Properties of the Material: Computational Approach
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Module No # 06
Lecture No # 27
Fermi Surfaces: Part 2

Hello friends we are going to continue our discussion on Fermi service. We already know how to draw first, second, third and fourth Brillouin zone of a square lattice. In this lecture we are going to learn about drawing the Fermi surface in different Brillouin zones of a square lattice starting with free electrons.

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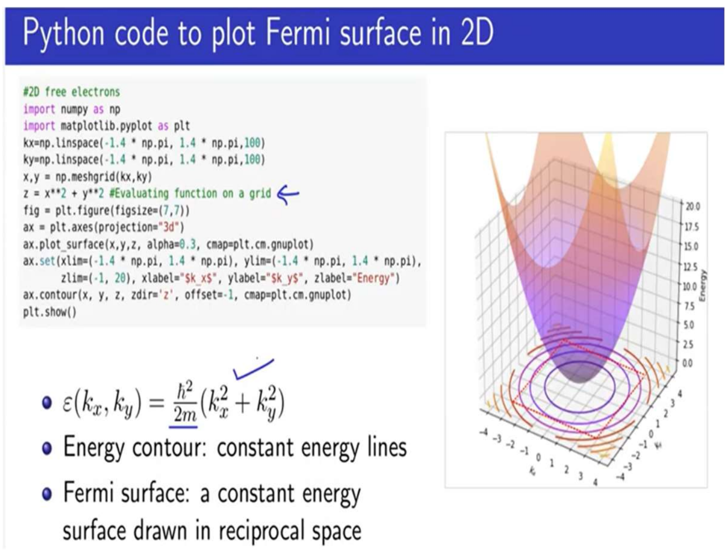

Let us write a python code to plot the Fermi surface of 2D free electrons. Note that this is an empty lattice approximation because we are going to use the blowing zones of a 2d square lattice while plotting the free electron Fermi surface. The energy dispersion relation is given by E = h cross square by 2m times k square + k y square setting h cross square by 2 m = 1 I calculate the energy in this line of the code. We have plotted this quadratic surface before this time in addition to the surface, we also plot the energy contours.

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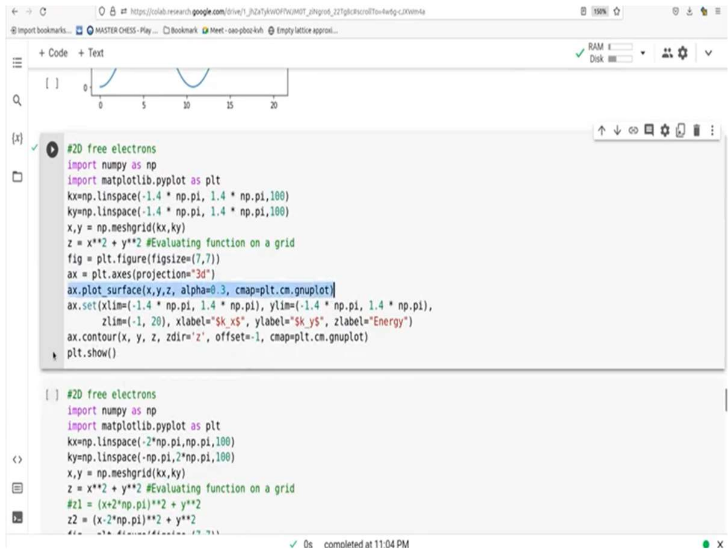

This is the code to plot the energy contours, this is where I define the range of k x and k y. And the range is extended slightly beyond the first below zone this is where I calculate the energy this is where the quadratic surface is plotted and this is where the energy contours are plotted.

