Electronic Properties of the Materials: Computational Approach
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Lecture: 24
Band Structure in 1D: Different Representation

Hello friends we have solved time independent Schrodinger equation for a periodic potential we now know the existence of energy bands and band gaps appearing due to the periodic potential. There is no unique representation of energy bands the same information can be presented in different ways. In this lecture I am going to discuss different representations of energy bands using energy versus wave vector or EK diagram.

This is also known as the band structure. I am going to start with 1D. So, that you can easily correlate with what I have discussed. So, far then I am going to discuss an alternate representation known as the energy pen diagram.

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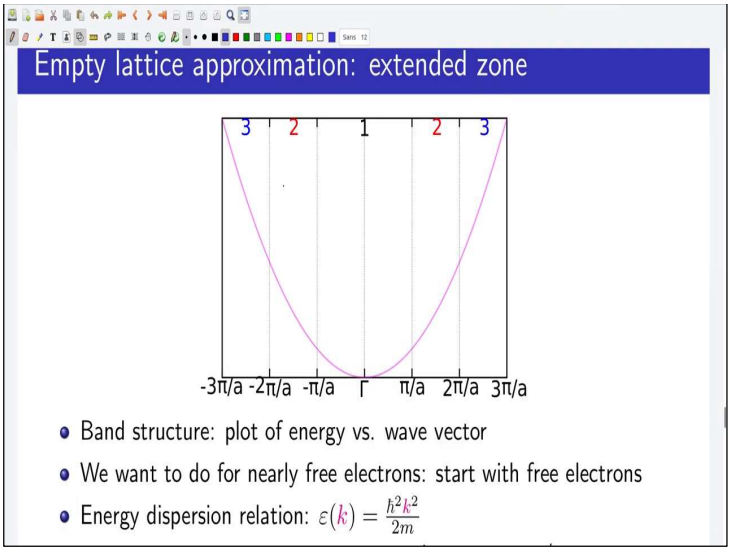

Here I show the free electron energy versus K Parabola in case of 1D block of energy versus wave vector k is known as the band structure. One denotes the first Brillouin zone 2 denotes the second Brillouin zone and three denotes the third Brillouin and so on. You may ask why we are talking about reciprocal lattice in case of free electrons this is why this is known as the empty lattice approximation although there is no potential but we still assume that there is some underlying lattice and reciprocal lattice.

You may wonder why we are doing so since we want to ultimately understand band structure of nearly few electrons it is not a bad idea to start with free electrons. For free electrons the energy dispersion relation is E k is equals to h cross by k Square by 2m. The wave vector k lie in first Brillouin zone second Brillouin zone and third Brillouin zone or any other Brillouin zone. So, however we know that we can map K back to some K Dash lying in the first Brillouin zone by adding some suitable lattice vector g.

For example take some point K in the second Brillouin zone. So, this is the point k now we subtract 2 pi by a such that this point is brought back to the first Brillouin zone and this is the equivalent Point K dashed in the first Brillouin zone. Similarly if we take some point say K in the third Brillouin zone then we can bring it back to the first Brillouin zone by subtracting 2 pi by a such that this point moves here. So, this is some point k dashed lying in the first Brillouin zone. Now let us see whether we can represent the band structure within the first Brillouin zone.

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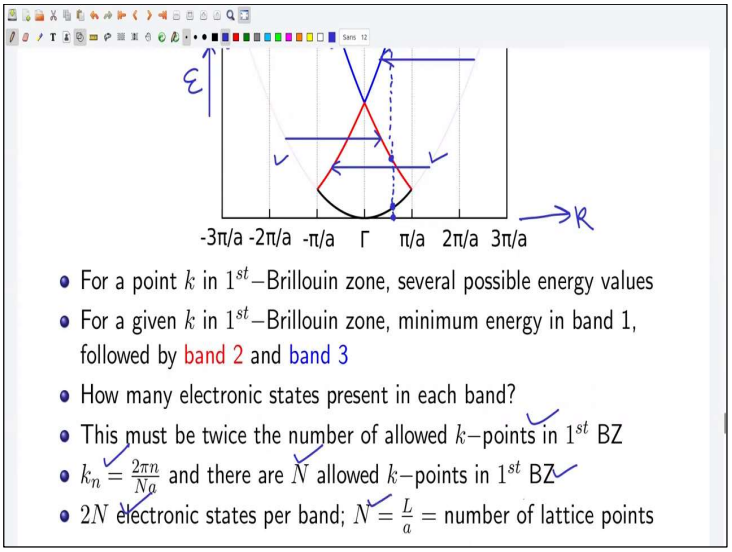

In this diagram I plot the free electron energy versus K Parabola portion of the parabola lying in the first Brillouin zone is shown in plank portion of the parabola lying in the second Brillouin zone is shown in red and portion of the parabola lying in the third Brillouin zone is shown in blue now I shift the portion lying in the second Brillouin zone and bring it back to the first Brillouin zone.

