Electronic Properties of the Materials: Computational Approach
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Lecture: 25
Band Structure in 2D and 3D

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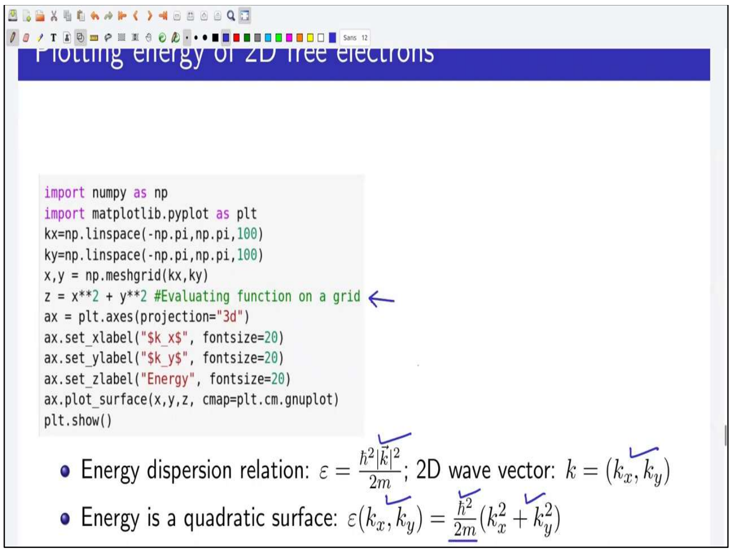

Hello friends we already have learned about different representations of band structure in one dimension using nearly free electron model. In this lecture we are going to learn about plotting the band structure in 2 dimension and three dimension. Let us start with 2D free electrons energy dispersion relation is e is equals to h cross square k square divided by 2m where k is a 2D wave vector having 2 components k x and k y energy is a quadratic surface in k space given by e is equals to h cross square by 2 M k x square + k y square. Taking h cross square by 2 M is equals to 1 I define energy in this line of the code.

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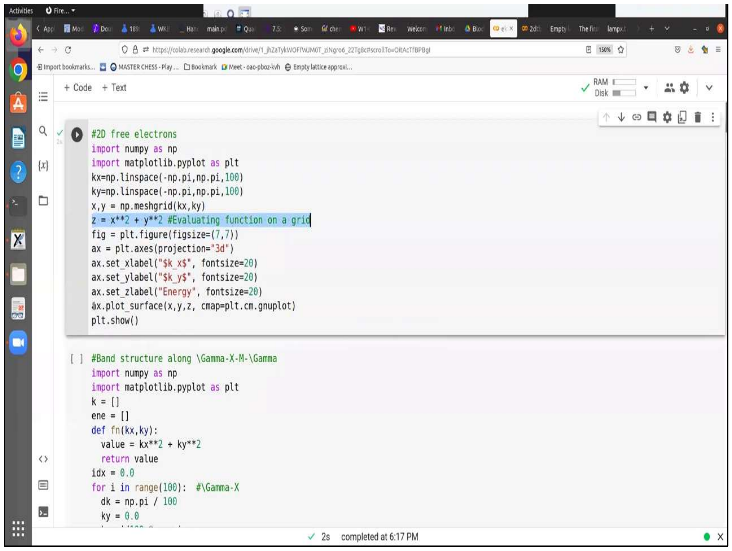

This is the code to plot the free electron energy in 2D. I take the range of k x from - pi to + pi similarly range of k y is from - pi to + pi this line is needed to plot a function on a 2D rate I define the energy in this line and the energy surface is plotted in this line let us run the code.

