Solid State Physics
Lecture 33
Periodic Boundary Condition

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So, we can consider something like a ring, just a geometrical consideration, nothing has to do with the constraints possibly coming from a ring, where the atoms are oriented this way, which gives us a periodic boundary condition. So, in a formal representation, the periodic boundary condition can be represented like this; $C_0 = C_N$ the coefficients of the basis elements and $C_{N+1} = C_1$. So, we will go by this definition of the periodic boundary condition ok. So, with this, the general solution becomes $e^{iN\theta} = 1$ which means $\theta = \frac{2m\pi}{N}$, where m can take the value from $0 \rightarrow N-1$ and the corresponding normalized Eigen states can be obtained by the expansion coefficients. So, the expansion coefficient $C_j^{(m)}$ for m^{th} state can be written as $\frac{1}{\sqrt{N}} e^{i\frac{2\pi jm}{N}}$. This is the coefficient. The Eigen values would be given as $E = \alpha + 2\beta\cos|\frac{2\pi m}{N}$. Now, if we go to the $\lim_{N\rightarrow\infty}$, you can see that θ represented this way becomes a continuous variable and the Eigen value will have a continuous spectrum. So, at the energy Eigen value is always $E = \alpha + 2\beta\cos\theta$. This quantity becomes a continuous spectrum, when $N \rightarrow \infty$. (Refer Slide Time: 04:05)

How can we plot this quantity? This is θ axis and this is the energy axis, it would look somewhat like this; a cosine function, where we have plotted it over $-\pi\ to\ \pi$, the value of theta which is in the first Brillouin zone of the system. The maximum value of energy here becomes $E_{max} = -\alpha - 2\beta$ and minimum value of energy here becomes $E_{min} = \alpha + 2\beta$ and the Eigen state of this infinite ring that can be ah. So, if we consider an infinite periodic system, the Eigen state can be represented by C_j's, the coefficients, this would be $\frac{1}{\sqrt{N}} e^{ij\theta}$. Here, we can examine the states and comment that at $\theta = 0$, we will have the maximum bonding state corresponding to this Eigen value at the bottom of the spectrum. At $\theta = \pm\pi$ which is the boundary of the Brillouin zone, edge of the Brillouin zone, there we will have the maximum antibonding state. And at $\theta = 0$, we will have neither bonding nor antibonding that is nonbonding state in this continuous spectrum. Now, since θ specifies the energy and the expansion of the Eigen state in terms of the basis states, it is appropriate quantum number for an infinite number of atoms and periodic boundary condition and if this is the spectrum in terms of theta, can we find out the density of states for this kind of a system? The density of states can be given as $D(E) = \frac{ds}{dE}$ which is the derivative of the number of states with respect to energy. (Refer Slide Time: 07:51)

And we can write $\theta = ka$ the crystal momentum times the distance between 2 hydrogen atoms that is the lattice constant. Why can we do that? If you go to the definition of reciprocal axis vectors, then you can understand this easily. Here $\theta \rightarrow -\pi\ to\ \pi$ and within the first Brillouin zone, we will have a certain range for the vectors in the reciprocal lattice and that would be precisely ka and if $ka = -\pi$ that is one edge of the first Brillouin zone; if it becomes $ka = \pi$ that is the other edge of the first Brillouin zone. So, in the reciprocal lattice, reciprocal space, this ka is the form of θ for one dimensional Brillouin zone. For more than one dimensional, it would be a vector ok. So, this quantity density of states can now be written as $D(E) = \frac{ds}{dk}\frac{dk}{dE}$the absolute value of this which is nothing but $\frac{\frac{ds}{dk}}{\frac{dE}{dk}}$; $\frac{dk}{dE}$ is the gradient of this energy band energy dispersion that we have plotted here because this axis is k now. It is $\theta = ka$. So, we can calculate for a cosine function, this quantity very easily and we can write that this quantity would be $D(E) = 2\frac{Na}{2\pi}(\frac{1}{2\beta a\sin ka})$ which is simplifies to $D(E) = \frac{N}{\pi}\frac{1}{\sqrt{4\beta^2-(E-\alpha)^2}}$. This is the density of states for the entire system. Now, if we want to find out the density of states for 1 atom, we represent that with small d. It is not the differential. The density of states for each atom, this can be represented just by removing this N from here $d(E) = \frac{1}{\pi}\frac{1}{\sqrt{4\beta^2-(E-\alpha)^2}}$. And if we plot this density of states, we will obtain the following. We will get this kind of a picture, where it

asymptotically reaches here and here this is the energy axis and this is d(E), the density of states, the middle point is α, extreme left is $\alpha + 2\beta$ and extreme right is $\alpha - 2\beta$. You can see from here, sorry this is not minus. So, $\alpha - 2\beta$ is here, $\alpha + 2\beta$ is here and these are the places, where the density of states peak and in between it, it is very flat, there are very few states in the region in between that is what we obtain by performing this calculation.