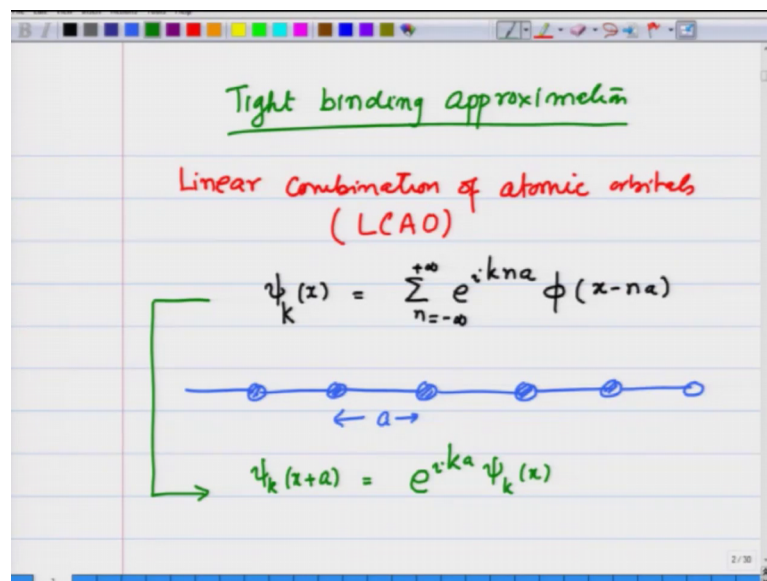


Introduction to Solid State Physics
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Lecture - 65
Tight Binding model - II

(Refer Slide Time: 00:18)



What we have done in the previous lecture is introduced the idea of Tight binding approximation which is nothing, but equivalent to Linear Combination of Atomic Orbitals or what is known as LCAO. And the idea is to combine them in such a way that Bloch's theorem is satisfied and therefore, we write ψ_k and I am first working in one dimension. So, $\psi_k(x)$ equals summation n $e^{ikna} \phi(x-na)$ n tends goes from minus infinity to plus infinity.

So, what we are doing is we are taking this crystal lattice where atoms have distance a between them and we are starting from some point n equals minus infinity to plus infinity, e^{ikna} and we also showed that if I take $\psi_k(x+a)$ it turns out to be equal to $e^{ika} \psi_k(x)$. So, this form of the wave function satisfies the Bloch's condition.

(Refer Slide Time: 02:10)

Calculate $E(k)$ using the tight binding wavefunction.

$$E(k) = \langle \psi_k(x) | H | \psi_k(x) \rangle$$

$\psi_k(x)$ is normalized

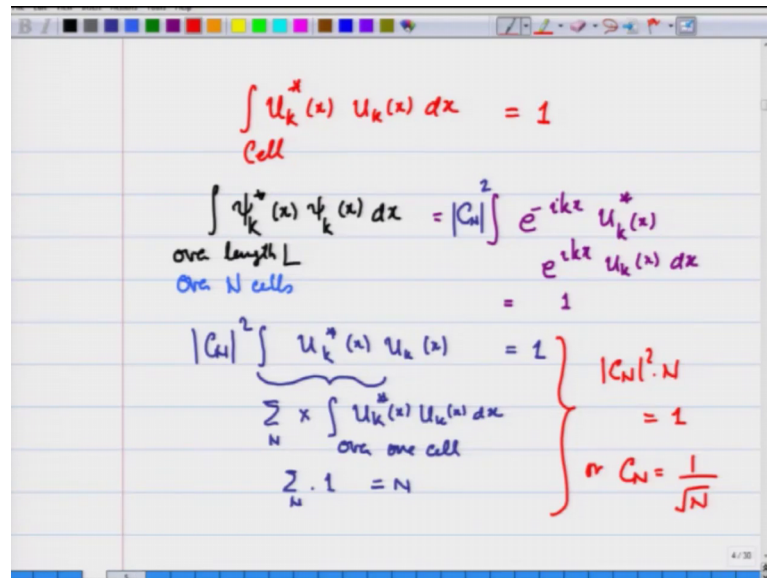
$$\int_L \psi_k^*(x) \psi_k(x) dx = 1 \quad L = Na$$
$$\psi_k(x) = e^{ikx} u_k(x)$$

(1) $u_k(x)$ is normalized over a cell

What we want to do now is calculate energy E as a function of k using the tight binding wave function and this will involve some approximations which we will spell out as we go along. The way to calculate the energy $E(k)$ is to calculate the expectation value $\langle \psi_k(x) | H | \psi_k(x) \rangle$, where $\psi_k(x)$ is normalized and what does that mean? Recall my earlier discussion of normalizing the block wave function which was related to normalization of plane waves.