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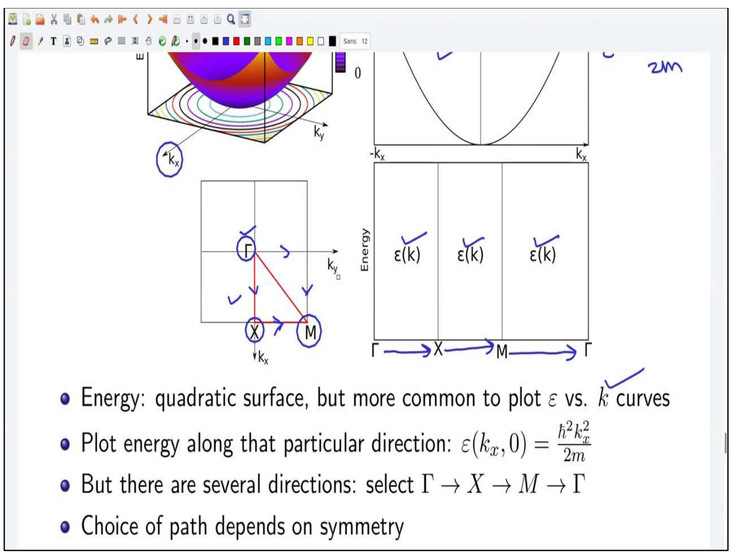

This is the EK diagram for 2D free electrons energy is a quadratic surface in 2D however it is more common to plot e versus k curves. For example we can calculate energy along a specific direction say k x direction. If we move along the k x line then k y is equals to 0 and energy is given by e is equals to h cross square k x square divided by 2m in that case we get a curve which is similar to the case of 1D.

However in 2D we can move along several directions like gamma 2x like gamma 2y like x 2m etcetera. We select some particular path like gamma 2x that is from this point to this point then x to M that is from x point to the M point and finally M 2 gamma that is from M point back to the gamma point. And we plot E k curves along this selected paths choice of path is not arbitrary but depends on symmetry.

For example in this case energy along the gamma x path is same as energy along the gamma y path thus if we plot energy along gamma x we need not plot energy along gamma y. Similarly energy along Y M path is same as energy along X M path. Thus if we plot energy along X M path we need not to plot energy along Y M path in other words because of symmetry gamma x and gamma y direction is equivalent. So, once we define gamma x we need not to define gamma y direction separately.

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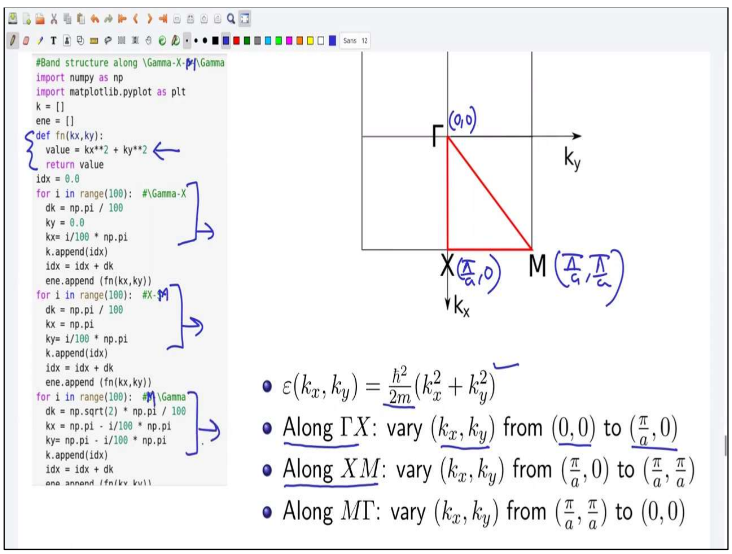

This is the code to plot the band structure along gamma xm gamma line energy is given by e equal to h cross square by 2m times k x square + k y square taking h cross square by 2 M to be equal to 1 we define the energy in this line we have a user defined function which returns the value of energy for a given value of k x and k y. To plot the EK diagram along gamma x k x k y is varied from 0,0 to pi by a, 0. So, gamma point is 0,0 and this point is pi by a, 0 in this portion we vary k x k y along the gamma x direction.

Then we plot EK diagram along XM direction where x is this point pi by a 0 and M is a point pi by a pi by a. In this portion we vary k along the X M direction. Finally we vary k in the M gamma direction in this portion of the code.