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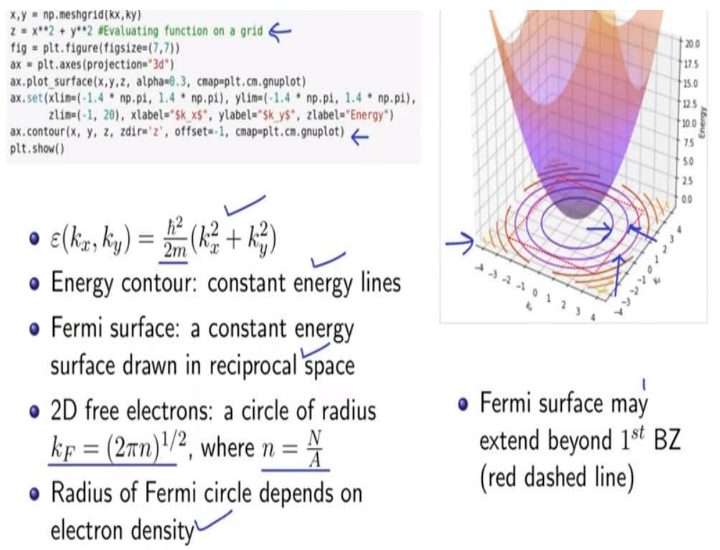

Let us run the code energy contours are constant energy lines it is a constant energy surface drawn in the reciprocal space. For 2D free electrons Fermi surface is one of the circles shown in this diagram. All the states lying outside the Fermi surface are empty and all the states lie inside the Fermi Circle are full. Radius of the circle is given by k f = 2 pi n whole to the power half where n is the number of electrons per unit area thus radius of the Fermi surface depends on the electron density higher.

The electron density more will be the radius take a small electron density such that radius of the Fermi surface is short. For example this one the red dashed line shows the boundary of the first Brillouin zone. Thus, if the Fermi surface has a short radius it will lie completely within the first pillowing zone consider higher electron density such that the radius of the Fermi surface is large.

For example this one in this case part of the Fermi surface lie within the first Brillouin zone and part of it lies outside the first Brillouin zone in conclusion the Fermi surface a circle in case of 2D free electrons may get extended beyond the first building zone or any other reloading zone depending on the electron density.

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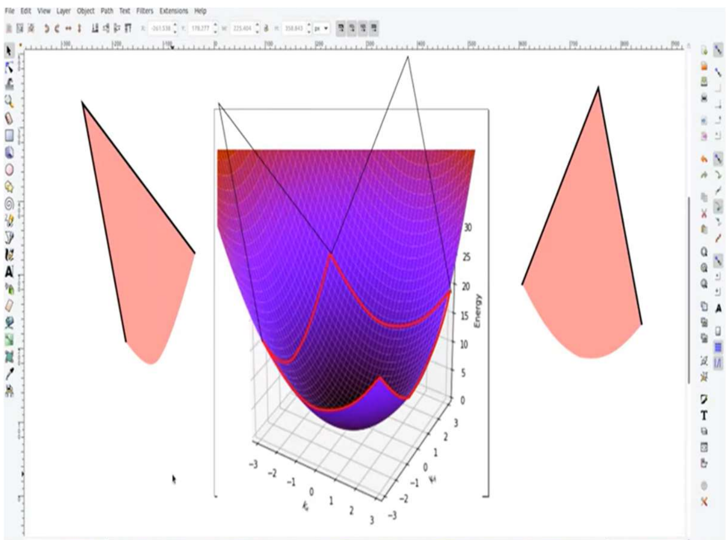

Let us understand how reduced zone scheme were in case of 2D, this is the quadratic energy surface for free electrons. In certain regions I have extended it beyond the first Brillouin zone regions within the first Brillouin zone are shown by the red border. Let us select some region beyond the first Brillouin zone let us say this region and shade it with some other colour. Now this region is lying outside the first building zone and let me bring it inside the first Brillouin zone.

Similarly I select another region which is lying outside the first Brillouin zone and shade it with some other colour and again I bring it inside the first below zone. Now below the red border we have the first bank and above the red border we have the second band shown by the red shaded regions. Now both of them are drawn in the first bloodline zone as per reduce zone scheme.