So, the way we do normalization these wave functions is by integrating $\psi_k^*(x) \psi_k(x) dx$ over length L where L is length of N cells and since $\psi_k(x) = e^{ikx} u_k(x)$, we normalize in 2 steps.

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$$\int_{\text{Cell}} u_k^*(x) u_k(x) dx = 1$$

$$\int_{\text{over length } L} \psi_k^*(x) \psi_k(x) dx = |C_N|^2 \int_{\text{over } N \text{ cells}} e^{-ikx} u_k^*(x) e^{ikx} u_k(x) dx = 1$$

$$|C_N|^2 \int u_k^*(x) u_k(x) dx = 1$$

$$\sum_N \int_{\text{over one cell}} u_k^*(x) u_k(x) dx = 1$$

$$\sum_N 1 = N$$

$$|C_N|^2 \cdot N = 1$$

$$C_N = \frac{1}{\sqrt{N}}$$

Number 1, step number 1 is $u_k(x)$ is normalized over a cell. So, what that means, is that integration $u_k^*(x) u_k(x) dx$ over a cell is equal to 1 and then I can write this normalization integration $\psi_k^*(x) \psi_k(x) dx$ over length L or equivalently over N cells as equal to integration $e^{-ikx} u_k^*(x) e^{ikx} u_k(x) dx$ and this is equal to supposed to be 1 right?

So, let me write a normalization constant that I want to determine in front of the wave function. So, I have this integration $e^{-ikx} u_k^*(x) e^{ikx} u_k(x) dx$ give me 1 and I have $u_k^*(x) u_k(x) C_N^2$ where C_N is the normalization constant, this should be 1. This integral I can write summation over N cells times integration over one cell and this integration over one cell is that of $u_k^*(x) u_k(x) dx$.

So, this gives me summation over N times 1 which is N . All this implies that $C_N^2 \cdot N = 1$ or the normalization constant is $1/\sqrt{N}$.

(Refer Slide Time: 06:16)

$$\psi_k(x) = \frac{1}{\sqrt{N}} e^{ikx} u_k(x)$$

$$\psi_k(x) = C_N \sum_{n=-\infty}^{\infty} e^{ikna} \phi(x-na)$$

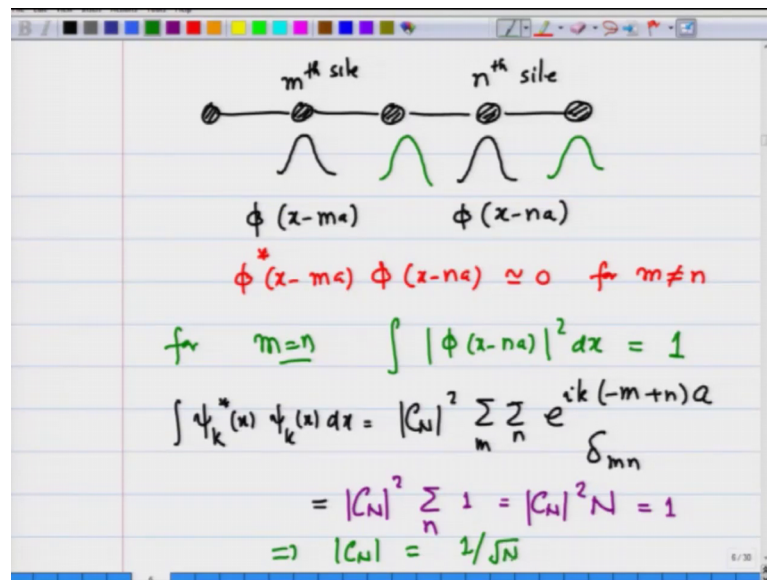
$$\int \psi_k^*(x) \psi_k(x) dx = |C_N|^2 \sum_m \sum_n \int e^{ik(-m+n)a} \phi^*(x-ma) \phi(x-na) dx$$

$$= |C_N|^2 \sum_m \sum_n e^{ik(-m+n)a} \int \phi^*(x-ma) \phi(x-na) dx$$

So, Bloch wave function is normalized like this $\psi_k(x)$ is written as $\frac{1}{\sqrt{N}} e^{ikx} u_k(x)$ where it is understood that $u_k(x)$ is normalized over a cell. Now, let us see how I am going to normalize the tight binding wave function and I have $\psi_k(x) = C_N \sum_{n=-\infty}^{\infty} e^{ikna} \phi(x-na)$. I have this wave function and I put in front of this a normalization constant C_N . C_N is for N cells. So, when I take $\psi_k^*(x) \psi_k(x)$ this comes out to be $|C_N|^2 \sum_m \sum_n \int e^{ik(-m+n)a} \phi^*(x-ma) \phi(x-na) dx$.