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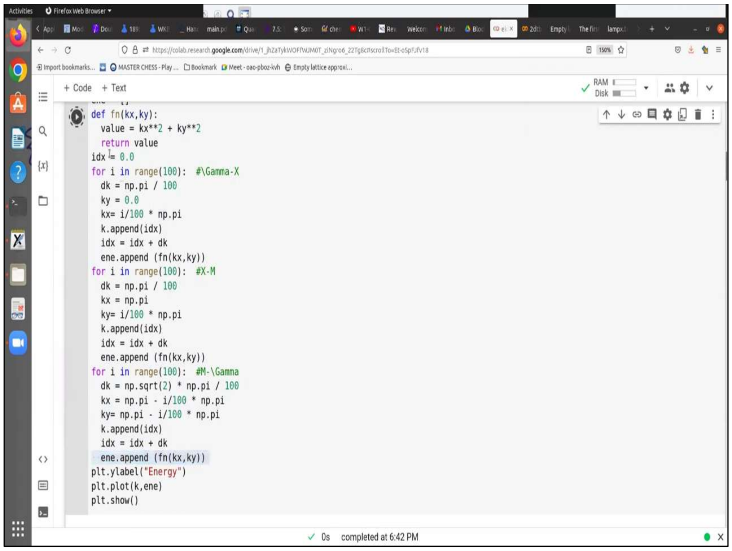

This is the code to plot the band structure along gamma X M gamma direction. This is the user defined function which returns the value of energy for a given value of k x and k y this is where we vary k x k y along the gamma x path and calculate energy along the gamma x path. This is where we vary k x k y along the X M path and calculate energy along the X M path this is where we vary k x k y along the M gamma path and calculate energy along the M gamma path. Let us run the code.

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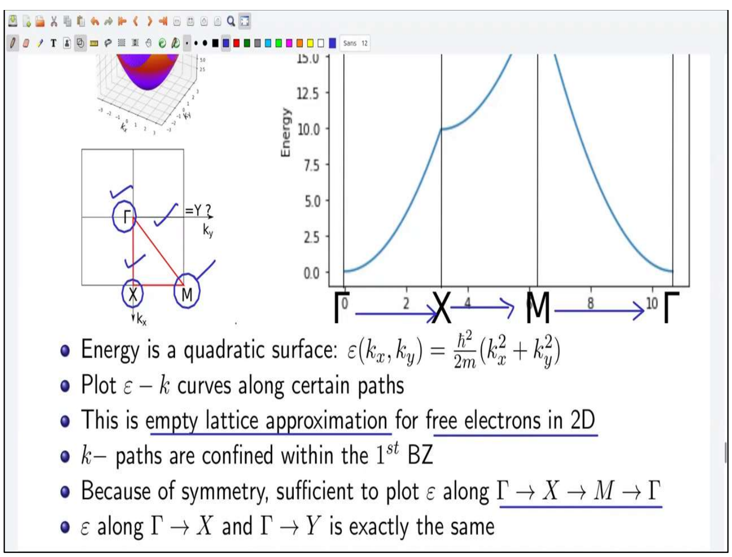

Energy is a quadratic surface in k space for 2D free electrons we plot E versus K curves along certain paths for example in this case we plot along gamma 2x that is the line joining gamma point and x point then from X to M that is the line joining X point and M point and finally from M to gamma that is the line joining the end point and the gamma point gamma X M are high symmetry points in the first Brillouin zone of the reciprocal lattice of a square lattice.

Thus this is empty lattice approximation for free electrons in 2D because we are introducing reciprocal lattice in a free electron model. Note that K paths are confined to the first Brillouin zone because of symmetry it is sufficient to plot EK curves along gamma to X to M to gamma for example EK curve along the gamma x direction is same as the EK curve along the gamma y direction. Thus if we plot along gamma x we do not need to plot along gamma y let me prove this to you.

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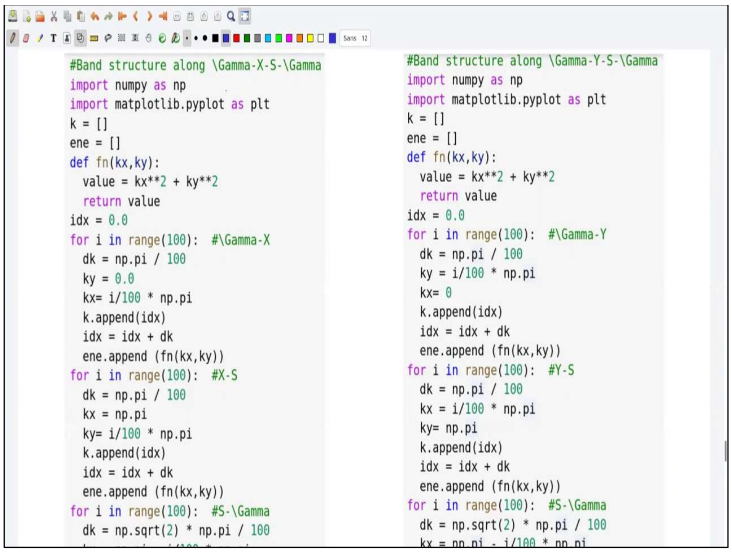