Similarly I take this portion lying in the second video and bring it back to the first Brillouin zone I do the same thing for the third Brillouin zone. So, I bring it back to the first Brillouin zone and similar thing for this portion. This is the band structure of free electrons represented in reduced zone scheme the vertical axis is the energy axis and the horizontal axis is the wave vector axis. So, we have mapped everything back to the first Brillouin zone.

For example this portion lying in the second Brillouin zone has been mapped here and this portion has been mapped here. Similarly this portion lying in the third Brillouin zone has been mapped here and this portion has been mapped here thus we have mapped everything to the first Brillouin zone and confine the relevant information to the first Brillouin zone only.

If we take a point in the first Brillouin zone we get several possible energy values. For example you can take this K point in the first Brillouin zone and the corresponding energy value in the first band is this; the corresponding energy value in the second band is this and the corresponding energy Brillouin zone in the third band is this. So, we have multiple energy values for a single key point in this representation.

Now let us find the number of electronic states in each band first we have to find the number of allowed K points in the first Brillouin zone because each K Point can accommodate two electrons as Pauli Execution principle number of electronic states must be twice the number of the K points in the first Brillouin zone. Along k points determined by the periodic boundary condition and given by K n is equals to 2 pi n divided by capital N times a and there are capital N number of allowed K points in the first Brillouin zone.

Thus there are 2N electronic states per band where capital N is the number of lattice points in a 1D solid of length L.

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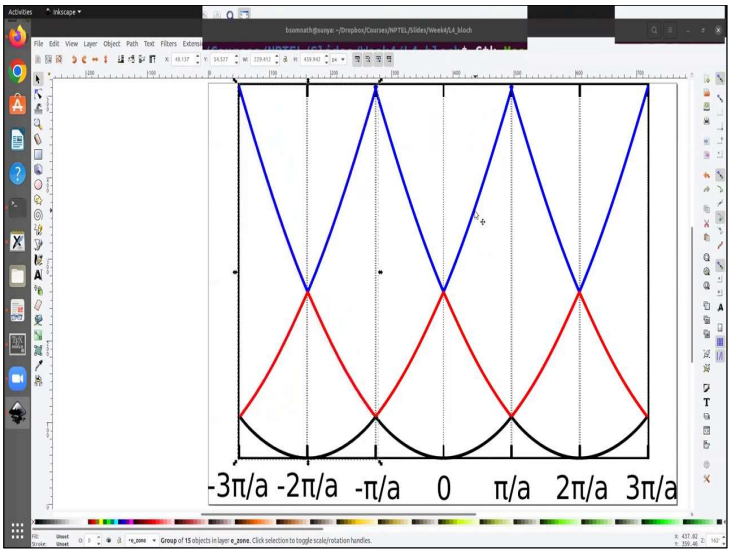

Now there is another scheme to represent energy dispersion known as the periodic or repeated zone scheme. Here we take the band structure in the first zone and repeat it in every other Brillouin zone. For example we just repeat this in every other Brillouin zone. Smilarly we do this.