Now, let us write this as again clearly $|C_N|^2 \sum_m \sum_n e^{ik(-m+n)a} \int \phi^*(x-ma) \phi(x-na) dx$. $e^{ik(-m+n)a}$ can be taken outside the integral and I have $\int \phi^*(x-ma) \phi(x-na) dx$.

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Let me show the approximation that we are going to make now. So, what we are doing is we are taking this atomic chain and here is my let us say the wave function out here let this be the nth site and let this be the mth site and here is the wave function phi which is concentrated near mth site and here is a phi concentrated near the nth site and what you can see is there is hardly any overlap between two.

So, what I can write is that if I have phi x minus m a star multiplying phi x minus n a it is almost equal to 0 for m not equal to n. So, even if I take the site right next to the nth site the overlap is nearly 0 and for m equals n, I am going to have mod phi x minus n a square d x and this I can take to be 1 because I am taking phi to be the atomic wave function which is normalized.

So, if I look at this integration psi k star x psi k x d x it comes out to be C N mod square summation m summation n e raised to i k minus m plus n a times delta m n, where delta m n is a function which is 0 if m is not equal to 1 and m equal to 1 it is equal to 1. So, this gives me C N mod square summation only one of the indices of m or n will be left times 1 which is equal to C N square times N, exactly like what we did for the free electron wave function and this should be 1 and this gives me that mod C N is equal to 1 over root N.

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Neglecting overlap between the atomic wavefunctions on two different atoms

$$\psi_k(x) = \frac{1}{\sqrt{N}} \sum_{n=-\infty}^{\infty} e^{ikna} \phi(x-na)$$
$$E(k) = \langle \psi_k(x) | H | \psi_k(x) \rangle$$
$$= \frac{1}{N} \sum_m \sum_n e^{ik(-m+n)a} \langle \phi(x-ma) | H | \phi(x-na) \rangle$$

Therefore, I can say that neglecting overlap between the atomic wave functions on two different atoms and this is an approximation I am neglecting the overlap between two atomic wave function. There are on two different atoms. I have the wave function tight binding wave function $\psi_k(x) = \frac{1}{\sqrt{N}} \sum_{n=-\infty}^{\infty} e^{ikna} \phi(x-na)$. This is my normalized tight binding wave function.

When I have normalized it, next I calculate $E(k)$ by taking the expectation value $\psi_k(x) | H | \psi_k(x)$ which will be equal to $\frac{1}{N} \sum_m \sum_n e^{ik(-m+n)a} \langle \phi(x-ma) | H | \phi(x-na) \rangle$. So, that is why I said integration $\phi(x-ma)$ keep in mind.

Now, that this term is independent of the Hamiltonian and therefore, it has been taken out of the expectation value and what we now are to focus on is calculation of this term here and again we will be making certain approximations when we calculate this.

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$$E(k) = \frac{1}{N} \sum_m \sum_n e^{ik(-m+n)a} \langle \phi(x-ma) | H | \phi(x-na) \rangle$$

where the Hamiltonian

$$H = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x)$$

$$V(x) = V(x+a) \text{ is periodic}$$

$$E(k) = \frac{1}{N} \sum_m \langle \phi(x-ma) | H | \phi(x-ma) \rangle + \frac{1}{N} \sum_m \sum_{\substack{n \\ m \neq n}} e^{ik(-m+n)a} \langle \phi(x-ma) | H | \phi(x-na) \rangle$$

So, let us do that now. So, we wish to calculate $E(k)$ equals $\frac{1}{N}$ summation m summation n $e^{ik(-m+n)a}$ $\langle \phi(x-ma) | H | \phi(x-na) \rangle$, where the Hamiltonian H equals $-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x)$ is periodic.

So, to facilitate this summation over all the sites what I am going to do is change what I am going to do is divide this sum into the same site m equals n and m not equal to n . So, what I am going to right now is $E(k)$ and there is a purpose for this. $\frac{1}{N}$ let us take the same side. So, I will just sum over m $e^{ik(-m+n)a}$ and now the same. So, that becomes $e^{ik(-m+n)a}$ which is 1, $\langle \phi(x-ma) | H | \phi(x-ma) \rangle$ plus one more term that includes both m and n , but m is not equal to n and now I have $e^{ik(-m+n)a}$ $\langle \phi(x-ma) | H | \phi(x-na) \rangle$. I will take both these contributions one by one and see how they work out.