I write 2 codes first one plots e k along the path gamma x M gamma the. Second one plots EK along gamma y M gamma in this code we vary K along the gamma x path whereas in the second code we vary k along the gamma y path. Then we vary along X M and along Y M. Finally we vary K along M gamma and M gamma the energy values are calculated in this user defined function for a given value of k x and k y.

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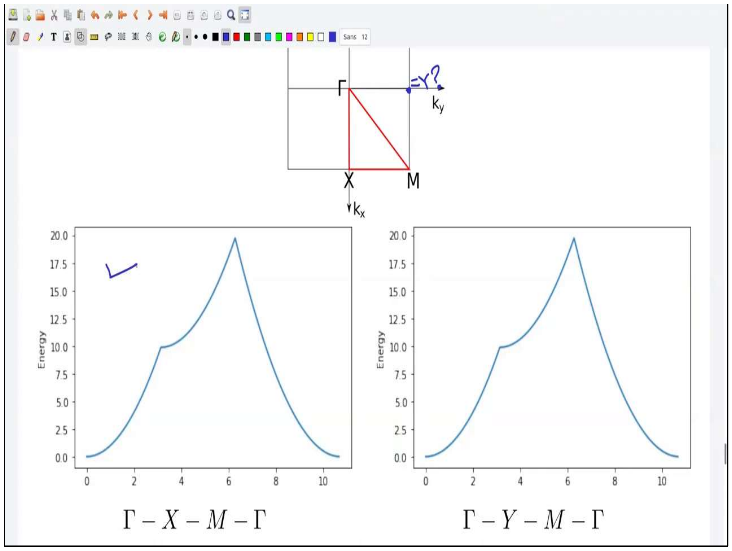

This is the EK diagram for 2D free electrons plotted along gamma X M gamma and this is the EK diagram for 2D free electrons plotted along gamma Y M gamma as mentioned previously they are exactly the same because of symmetry. Thus we can choose to show EK along either gamma X or gamma Y. We do not need to show both gamma to X and gamma to Y and this happens because X point and Y point is equivalent because of the symmetry of the square lattice. Thus if we show EK diagram along gamma x we need not to show e diagram log gamma y.

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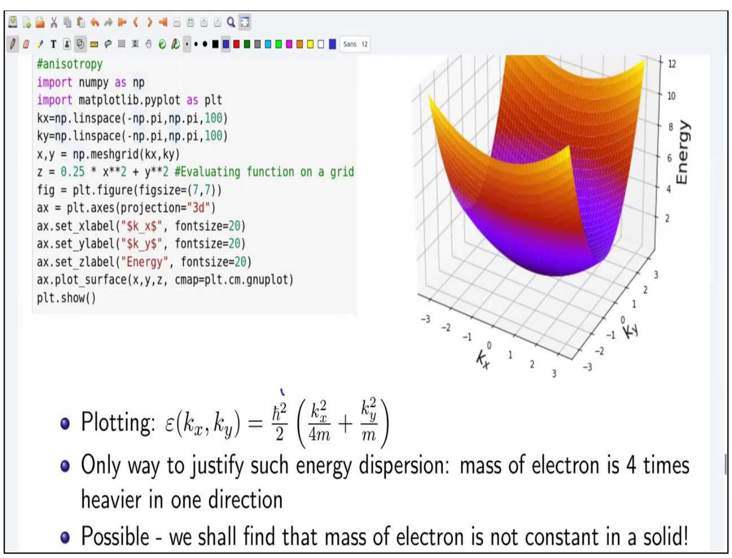

Let us consider a case where energy dispersion relation is given by e is equals to h cross square by 2 times k x square by 4 M + k y square by M clearly energy is not symmetric along k x and k y energy increases slowly in the k x direction and energy increases rapidly in the k y direction. How we can get such energy dispersion only way to justify such a dispersion is to assume that mass of electrons is 4 times heavier along k x that is we can write this as h cross square by 2 k x square by M + k y square by small m.