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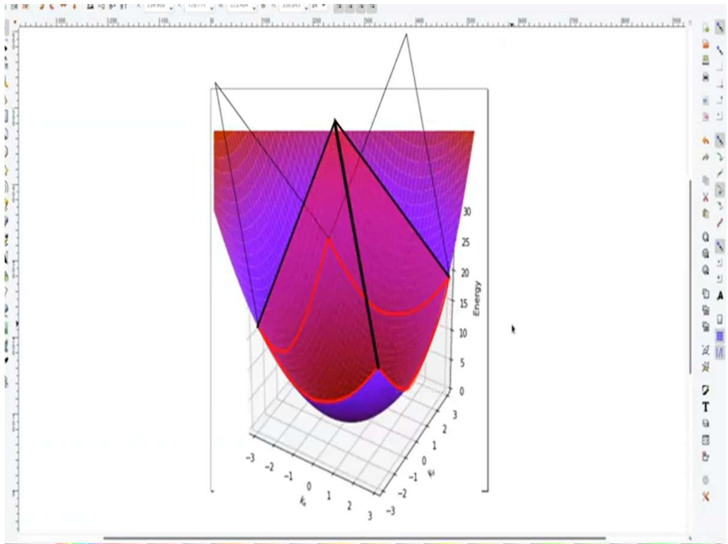

Thus, we know that constant energy contours may span more than one Brillouin zone depending on the electron density. A constant energy contour going beyond the first Brillouin zone what does it mean it implies that certain regions of the second band have same energy as certain regions in the first band at least in case of empty lattice model which deals with free electrons. In fact certain regions in the second band can have lower energy than certain regions in the first band.

For example, in the right-hand side diagram red region in the top is the second band remember that the second band is the part of the quadratic energy surface which was originally in the second Brillouin zone and has been brought to the first Brillouin zone as per reduce zone scheme. Clearly this region of the second band or this region of the second band has less energy than this region of the first band this is known as band overlap

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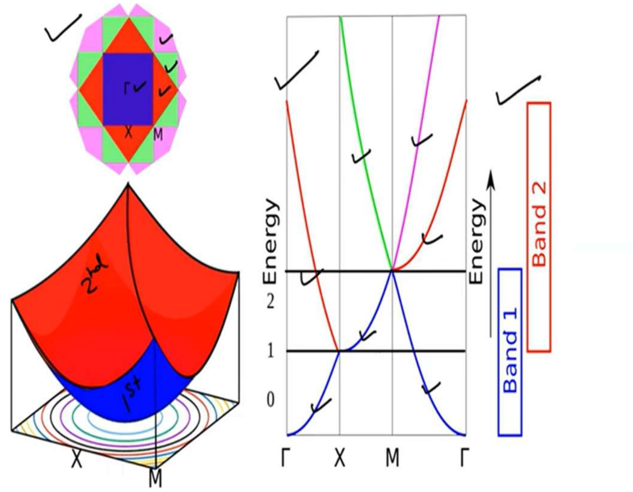

Band overlap

Let us try to understand band overlap in terms of e k diagram top figure shows the Brillouin zone of the 2D square lattice. Bottom figure in the left shows the quadratic energy surface for free electrons in reduced zone scheme. The blue surface is the first band and the red surface is the second band remember that the red surfaces were lying originally in the second Brillouin zone and have been brought to the first Brillouin zone.

As per reduced zone scheme this figure is the e k diagram along the high symmetry points in the first below zone. The blue lines correspond to the first band, they correspond to the energy within the first Brillouin zone. The red lines correspond to the second band they correspond to energy values in the second reloading zone. Similarly the green and the magenta line correspond to energy values in the third and fourth Brillouin zone.

Clearly within this energy window part of the first band and second band have same energy. Thus, we can say that the first and second band overlap this becomes very clear in the energy band diagram as shown here Band 1 and Band 2 has some over lapin certain energy window.

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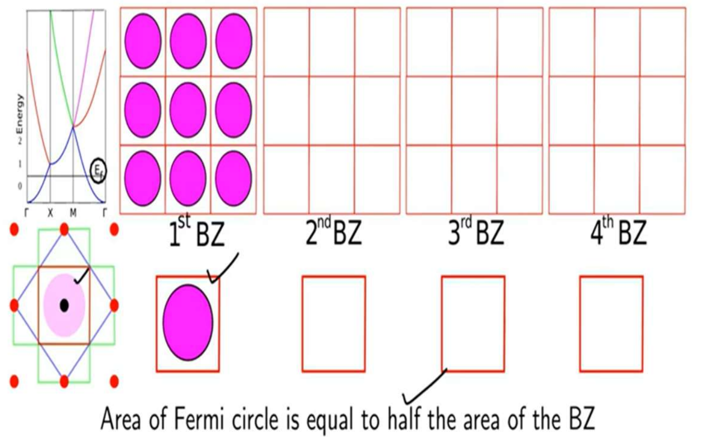