(Refer Slide Time: 15:46)

$$\frac{1}{N} \sum_m \langle \phi(x-ma) | H | \phi(x-na) \rangle$$

$$\phi(x) \text{ is the atomic orbital}$$

$$(LCAO \text{ satisfying Bloch's theorem})$$

$$H = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x)$$

The diagram shows a series of potential wells. A horizontal black line represents the zero potential level. Below it, a series of green wells represent individual atomic potentials $V(x)$. A series of red wells represent the total potential $V(x)$, which is the sum of the atomic potentials. A series of dark blue wells represent the difference potential $\Delta V(x)$, which is zero near the atomic sites and positive in the interstitial regions.

So, let us first focus on the first term which is $\frac{1}{N}$ summation m $\phi(x-ma)$ the Hamiltonian $\phi(x-na)$. Now recall that $\phi(x)$ is the atomic orbital at each site because what we have done is made the linear combination of atomic orbitals satisfying Bloch's theorem. So, each ϕ is an atomic orbital. Let us look at the H the Hamiltonian. The Hamiltonian consist of 2 parts; the kinetic energy part plus $V(x)$. If you look at $V(x)$ this is how it looks. So, let me make this chain in one dimension of atoms $V(x)$ is nothing, but the sum of these atomic potentials.

So, atomic potential would have been something like what I show in green for each site and when I add these the $V(x)$ potential that I get I am going to show it in red it is pretty much atom like near the site and in between it becomes little lower because we are adding a negative potentials. So, it differs a bit, but mainly in the interstitial region; if I were to plot the difference $\Delta V(x)$ between the two potentials $\Delta V(x)$ will be something like this, almost 0 near the atomic sites and quite large in between. So, keep this picture in mind because this will help us calculate these matrix elements.

So, this is $\Delta V(x)$ the one shown in dark blue it is quite large in between and very small near the sites.

(Refer Slide Time: 18:43)

$$\frac{1}{N} \sum_m \int_0^L \phi^*(x-ma) \left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \right) \phi(x-ma) dx$$

$$H |\phi(x-ma)\rangle \approx E_{\text{atomic}} \phi(x-ma)$$

H is not the atomic Hamiltonian

Now, let us go back to the calculation of this matrix element $\frac{1}{N} \sum_m \int_0^L \phi^*(x-ma) \left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \right) \phi(x-ma) dx$. $\phi^*(x-ma)$ is the complex conjugate of $\phi(x-ma)$. $\phi(x-ma)$ is the atomic orbital. H is the Hamiltonian. E_{atomic} is the energy of the atomic orbital. $\phi(x-ma)$ is the atomic orbital. H is not the atomic Hamiltonian.

Now, I can say that this Hamiltonian acting on $\phi(x-ma)$ will give me about E_{atomic} times $\phi(x-ma)$. I am saying this about because H is not the atomic Hamiltonian. $\frac{1}{N} \sum_m \int_0^L \phi^*(x-ma) H \phi(x-ma) dx$.

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$$\frac{1}{N} \sum_m \int_0^L \phi^*(x-ma) H \phi(x-ma) dx$$

$m: ma \leq L$

$$\int_0^L \phi^*(x-ma) H \phi(x-ma) dx = E_{\text{atomic}}$$

$$\sum \int_0^L = N E_{\text{atomic}} \quad (\text{Kittel calls it } -\alpha)$$

$$\frac{1}{N} \cdot N \cdot E_{\text{atomic}} = E_{\text{atomic}}$$

Now this integral will contribute only for m such that ma is less than or equal to L . So, m will give you a count of n integral 0 to L $\phi^* (x - ma) H \phi (x - ma) dx$ will be about E_{atomic} as I argued earlier and sum over m of this integral 0 to L , then it is going to give me N times ϵ_{atomic} . It is understood that ϵ_{atomic} is not exactly the orbital I can value of the atom, but very close to it. Kittel calls it minus α ; α being greater than 0 . And therefore, this whole expression comes out to be 1 over N times N times ϵ_{atomic} and I can cancel this N and N , so, this is equal to ϵ_{atomic} .