Where m is the mass of electron along the k x direction and small m is the mass of electron along the k y direction and capital M is four times the small m. Is this just a toy model it turns out that such dispersion is indeed possible and mass of electron is not constant in a solid. Mass of electron can be heavier or lighter compared to free electron mass along certain directions in a crystal.

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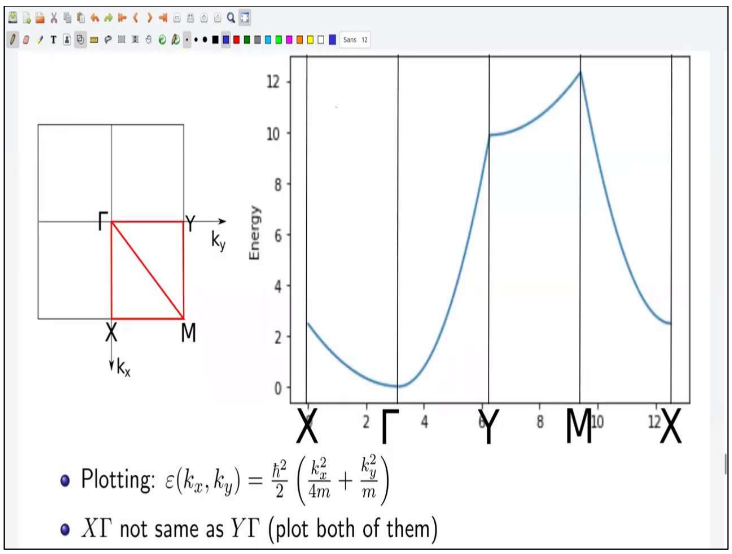

This is the EK diagram along the high symmetry directions in the first Brillouin zone in case of anisotropy because of anisotropy now gamma 2x and gamma 2y directions are not equivalent thus we need to show EK curve along X to gamma as well as gamma to Y. Similarly M to Y and M to X are not equivalent because of an isotropy and we have to show E versus K curves along M to X as well as M to Y.

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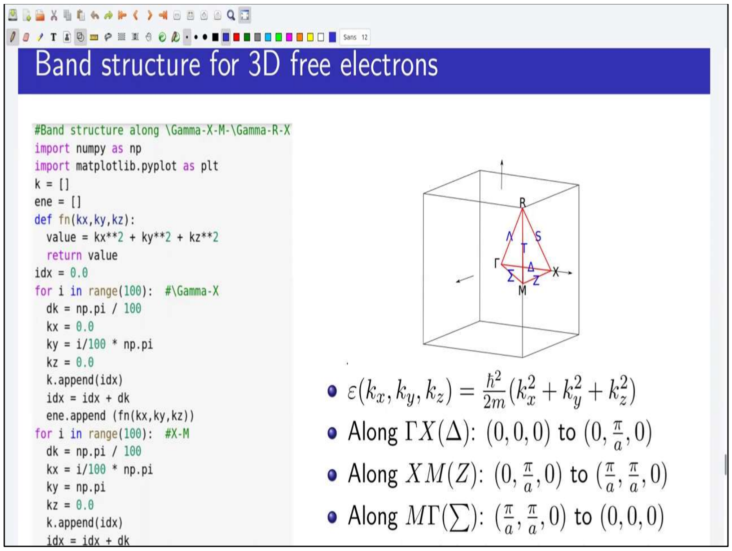

Let us now plot the electronic band structure of free electrons in 3D using a python code. The energy dispersion relation is equal to h square by 2m times k x square + k y square + k z square I set h cross square by 2m to be equal to 1 and then calculate the energy using a user defined function in the code for a given value of k x k y and k z the function returns the value of energy. We have to plot energy versus K along gamma 2x this is known as the delta path.

In the code I vary K along the gamma x direction in this portion. Then we have to plot energy versus K along X to M the line joining X to M is known as the set line in the code I vary K along X M direction in this portion then we have to plot energy versus K along M to gamma the line joining M 2 gamma is known as the sigma line I vary K along M to gamma in this portion of the code.