Let us now draw the Fermi surface for a monovalent metal in case of a monovalent metal area of the Fermi circle is half the area of the Brillouin zone thus the Fermi circle lies completely within the first Brillouin zone. So, in the e k diagram this is the Fermi energy and note that the Fermi energy line crosses only one band the first band. This also implies that the Fermi circle lies completely within the first Brillouin zone. If we repeat this diagram like we did for periodic or repeated zone scheme then this is what we get?

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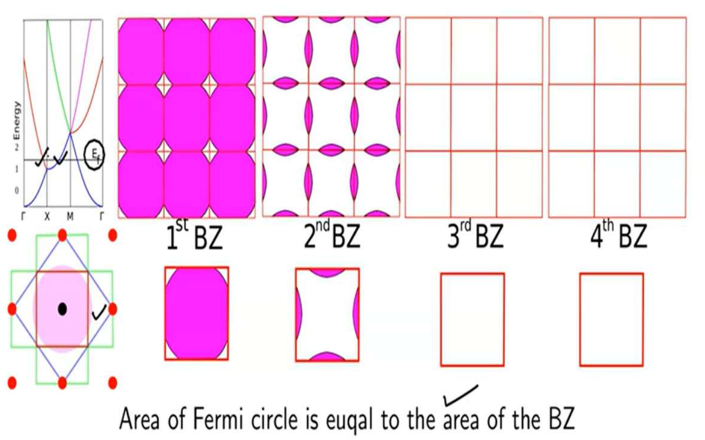

Now let us draw the Fermi surface of our divalent metal in case of a divalent metal area of the Fermi circle is equal to the area of the Brillouin zone. Now if we draw the Fermi circle which has same area as the Brillouin zone it crosses over from the first Brillouin zone in the second Brillouin zone. In the e k diagram we also find the line corresponding to the Fermi energy crosses 2 bands the first band and the second band. This also implies that the Fermi circle goes beyond the first Brillouin zone and crosses over to the second building.

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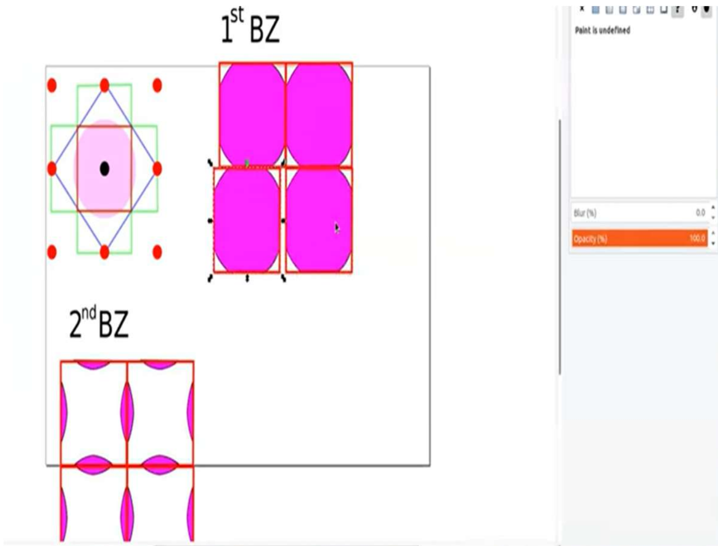

Let me show how to draw the Fermi surface in different blowing zones. In this case the red box denotes the first below in zone and the blue box denotes the second reloading zone clearly the Fermi circle crosses over from the first Brillouin zone to the second blowing zone. In this diagram I show only the part of the Fermi circle inside the first Brillouin zone and in this diagram, I show the part of the Fermi circle outside the first below zone.