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Second term $\frac{1}{N} \sum_m \sum_{n \neq m} e^{ik(-m+n)a} X \langle \phi(x-ma) | H | \phi(x-na) \rangle$

$m \neq n$

$$\int \phi^*(x-ma) \left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \right) \phi(x-na) dx$$

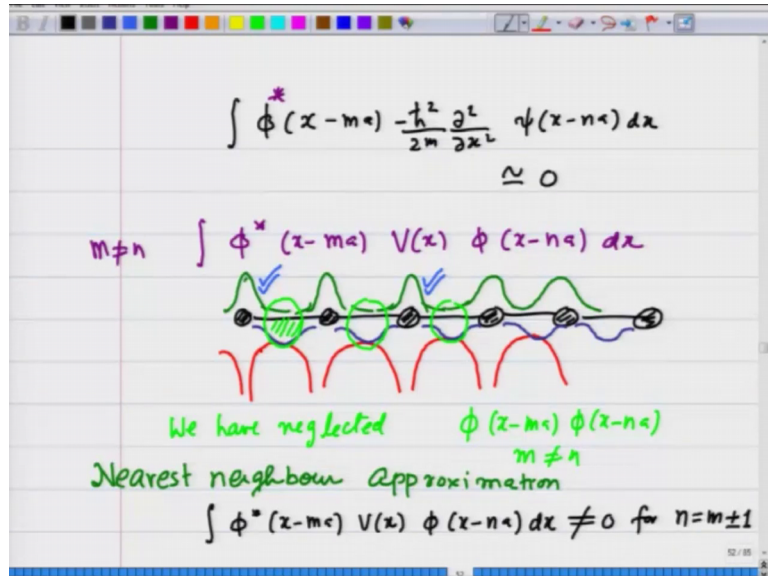
$$\frac{\partial^2 \phi}{\partial x^2} \propto \phi \quad (\phi \sim e^{ikx})$$

Let us now look at the second term; the second term which is $\frac{1}{N} \sum_{m \neq n} e^{ik(n-m)} \langle \psi_n | H | \psi_m \rangle$. Let us look at this term. Now m is not equal to n . So, let me again just to visualize make that atomic chain and the potential that we drew earlier is something like this and symbolically I have the wave function right on each site this is my ϕ .

Now, when I calculate this term, I am actually talking about a ψ at some site which I am showing by shaded by this purple color and ψ some other site at some other site. Here could be right the next site or could be farther out. When I write this expectation value this is going to be just the expectation value term it is going to be $\int \psi^* \left(-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x) \right) \psi dx$ and m is not equal to n .

Most of the time the atomic orbitals are you know exponentially decaying. So, even this term $\frac{d^2 \phi}{dx^2}$, if you go to the region between the atoms is going to be proportional to ϕ itself that you can check if ϕ is exponentially decaying maybe αx . So, for the first term what you will see is that the overlap in between out here is negligible. If m is not equal to n then the first term should give me roughly 0. This also makes sense according to the approximation that we have been making in normalizing the wave function we have been neglecting the overlap of wave functions from sites which are different.

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So, the only term which will contribute in this is the $V \times$ term. So, let us just slowly understand. So, I conclude by looking at this picture that this $\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi(x-na) dx$ is roughly equal to 0. Let me see if I put the minus sign will be changes is roughly equal to 0 and for the second term if I look at this ϕ . So, there should be a star here, $\phi^*(x-ma) V(x) \phi(x-na) dx$ is not equal to 0. Let me look at these atoms again this is the potential it has some value in between remember I had plotted it earlier. So, the $\Delta V(x)$ is quite large in between and here are the wave functions.

So, although we have neglected right let me just point out we have neglected $\phi(x-ma) \phi(x-na)$ when m is not equal to n . Now you see this product yes when it is multiplied by $\Delta V(x)$ is going to be large only from this intermediate region. So, this part cannot be neglected if I did that the only value for the expectation value of the Hamiltonian I will get is the atomic E atomic orbitals and the band would be flat.

So, we are not going to neglect this term and what we are going to do is make what is known as the nearest neighbour approximation and by looking at the picture you can make out it is when we look at the atomic orbitals next to each other then this term is appreciable otherwise it becomes negligible because if I look at this site I am now taking and the site one removed from the next site you will see that the overlap is going to be very small.

So, a nearest neighbour approximation what I am going to say is that the integral $\langle \phi(x-ma) | H | \phi(x-na) \rangle$ is not equal to 0 for $n = m \pm 1$ that means, right next to each other for others it is going to be 0.