This is followed by gamma 2 R and the line joining gamma and R is known as lambda finally we plot E versus K along R to X and the line joining R to X is known as the S line.

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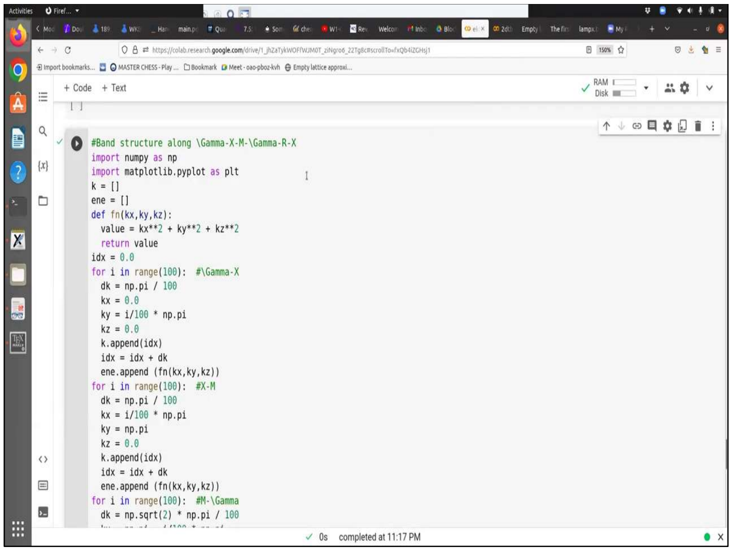

This is the code to plot the band structure along gamma 2x to M to gamma to R to X this is the user defined function where I calculate the value of energy for a given value of k x k y and k z. This is where I vary K along the gamma x line and calculate energy along the gamma x line. This is where I vary k along the x M line and calculate energy along the xm line. This is followed by M gamma gamma R and R x let us run the code.

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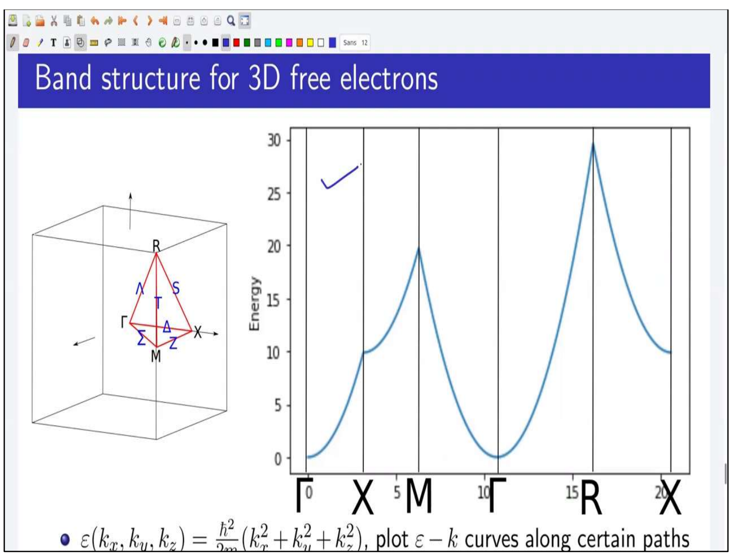

This is the band structure of 3d free electrons plotted along gamma to X, X to M, M to gamma, gamma to R and R to X. Note that gamma X, M and R are high symmetry points in the first Brillouin zone of the reciprocal lattice of a simple cubic lattice. We are using reciprocal lattice in case of free electrons and this is known as the empty lattice approximation K paths are confined within the first Brillouin zone because of symmetry it is sufficient to plot energy versus K along gamma to X, X to M, M to gamma, gamma to R and R to X. I have skipped energy versus k plot along R to M path and this is left as an exercise for U.