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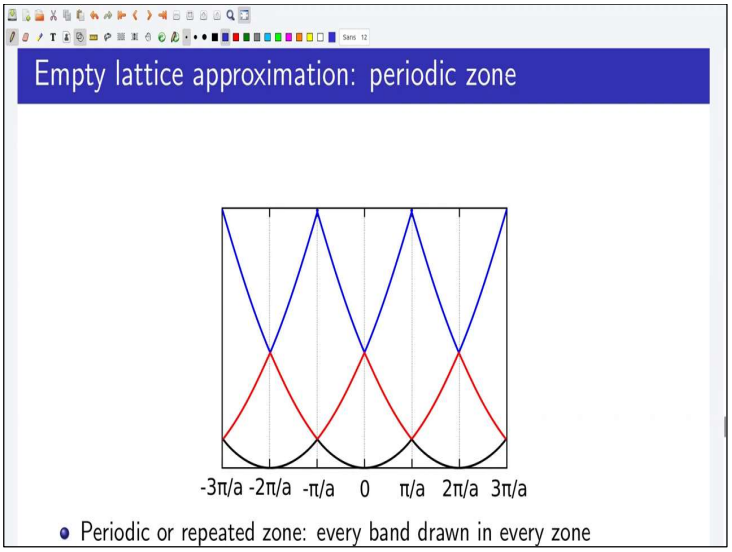

This is the periodic scheme where every band is drawn in every zone this is also known as the repeated zone scheme.

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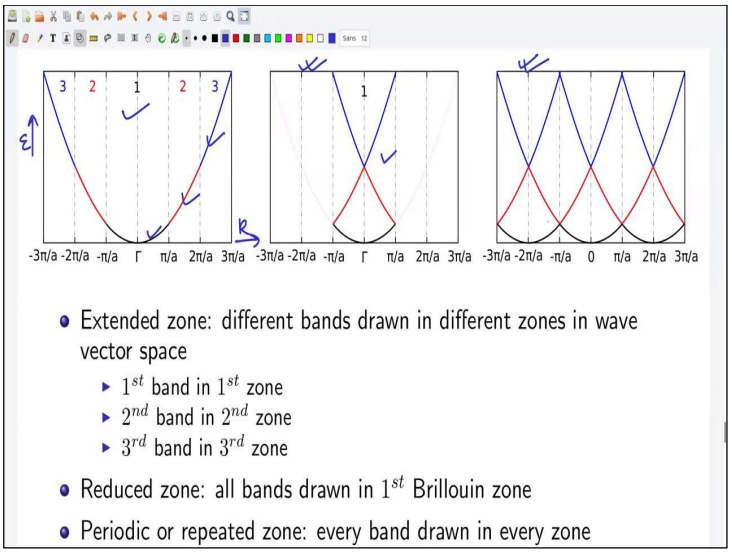

Here I show the comparison among different schemes energy lies along the vertical axis and wave vector is along the horizontal axis. The first one is the extended zone scheme where different bands are drawn in different zones in wave vector space. For example the first band is drawn in the first zone the second band is drawn in the second zone and the third band is thrown in the third zone.

Next one is the reduced zone scheme where all bands are drawn in the first Brillouin zone. The last one is the periodic or repeated zone scheme where every band is drawn in every zone.

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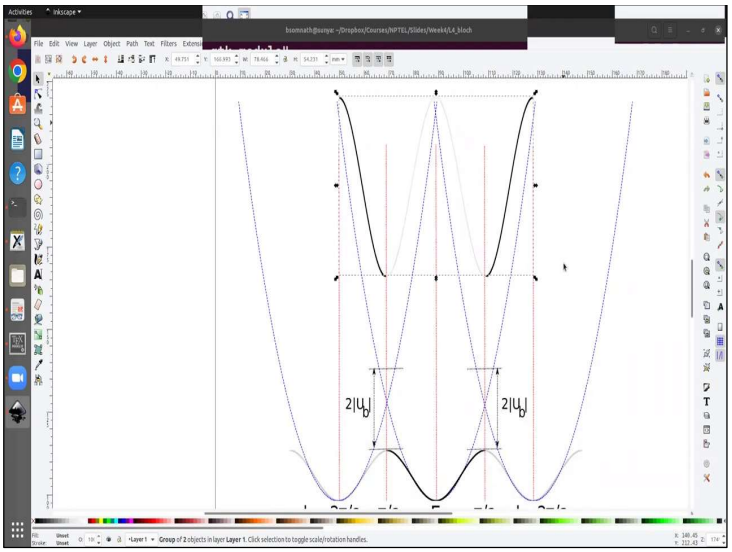

We have discussed about band structure of free electrons using empty lattice approximation now let us get back to the actual problem that is representing the band structure for nearly free electrons the advantage of nearly free electron model is its simplicity we can start with the free

electron band structure and modify it only near the Brillouin zone boundary to get the actual band structure for a weak periodic potential. Let me explain how to do it systematically.