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The image shows a whiteboard with the following handwritten mathematical expressions:

$$\frac{1}{N} \sum_m \sum_n e^{+ik(-m+n)a} \langle \phi(x-ma) | H | \phi(x-na) \rangle$$

$$\langle \phi(x-ma) | H | \phi(x-na) \rangle$$

$$= \int_0^L \phi^*(x-ma) H \phi(x-na) dx$$

$\neq 0$ for $n = m \pm 1$
 $= 0$ for all other terms

$$\langle \phi(x-ma) | -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} | \phi(x-na) \rangle \approx 0$$

$$\langle \phi(x-ma) | \Delta V(x) | \phi(x-na) \rangle \neq 0$$

So, if I look at the term again the term I am after is $\frac{1}{N} \sum_m \sum_n e^{+ik(-m+n)a} \langle \phi(x-ma) | H | \phi(x-na) \rangle$. So, what we are going to say is that this term $\langle \phi(x-ma) | H | \phi(x-na) \rangle$ which is equal to $\int_0^L \phi^*(x-ma) H \phi(x-na) dx$ is not equal to 0 for $n = m \pm 1$ and 0 for all other terms.

And in this also what we said earlier is that the kinetic energy term $\langle \phi(x-ma) | -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} | \phi(x-na) \rangle$ is going to be almost 0 and it is the second term that contributes and that is $\langle \phi(x-ma) | V(x) | \phi(x-na) \rangle$ is not equal to 0 and in this $V(x)$ also as I showed in the previous slide actually is the $\delta(x-na) V_0$ term I am putting a little $\delta V(x)$ here I am emphasizing ok.

Let me just encircle this term is the $\delta V(x)$ term which is large between the two atomic sites that is the main contributor this nonzero term. So, it is because of the $\delta V(x)$ that the bands arise if this was not there the bands would not arise. Suppose $\delta V(x)$ was 0, each atomic site was independent all I would have gotten is E_{atomic} as the expectation value of the Hamiltonian and the total band would be flat energy will be equal to a atomic for each k .

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$$\int_0^L \phi^*(x-ma) \left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V(x) \right) \phi(x-na) dx \neq 0 \text{ for } n = m \pm 1$$

(nearest neighbour approximation)

$$\int_0^L \phi^*(x-ma) H \phi(x-na) dx = \gamma$$

And this is non-zero (=γ) for $m = 0 \text{ to } N-1$ or $1 \text{ to } N$

$$\frac{1}{N} \sum_m \sum_n e^{ik(-m+n)a} \langle \phi(x-ma) | H | \phi(x-na) \rangle$$

But now this is what we have. So, we are calculating this term integration 0 to L phi star x minus m a the Hamiltonian minus h cross square over 2 m d 2 by d x square plus V x phi of x minus n a d x and we are saying this is nonzero for n equals m plus or minus 1 which is I am calling the nearest approximation.

So, you see again that the main contribution to this term comes from that delta V x term that I talked about earlier and what I am now going to call this as 0 to L phi star x minus m a H phi x minus n a d x. I am going to call is equal to gamma. Since I am integrating from 0 to L and this is nonzero that is equal to gamma for m equal to 0 to N minus 1 or 1 to N because that is where we are integrating from 0 to L if the orbit lies or the atom lies outside it its contribution within the region it is going to be very small.

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$$\frac{1}{N} \sum_m \left[e^{ik(-m+m+1)a} \gamma + e^{ik(-m+m-1)a} \gamma \right]$$

$$= \frac{1}{N} \cdot N \cdot 2\gamma \cos ka$$

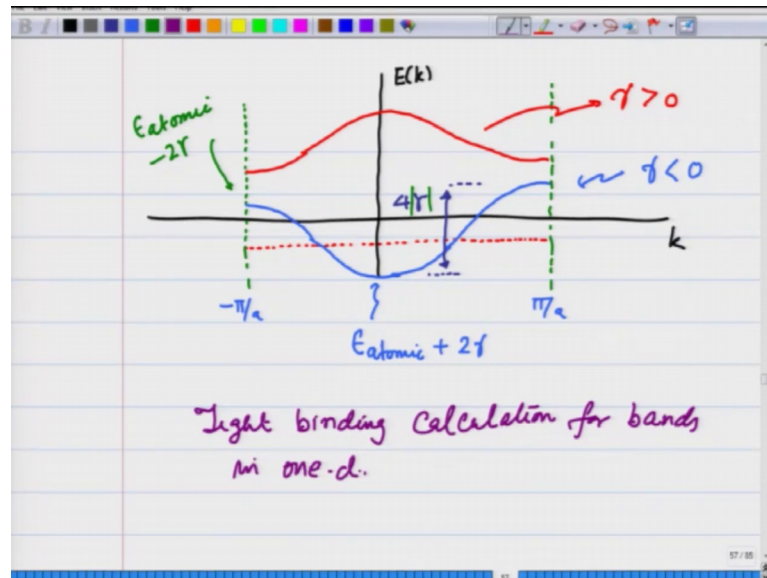
$$E(k) = \frac{1}{N} \sum_m \sum_n e^{ik(-m+n)a} \langle \phi(x-ma) | H | \phi(x-na) \rangle$$