Now let me bring this portion from the second below end zone to the first Brillouin zone. Similarly let me bring this portion from the second below zone to the first Brillouin zone. Now I bring this portion from the second Brillouin zone to the first Brillouin zone and finally I bring this portion from the second bridge zone to the first Brillouin zone. I just followed the reduced zone scheme.

Now let me apply the repeated zone scheme and repeat the reload zone periodically in space. For example, I take this Brillouin zone and I repeat it in space like this. Similarly, I can do it for the first period. So, this is how the Fermi surface looks like in the first prevention and this is how the Fermi surface looks like in the second blue line.

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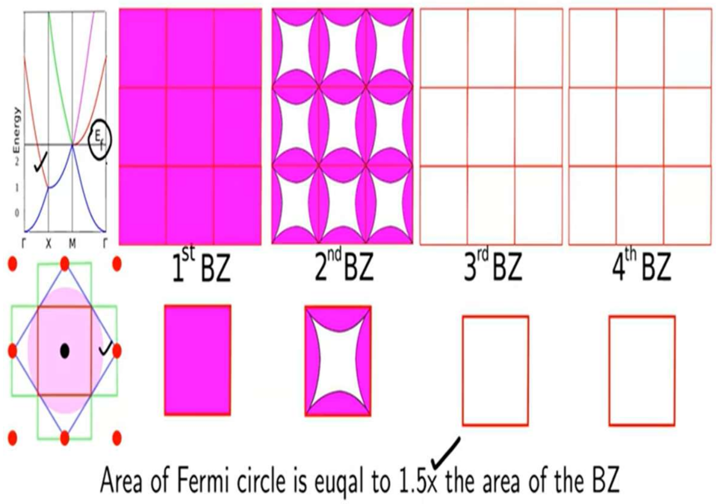

So now let us draw the Fermi surface of a trivalent metal in this case area of the Fermi circle is equal to 1.5 times the area of the Brillouin zone. If we draw the Fermi circle obviously it crosses the first Brillouin zone and goes to the second Brillouin zone. However, it does not cross over to the third between zone in e k diagram. Also, we find that the line corresponding to the Fermi energy process the second band but does not cross the third band this implies that the Fermi circle does not cross over to the third building zone.

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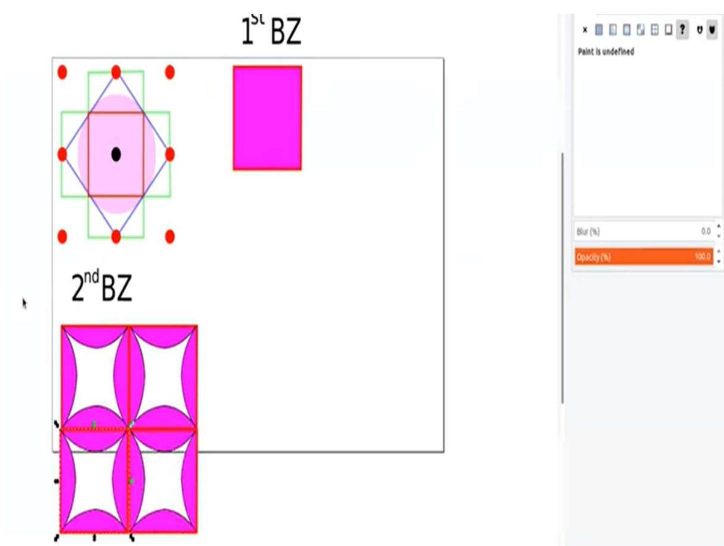

Let me show how to draw the Fermi surface in different Brillouin zone in this diagram I show the portion of the Fermi circle only within the first Brillouin zone. This is not so interesting as the first Brillouin zone is completely occupied. In this diagram I show the portion of the Fermi circle lying outside the first Brillouin zone. Let me bring this portion from the second Brillouin zone to the first Brillouin zone.

Now let me map this portion from the second below zone to the first Brillouin. So, then I map this portion from the second Brillouin zone to the first Brillouin zone and finally I map this portion from the second Brillouin zone to the first Brillouin zone. I just followed the reduced zone scheme why mapping from the second to the first Brillouin zone. Now let me apply repeated zone scheme and repeat the Brillouin zone periodically in reciprocal space. So I take this object and repeat it periodically in space in case of a trivalent metal the first Brillouin zone is completely full.