We start with the free electron energy versus K Parabola shown by the blue dashed curve. We repeat it periodically in reciprocal space such that the parabola is centered at every reciprocal lattice point for example we shift the parabola to the reciprocal that is located at 2 pi by a. Similarly we shift the parabola to the reciprocal that is Point located at -2 pi by a vertical red dotted lines denote the location of the reciprocal lattice points as well as Brillouin zone boundaries.

The first Brillouin zone boundary is at Pi by a and minus Pi by a the second Brillouin zone boundary is at 2 pi by a and minus 2 pi by a. Note that Parabola centered at two adjacent reciprocal lattice point are crossing each other at the Brillouin zone boundary. For example take the parabola centered at the gamma point and at 2 pi by a. They cross each other at the first Brillouin zone boundary located at Pi by a. Due to periodic potential energy gap will open at the Brillouin zone boundary where free electron parabolas are crossing each other.

Remember that black planes are located at every Brillouin zone boundary. The free electron Parabola will get distorted near the black planes due to the weak periodic potential. We have to change in such a way that energies deviate from the free electron values only near the Brillouin zone boundaries. Let us do it for the first band the black curve is the energy of electrons in a periodic potential.

Note that for the first band energy is same as free electron energy near the gamma point as we move close to the first Brillouin zone boundary the curvature changes and first derivative of energy becomes zero at the first Brillouin zone boundary in case of the black curves. We do similar thing for the second band also.

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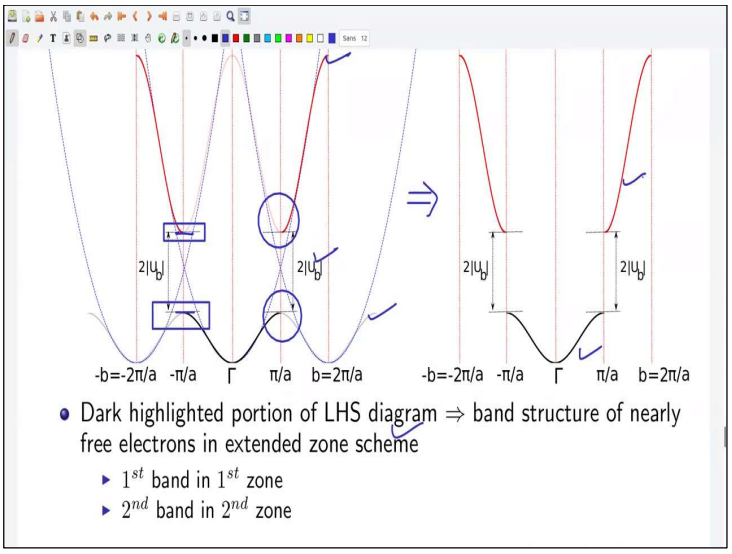

Again note that the deviation from the free electron energy occurs only near the first and second Brillouin zone boundary as a result of the deviation from the free electron energy band Gap opens up at every Brillouin zone boundary. The magnitude of the Gap depends on the Fourier component of the periodic potential. Starting with free electron energy versus K parabolas we have learned how to distort them near the Brillouin zone boundaries and get the band structure for a weak periodic potential.

Note that we have not done any calculation at all we just took free electron parabolas and change the free electron energies close to the Brillouin zone boundary. For example in this region or in this region the distortion shown by the black line for the first band and shown by the red line for the second band are done in such a way that the band gap matches with 2 times U b where U b is the Fourier component of the periodic potential.

Note that at the Brillouin zone boundary slope of E versus K curve for the electron in a periodic potential goes to zero. For example here and here if we take only the dark highlighted portion from the left hand side diagram then we can construct the band structure shown in the right hand side. Clearly this is the extended zone scheme as the first band is plotted in the first Brillouin zone and the second point is plotted in the second Brillouin zone.