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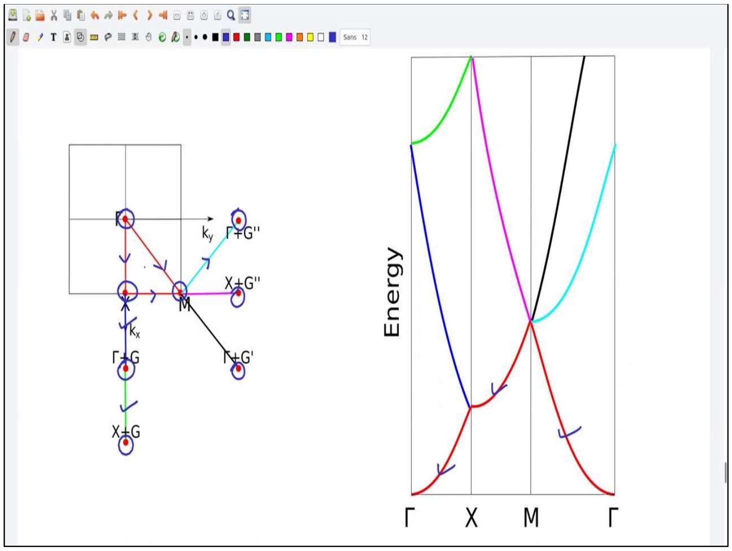

So, far we have plotted only one band in the EK diagram using python code. However in case of 1D we have seen that all the bands are plotted in the first Brillouin zone in case of reduced zone scheme how do we do it for higher dimension. For example take the case of 2D we have plotted the band structure along gamma to X, X to M and M to gamma shown by the red lines in this diagram. If we keep going along gamma x then we reach a point gamma + G and finally reach a point X + G which is outside the first Brillouin zone.

How do we map the EK curves in these zones to the first Brillouin zone. Similarly if we keep moving along gamma M then we reach a point gamma + G dashed and if we keep moving along XM then we reach a point X + G 2 dashed and if we keep moving along this line then we reach a point gamma + G 2 dash. How do we map the EK curves along these lines to the first Brillouin zone let us learn that.

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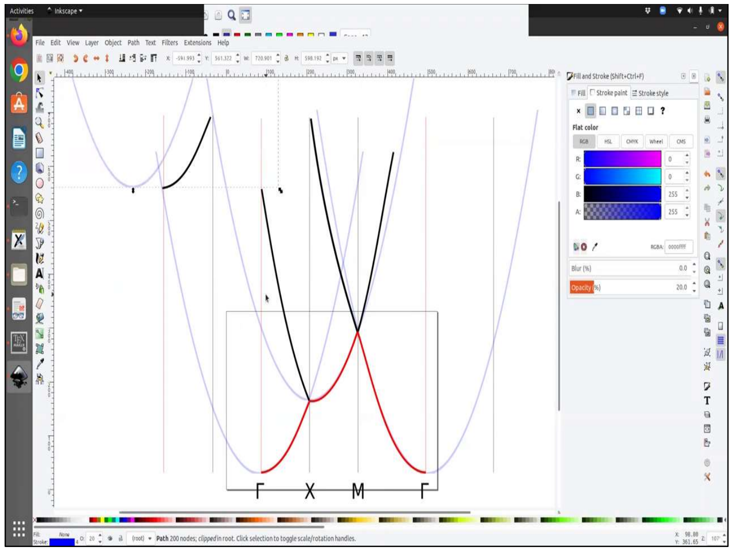

In this diagram red lines are the actual E versus K curves we obtained from our code let us start at this gamma point we draw a parabola which fits the red line along the gamma x direction. The black region is the portion which is lying outside the first Brillouin zone we have to bring it inside the first Brillouin zone. Next we draw a curve that fits the actual E versus K curve in the X M region.

Now this black portion is lying outside the first Brillouin zone and we have to bring it inside the first Brillouin zone then we focus on the other gamma point and draw a parabola that fits the actual EK curve along the gamma M direction. Now this black region lies outside the first Brillouin zone and we have to bring it inside the first Brillouin zone. If we keep moving along the gamma x direction ultimately we reach another reciprocal lattice point,

Here we draw a E versus K parabola at this reciprocal lattice point and this black portion of the parabola we bring it inside the first Brillouin zone. So, we can keep doing this and bring all the EK curves lying outside the first Brillouin zone to inside the first Brillouin zone this is the E versus K diagram for 2D free electrons in reduced zone scheme. The red portion of the curves are energy for K paths within the first Brillouin zone.