$$E(k) \cong \epsilon_{atomic} + 2\gamma \cos ka$$

So, this term summation $\frac{1}{N} \sum_m e^{ik(-m+m+1)a} \gamma + e^{ik(-m+m-1)a} \gamma$ this is the summation over n also n equals m plus minus 1. Now, can be written as $\frac{1}{N} \sum_m$ and for the other term I am going to have $e^{ik(-m+m+1)a} \gamma + e^{ik(-m+m-1)a} \gamma$ and that is it. So, this will turn out to be $\frac{1}{N}$ times sum over m . Now each term is the same is going to give me a factor of N times $2\gamma \cos ka$.

So, recall what we were calculating. We were calculating $E(k) = \frac{1}{N} \sum_m \sum_n e^{ik(-m+n)a} \langle \phi(x-ma) | H | \phi(x-na) \rangle$. And by splitting it into m equals n term and not equal to n term and making the nearest neighbour approximation, we have gotten this to be about $\epsilon_{atomic} + 2\gamma \cos ka$. That is your $E(k)$. Notice that this γ term arises because of that ΔV mainly.

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So, if I were to plot it, $E(k)$ versus k , E_{atomic} is some number which your book Kittel calls ϵ . There is some ϵ_{atomic} and I am plotting the Brillouin zone. The band in the first Brillouin zone and if γ were negative this is how it is going to look. This is being plotted between $-\pi/a$ to π/a . This is a cosine curve.

The lowest value here is going to be $E_{\text{atomic}} + 2\gamma$, I am taking four here $\gamma < 0$. The overlap integral is giving me 0 and the width of the band from its bottom to the top is $4|\gamma|$. The top value out here is $\epsilon_{\text{atomic}} - 2\gamma$. I should put this $4|\gamma|$ as $|\gamma|$ because I am taking γ to be negative. If on the other hand γ was positive, then the curve would look like this. This will be for $\gamma > 0$.

So, you see similar kind of bands that we obtained earlier in the other extreme limit of nearly free electron model is obtained when we take LCAO, the Linear Combination of Atomic Orbitals and make appropriate combinations to make it satisfy Bloch's theorem. So, this what we have done is calculation Tight binding calculation for bands in one d.

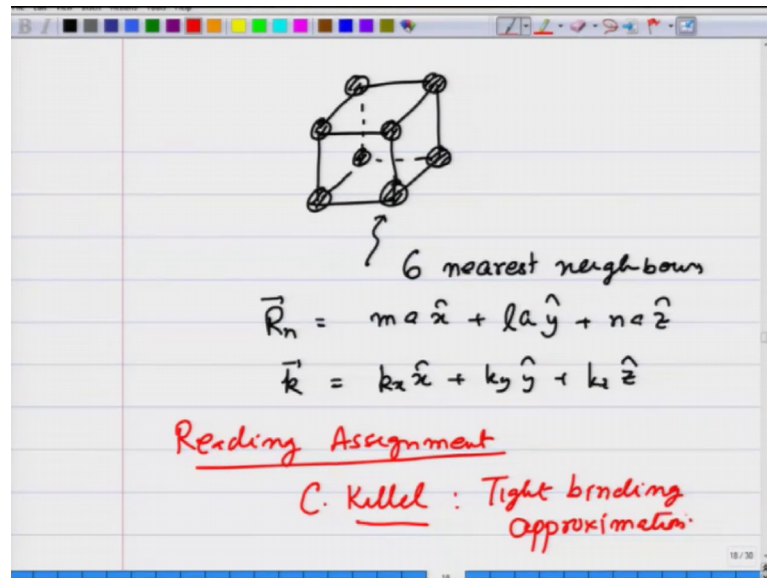
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The image shows a whiteboard with handwritten notes in green and red ink. At the top, it says "One-d calculations" in green, followed by the equation $\psi_k(x) = \sum_{n=0}^{N-1} e^{ikna} \phi(x-na)$. Below that, it says "Two or three dimensions" in red, followed by the equation $\psi_{\vec{k}}(\vec{r}) = \sum_{n=0}^{N-1} e^{i\vec{k} \cdot \vec{R}_n} \phi(\vec{r} - \vec{R}_n)$. At the bottom, there is a diagram of a 2D square lattice with a central atom circled in red. To the right of the diagram, it says "4 nearest neighbours" and the equation $\vec{R}_n = m\hat{x} + n\hat{y}$. The whiteboard has a toolbar at the top and a status bar at the bottom right showing "17/30".