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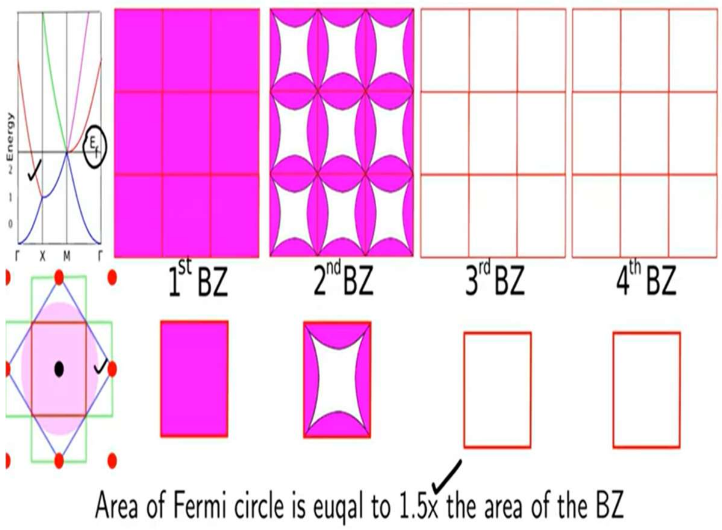

This is how the Fermi surface looks like in the second Brillouin so finally

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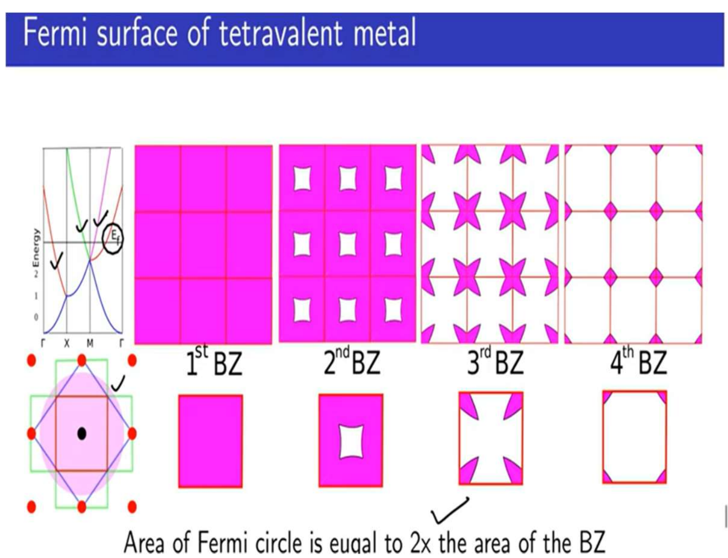

Let me show you how to draw the Fermi surface for a tetravalent metal. In this case area of the Fermi circle is twice the area of the Brillouin zone. When we draw the Fermi circle it extends all the way to the fourth Brillouin zone in ek diagram. Also, we find that the line corresponding to the Fermi energy crosses the second third and fourth band which implies that the Fermi circle extends to the second third and fourth Brillouin zone.

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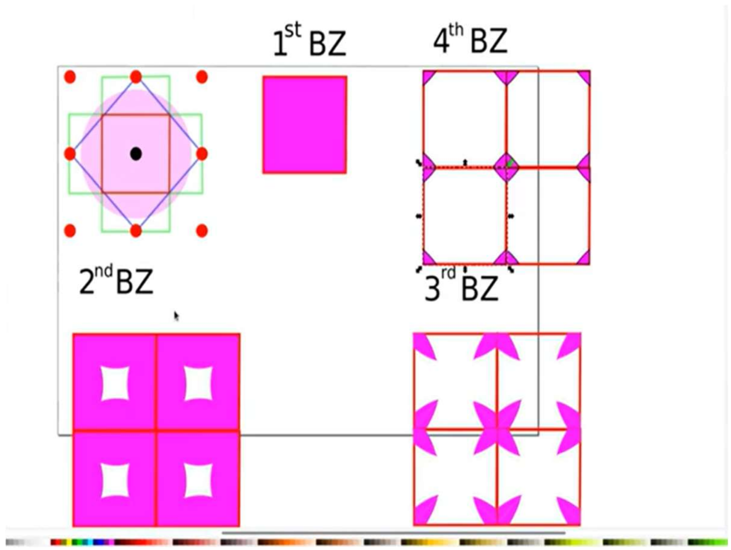