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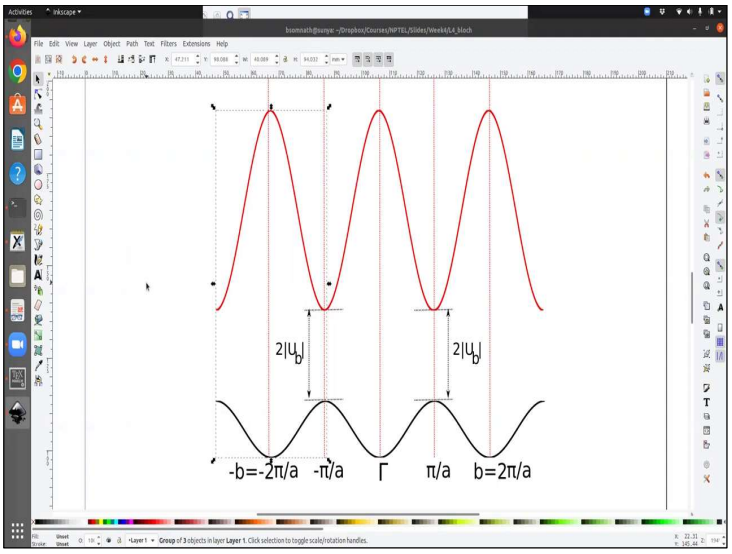

So, as we did for the free electrons we can plot all the banks in the first Brillouin zone to do that we need to shift this portion of the second band to the first Brillouin zone. Similarly we need to shift this portion of the second band to the first Brillouin zone. Finally we can plot all the bands in all the zones by repeating the bands in the first zone to all the other zones. This is the periodic or repeated zone scheme.

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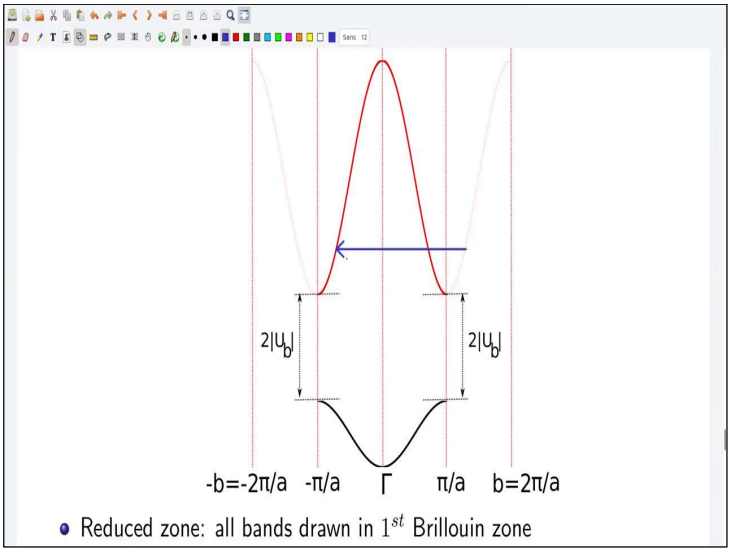

This is the reduced zone scheme where all the bands are drawn in the first Brillouin zone to do that we need to shift this portion of the second band to here in the first Brillouin zone and this portion is shifted here.

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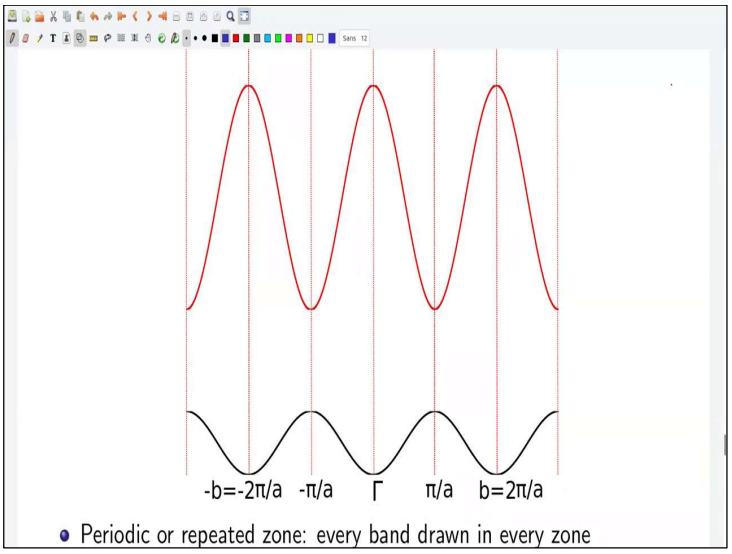

This is the periodic or repeated zone scheme where every band is drawn in every zone.