Now, we have focus so far on one dimension calculations and we have taken $\psi_k x$ to be of the form summation n equals 0 to N minus 1 or N equals 1 to nN the same thing e raised to $i k n a$ $\phi(x - na)$. Now, this is easily extended to two or three dimensions. So, in two or three dimensions, I am going to have ψ_k vector, r vector is equal to summation n equals 0 to N minus 1 e raised to $i k \cdot R_n$, where R_n is the position of the n th cell $\phi(r - R_n)$.

This is going to be the form of the wave function and rest of the calculations go exactly in the same way as we did for one dimensional calculations except that when you take two dimensions. For example, if I take a square lattice and the atoms are at the corners number of nearest neighbours becomes larger for example, in two d for the central atom which I will encircle I have 1, 2, 3, 4 nearest neighbours and R_n the n th vector is going to be R_n which is some $m a_x$ plus some $n a_y$.

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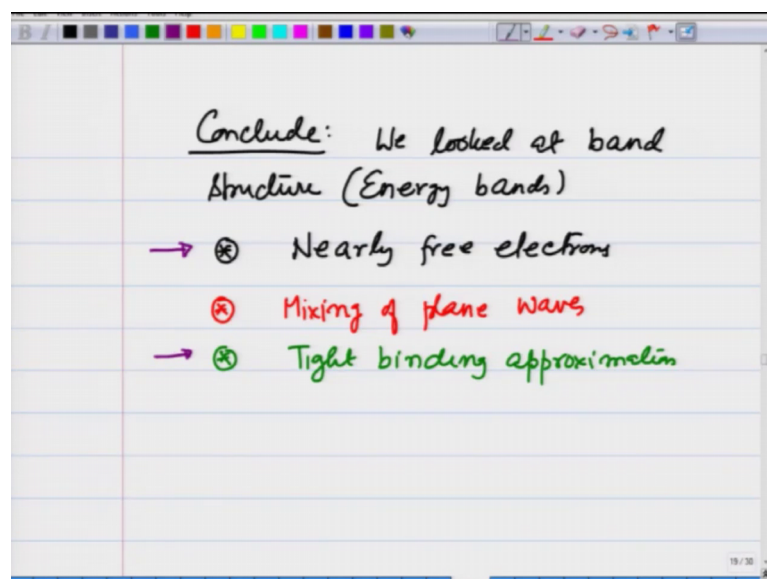
A handwritten diagram of a cubic lattice unit cell. The unit cell is a cube with atoms at the corners. A central atom is shown with dashed lines connecting it to the six nearest neighbor atoms on the faces of the cube. A bracket below the diagram indicates "6 nearest neighbours". Below the diagram, the position vector \vec{R}_n and the wave vector \vec{k} are defined in terms of their Cartesian components:

$$\vec{R}_n = m a \hat{x} + l a \hat{y} + n a \hat{z}$$
$$\vec{k} = k_x \hat{x} + k_y \hat{y} + k_z \hat{z}$$

Below the formulas, the text "Reading Assignment" is written in red and underlined. Underneath that, "C. Kittel : Tight binding approximation." is written in red.

Similarly, when I go to three dimensions suppose I take a cubic lattice and here are the atoms at the corners for each atom there are going to be 6 nearest neighbours and R_n is going to be of the form some $m a x$ plus $l a y$ plus $n a z$ and k is also going to have three components. $k_x x$ plus $k_y y$ plus $k_z z$ and it will require a little more book keeping, but procedure is exactly the same. I will be giving you problems related to this and I urge you to read this from Kittel's book Tight binding approximation.

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Conclude: We looked at band structure (Energy bands)

- ⊗ Nearly free electrons
- ⊗ Mixing of plane waves
- ⊗ Tight binding approximation

So, this winds up our you know different ways of looking at bands. So, I conclude this lecture by noticing that we looked at band structure or energy bands from the point of view of nearly free electron in which I applied the perturbative approach, then I looked at it from the mixing of plane waves where we mix many many plane waves to get the wave function in a periodic structure and third we have looked at it from the tight binding approximation point of view.

And if you look at it the first one the nearly free electrons model and the tight binding approximation. These are at the two extremes of band structure calculations in one we have electrons moving freely and then we apply a very weak perturbation and see how bands arise. In the tight binding case we have electrons tight bound to atoms and then we delocalize them a bit so that the electrons interact with only neighbouring potentials. In the next lecture I will be talking about how particles move in a band when a force is applied.

Thank you.