px}{a}$, we put this as ϕ then from the above we can write n_p. I am just expanding the $\exp i\phi = (\cos\phi + i\sin\phi) + n_{-p}(\cos\phi - i\sin\phi) = (n_p + n_{-p})\cos\phi + i(n_p - n_{-p})\sin\phi$. Now, this function becomes a real function that means, this quantity goes to 0, provided this condition is satisfied, ok. After arguing this, let us take the next step that is let us extend this analysis to 3 dimension. We have done this analysis in a simple 1 dimensional fashion, now, let us extend it to 3 dimension. The extension is straightforward. (Refer Slide Time:

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Instead of $e^{x/a}$, we need to put. So, instead of n_x we are putting n_r that generic function that is obtained by a Fourier transform that is $\Sigma_{\overrightarrow{G}}$. So, if a Fourier series $\Sigma_{\overrightarrow{G}} n_{\overrightarrow{G}} \exp{(i\overrightarrow{G}\cdot\overrightarrow{r})}$ and this must be invariant under all the allowed translations that is there in the crystal. So, whatever translation the crystal allows this function should be invariant under that. Now, what if we invert this Fourier transform? So, the coefficients n_p that can be written as $a^{-1}\int_0^a dx\ n(x)\exp{(-i\frac{2\pi px}{a})}$ in the 1 dimensional case. I have just written it, I want to show it now. If we put the value of $n(x)$ that we have written earlier, $n(x)$ was given as $\Sigma_p n_p \exp{(i\frac{2\pi px}{a})}$. Now, if we put this in the case of in the expression for n_p that we have written it is $a^{-1}\Sigma_{p'}$ because there would be repeated indices and to preserve the generality we need to introduce a prime here $n_{p'}\int_0^a \exp{(i\frac{2\pi(p'-p)x}{a})}$. Now, if we have $p' \neq p$ then we can see that this integral will go to 0. You can work out how this integral goes to 0, if $p' \neq p$ and if $p' = p$ then the integrand becomes $e^{i\times 0}$ that is 1. So, performing this integral we will get $n_{p'} \times a$, that is what we will get and so, everything becomes consistent with this. $\Sigma n_{p'}$ we would just get n_p from this. So, only one value of p was allowed and therefore, we will get $n_p = n_p$ and this expression that we have written for n_p is valid, everything becomes consistent. (Refer Slide Time: 16:31)

And at this stage it becomes important to write down the inverse Fourier transform after knowing n_p's. So, the inverse coefficient $n_{\overrightarrow{G}}$ that can be written as $\frac{1}{V_c}\int_{cell} dV\ n(\overrightarrow{r})\exp{(-i\overrightarrow{G}\cdot\overrightarrow{r})}$, V_c is the cell volume. Now, we have also we have also defined the inverse transform what we do not know in here is what are these $\overrightarrow{G}$. So, the $\overrightarrow{G}$ are called reciprocal lattice vectors. What do we mean by reciprocal lattice vectors? So, we must define what it is. It is like the $\overrightarrow{T}$ that we defined in the case of real space that is a linear combination of. So, with integer coefficients a linear combination of the axis vectors in the real space and G would be with integer coefficients linear combination of the axis vectors in the reciprocal space. So, we must define the axis vectors in the reciprocal space. We call it $\overrightarrow{b_1}, \overrightarrow{b_2}$ and $\overrightarrow{b_3}$. $\overrightarrow{b_1}, \overrightarrow{b_2}$ and $\overrightarrow{b_3}$ can be defined as; so, $\overrightarrow{b_1}, \overrightarrow{b_2}$ and $\overrightarrow{b_3}$ they must satisfy certain conditions. And I am just telling the definition the way we can define them and exactly what conditions they must satisfy and how this 1 is a possible choice we will discuss that later. So, the numerator will have a cyclic order and the denominator is nothing but the scalar triple product that is the cell volume of the real cell and $\overrightarrow{b_3}$ can be similarly written as $2\pi\frac{\overrightarrow{a_1}\times\overrightarrow{a_2}}{\overrightarrow{a_1}\cdot(\overrightarrow{a_2}\times\overrightarrow{a_3})}$. So, with $\overrightarrow{a_1}$, $\overrightarrow{a_2}$ and $\overrightarrow{a_3}$ being the primitive lattice vectors for the real cell, $\overrightarrow{b_1}, \overrightarrow{b_2}$ and $\overrightarrow{b_3}$ are the primitive lattice vectors for the reciprocal cell and it will hold a property $\overrightarrow{b_i}\cdot\overrightarrow{a_j}$ that becomes $2\pi\delta_{ij}$. So, if $i = j$, $\delta = 1$. If $i \neq j$, $\delta = 0$ and this is something you must verify. For this definition that this holds good and this is one of your home works. And later on we will show you why we require this condition to hold and why this definition of $\overrightarrow{b_1}, \overrightarrow{b_2}$ and $\overrightarrow{b_3}$ could be an acceptable definition. That is all for now.