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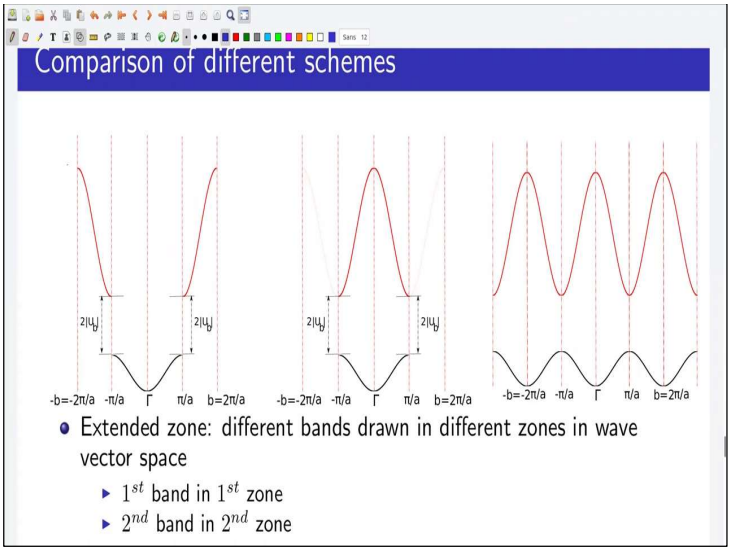

This is the comparison of different schemes for representing band structures vertical axis is energy and horizontal axis is the wave vector. In extended zone scheme different bands are drawn in different zones in wave vector space for example the first band is drawn in the first Brillouin zone and the second band is drawn in the second Brillouin zone in the reduced zone scheme all the bands are drawn in the first Brillouin zone. And in the periodic or repeated zone scheme every band is drawn in every zone.

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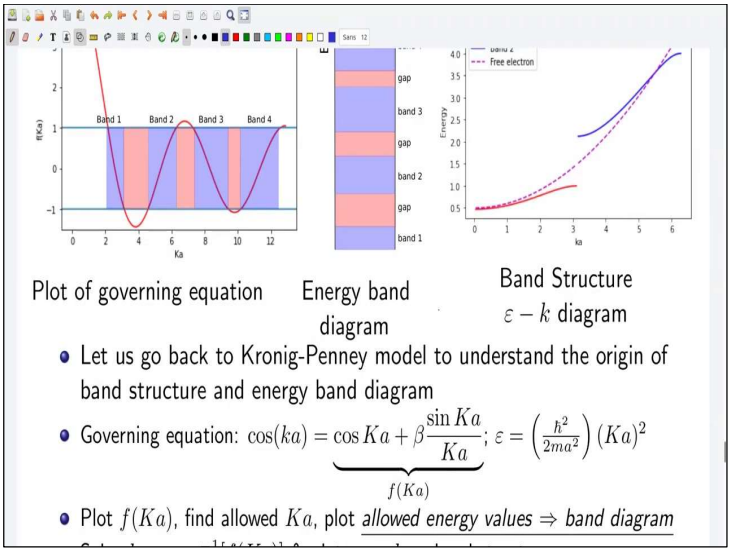

There are two different ways of representing the electronic bands band structure or EK diagram and energy band diagram. To understand the origin of band structure and energy band diagram let us go back to the Kronig-Penny model. The governing equation in Kronig-Penny model is this where capital K is related to the energy small k is the wave vector and small a is the distance between two adjacent lattice points and beta is the strength of the periodic potential.

Plot of f of Ka is shown in the first diagram since f of Ka has to lie in a range of plus 1 and -1, we can easily identify the allowed regions of f of Ka as shown by the blue shaded regions in the figure. Once we have identified the allowed K values we can use this equation to get the allowed energy values. Allowed energy regions are termed as energy bands like Band 1 Band 2 Band 3 etc. Energy values lying between two allowed regions are forbidden and we call them as gaps as shown here.

This type of representation of allowed energy value is known as the energy band diagram. Using the governing equation we can also find the value of the wave vector of block electrons by solving small K times a is equals to cos inverse f capital K of a. Then we can plot energy versus wave vector. This type of representation of allowed energy values is known as the electronic band structure or EK diagram.