Let me show how to draw the Fermi surface in different drilling zone in this diagram I show the part of the Fermi circle only within the first Brillouin zone it is completely full and not so interesting. Next, we show part of the Fermi circle in the second Brillouin zone I map each portion back to the first Brillouin zone one by one starting with this followed by this and this. In this diagram I show the portion of the Fermi circle lying in the third Brillouin zone as I did for the second blue line zone.

In this case also I map each portion to the first Brillouin zone so this portion is mapped to the first pre-line zone next this portion is mapped to the first Brillouin zone. Next portion is mapped to the first below and zone next this portion is mapped to the first Brillouin zone next portion and finally we map this portion to the first Brillouin. So, in this diagram I show the portion of the Fermi circle lying in the fourth Brillouin zone again I map each portion back to the first below zone.

So, this portion is mapped to the first below this portion is mapped from the foreign and finally this portion is mapped from the fourth window to the first below. So, after mapping the portions of the Fermi circle lying in higher relevant zone to the first below zone according to the reduced zone scheme,I apply periodic zone scheme and repeat each below zone periodically in reciprocal space.

So let me start with the second blowing zone I take this portion and repeat it periodically in reciprocal space take this portion and repeat it take this portion and then I do it for the third blue line zone. Then I do it for the fourth Brillouin zone takes this portion and repeat it periodically in reciprocal space repeats it.

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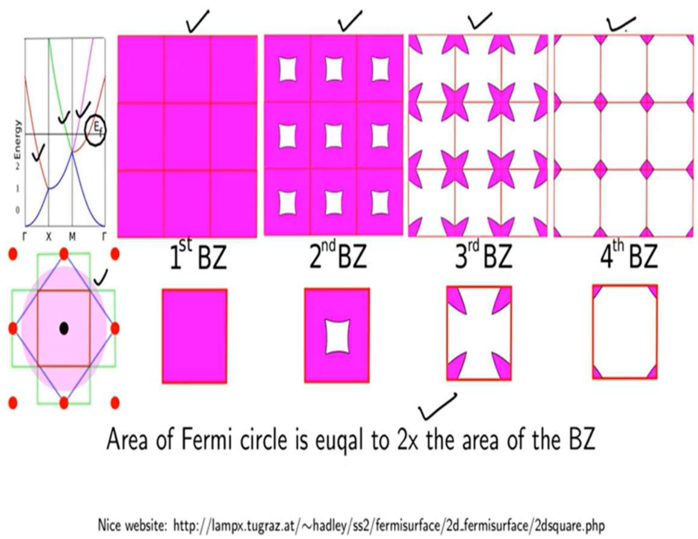

In case of a tetravalent metal the first billion zone is completely full and this is how the Fermi surface looks like in second third and fourth Brillouin zone.

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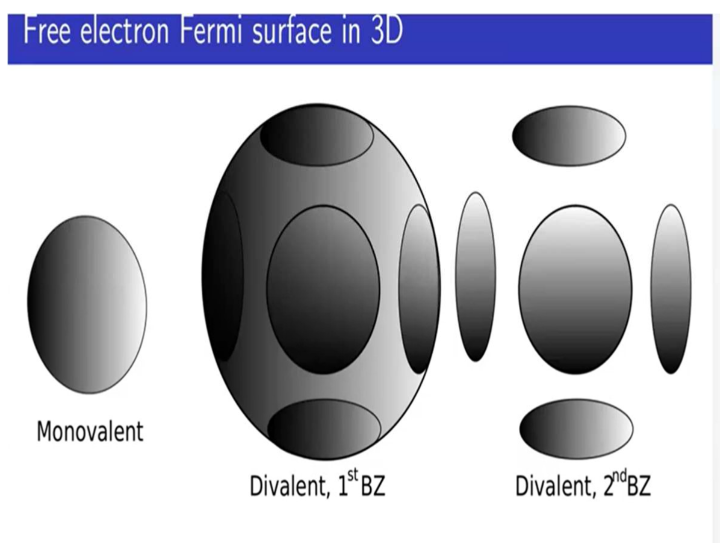