The dark blue portion is the energy along X to gamma + G the green portion is energy along gamma + G to X + G. The magenta portion is energy along m2 x + g 2 dashed the black portion is energy along M to gamma + G dashed and finally the light blue portion is energy along M to gamma + G dash.

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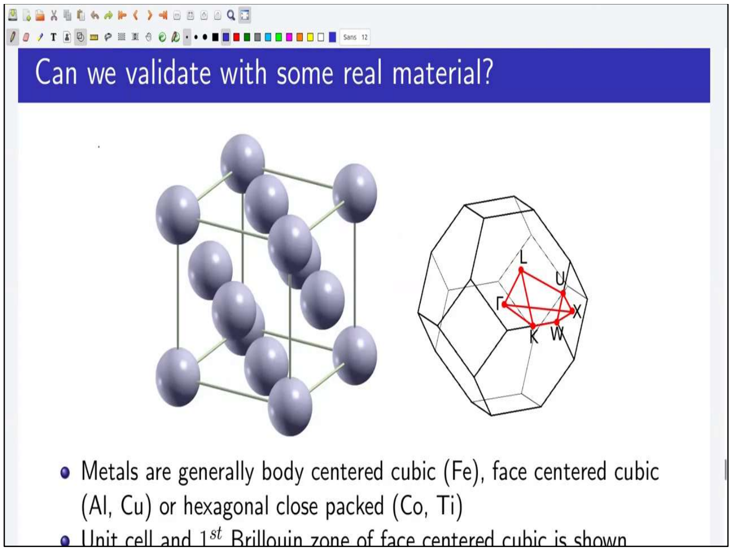

Let us try to understand how good is empty lattice approximation does it work for metals where valence electrons are like free electrons or does the periodic potential have very significant effect in case of metals also. Most of the metals we know are either body centered cubic like iron or face centered cubic like aluminum copper or hexagonal close packed like cobalt and titanium.

Unit cell of face centered cubic lattice and corresponding first below in zone and high symmetry points are shown in the diagram. Let us plot empty lattice band structure along l to gamma to x to u to gamma and compare with actual band structure of aluminum.

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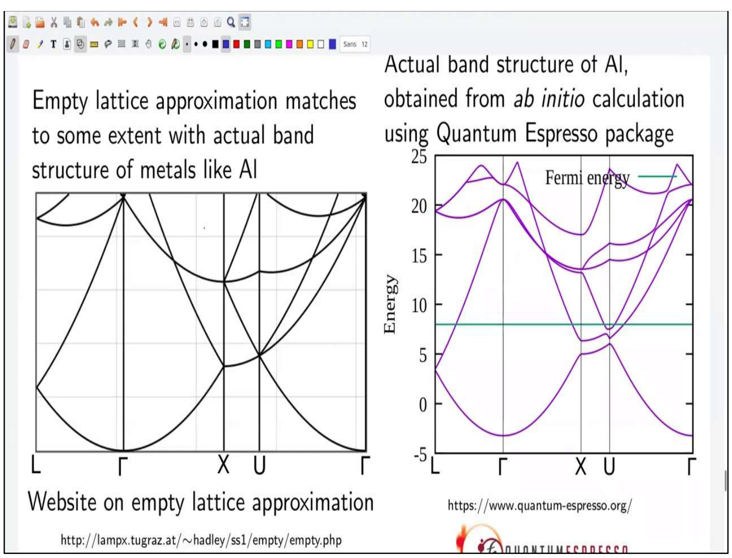

In case of a square lattice I showed you how to plot the band structure using empty lattice approximation we can use the same principle and do it for a face centered cubic lattice.

Obviously doing it for a face centered cubic lattice is going to be much more complicated than a square lattice. So, I am going to just show the result the first diagram from the left hand side shows the empty lattice approximation for a face centered cubic lattice.

You can find the empty lattice band structure for different lattice in this website in the right hand side diagram I show that actual electronic band structure of aluminium I calculated this using ab initio package quantum express. So, details of the calculation is beyond the scope of this course. So, let us just focus on the plot comparing the empty lattice and actual band structure we find good qualitative match.

Periodic potential definitely has some effect but still the overall agreement is very good. In conclusion for metals like aluminium nearly free electron model works very well the weak periodic potential indeed modifies the empty lattice band structure to some extent but the overall agreement is very good.