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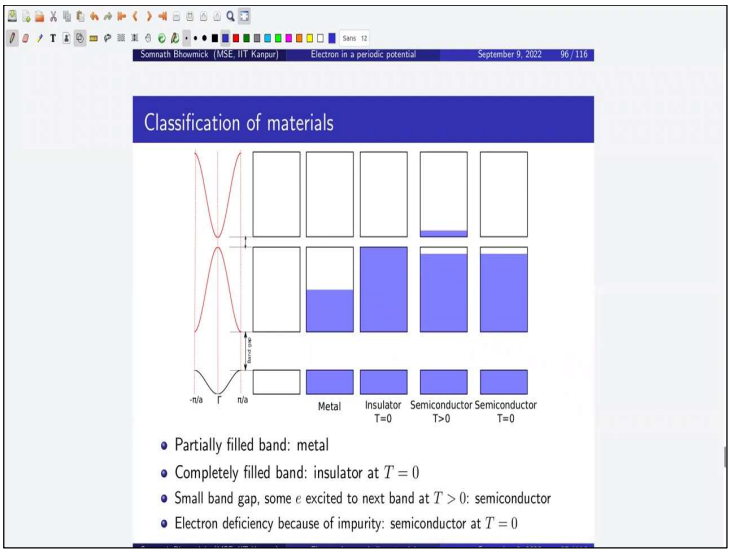

Now let me show you a broad classification of materials represented by energy band diagram. The first figure is a band structure or EK diagram shown using the reduced zone scheme. The corresponding band diagram is shown in the adjacent figure. Next we start filling the energy levels with electrons if we end up getting some partially field band we call it a metal for example in case of a metal the first band is completely full and the second band is partially full.

So, this is a metal partially filled bands have electrons that can take part in electronic transport. If all the bands are either completely full or completely empty we call it an insulator. Since these bands are completely full they cannot take part in electronic transport. If some of the electrons can be thermally excited to the next energy band then they can take part in electronic transport.

This is possible if the energy gap is not too high and such materials are classified as semiconductors. Finally we can artificially create some electron deficiency by doping. Example of yore and dope semiconductors will be discussed later in detail. Note that the energy band diagram looks similar in one dimension and in higher dimension as well.

However EK diagrams in higher dimension is more complicated than 1D EK diagrams. In the next lecture we shall learn how to construct EK diagram for 2D and 3D solids.

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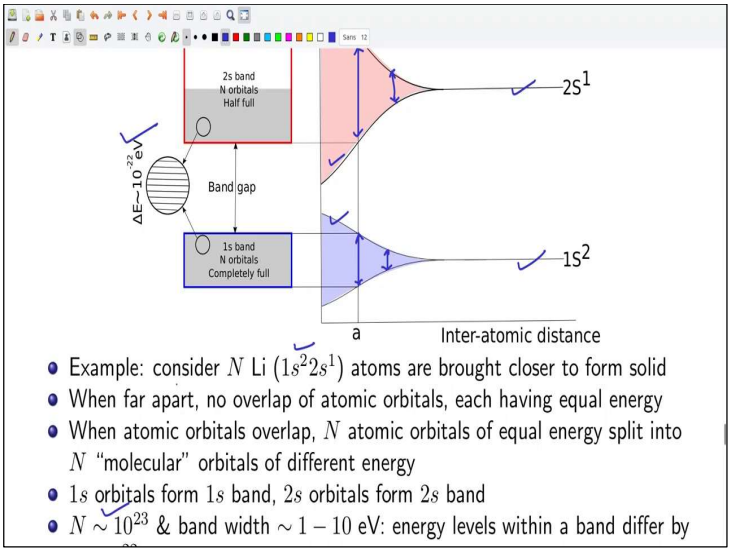

We can also understand the origin of energy band diagram starting from the atoms and atomic orbitals. Consider we start with isolated lithium atoms and being them close to each other to form a solid. Electronic configuration of Lithium is 1s2 2s1 when far apart Atomic orbitals do not overlap and all of them have same energy. When we bring the atoms closer Atomic orbitals start to overlap as a result n atomic orbitals of equal energy split into n molecular orbitals of different energy.

As a result of this 1s orbitals form 1s band 2s orbitals form 2s band. Bandwidth is given by the amount of splitting at the equilibrium distance a. Each band has N molecular orbitals where N is the order of 10 power 23. Typical bandwidth is 1 to 10 electron volt thus gap between two molecular orbitals within a band is of the order of 10 power -22 electron volt. This is a very small number in conclusion energy levels within a band can be considered as continuous.