It is not an easy task to show how to draw Fermi surface in 3 dimensions. However, let me illustrate one simple example I draw the Fermi surface assuming Brillouin zone of a simple cubic lattice Fermi surface is spherical for 3d free electrons. If we have a monovalent atom then the Fermi surface does not cross the first Brillouin zone boundary volume of the Fermi sphere is equal to the half the volume of the Brillouin zone the Fermi sphere is a spherical surface lying completely within the first Brillouin zone.

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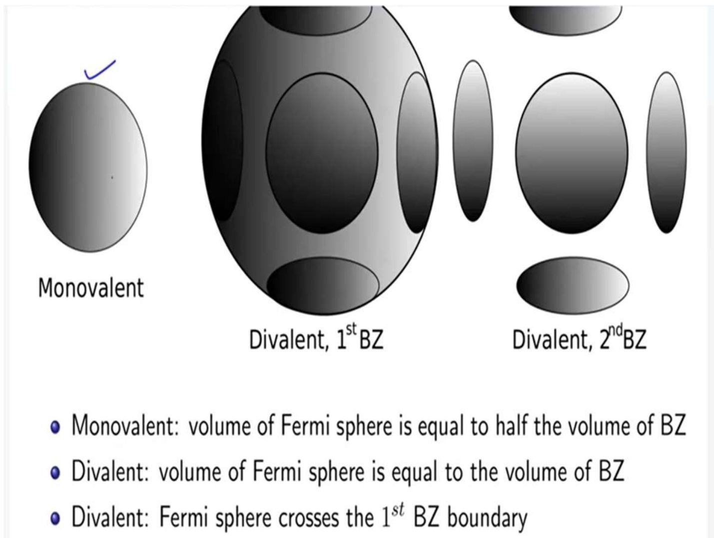

In case of a divalent metal volume of Fermi sphere is equal to the volume of the Brillouin zone it crosses the boundary of the first Brillouin zone. As a result part of the Fermi surface lies in the first Brillouin zone and part of it lies in the second Brillouin zone. This is how the Fermi surface looks like in the first Brillouin zone and this is how it looks like in the second Brillouin zone.

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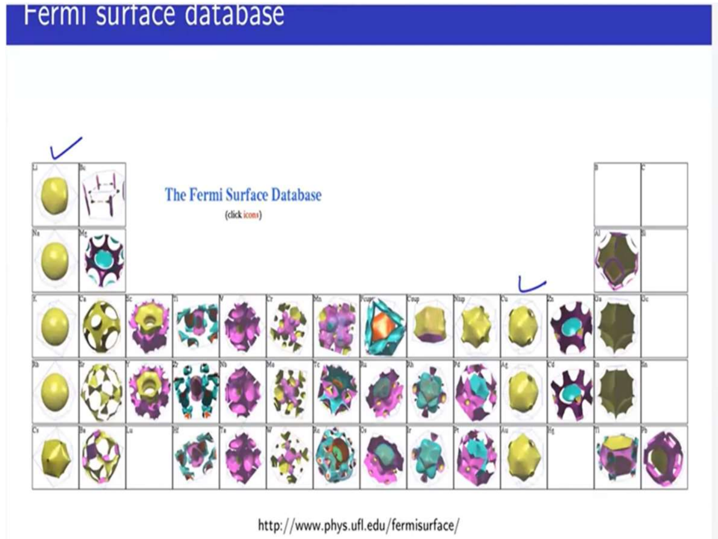

So far, I have drawn free electron for me surfaces however periodic potential may deform the free electron Fermi surfaces. We are going to learn how to draw Fermi surfaces in case for weak periodic potential in the next lecture. Fermi surfaces for the actual metals can look like spherical Fermi surface of free electrons for some metals. However, for most of the metals it looks very complicated to get a feeling of how the Fermi surface looks like for actual metals you are advised to visit this website.