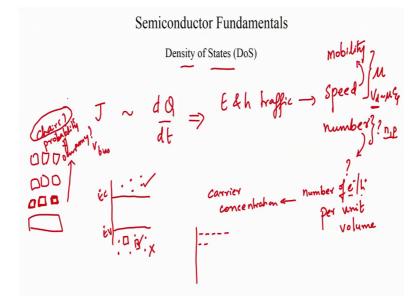
## Semiconductor Devices and Circuits Prof. Sanjiv Sambandan Department of Instrumentation and Applied Physics Indian Institute of Science, Bangalore

## Semiconductor Fundamentals Lecture – 09 Density of States (DoS)

We now proceed to the next important topic with regards to Semiconductor Fundamentals and this is got to do with something called as the Density of States ok.

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And the idea behind this are if you remember I see our main goal in this subject is to calculate the current or the current density let us say and in essence. This current density is dependent upon the traffic of electrons and holes right. It depends upon the rate of change of charge ok. To first order this is what we would like to calculate when we apply you know when we subject the semiconductor device to different bias conditions.

Now this traffic of electrons electron and whole traffic it depends not only on the speed, but also on the number ok. Now the speed was very nicely characterized by something called as the mobility of semiconductor of the carriers ok, but you have still not discuss anything to do with the count on the number of carriers ok. In particular we would like to calculate the number of electrons or holes per unit volume of the semiconductor and this is something called as the carrier concentration ok. So, when we say carrier concentration we imply the number of free electrons and holes per unit volume. So, we are not interested for example, if this is the conduction band edge and that is the valence band edge ok. We are only interested in the electrons above the conduct in the in the conduction band and we are interested in the holes in the valence band we are not interested in the holes in the conduction band there are plenty of holes in the conduction band plenty of vacant states, but that is not going to contribute the current.

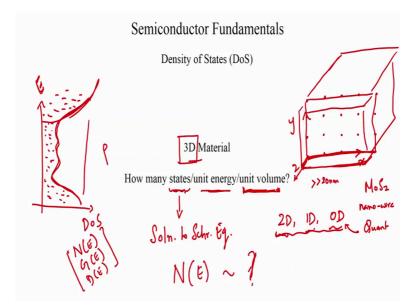
And similarly there are plenty of electrons you know that are bound to the atoms sitting inside the valence band and they are not going to contribute to the current. So, we are not interested in the electrons we are interested in the holes in the valence band and the electrons in the conduction band. So, we want to get a gauge on the number of electrons and holes per unit volume again how do we do this. So, this is what our next goal is in how do we when we know how to calculate speed to some extent ok.

Because we know this parameter called mobility and we know that the drift velocity is the mobility times the electric field. So, we know how to calculate the velocity, but we do not know the number we left that we you know we simply use the symbols n and p and we left those undefined now the way you go about calculating number is to. Firstly, identify the number of seats or the number of solutions to Schrodinger equation that electrons and holes can occupy ok. So, if you imagine a classroom which is got which is got let us say there is a classroom and let us say there are lots of chairs in the classroom.

And the students can come and occupy consider in the classroom, but you make a rule that a student has to sit on a chair, he cannot stand he or she cannot stand in the classroom. So, if the student has to sit on a chair and if the students can be imagined to be electrons and you ask the question you know how many students can you take a guess as to how many students are present in a classroom? Ok. So, the you need two parts to answer that question the first is how many chairs are present in that classroom how many chairs and the second is what is the probability that the chair is occupied?

So, if you know what these two numbers are then you have a good estimate as to the number of students in the classroom and the density of states is going to give you an answers to the number of chairs or. In fact, more accurately it is the number of states per unit energy per unit volume in a 3D material.

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So, if you are looking at 3D semiconductors ok.

So, 3D semiconductors imply your crystalline lattice is quite large it is much larger than the size of the atom in all three dimensions ok. So, let us say for example, if you are interested in a number let us say it is greater than much greater than 20 nanometers I mean the atom is much smaller than 20 nanometers, but nevertheless as a practical estimate you can consider all these materials to be three dimensional.

So, you have a lattice that is significantly large in all three dimensions, if you have a Cartesian coordinate system and you label this as x that is y and this is z then you have a lattice that is significantly large in x and y and z directions. So, the density of states is going to give you an answers to the number of chairs. So, that you know the number of students ok. So, it is an important question to answer if you want to calculate the concentration.

So, we want to know how many states and what are states? States are basically the solutions to Schrodinger's equation ok. How many solutions are there to Schrodinger's equation per unit energy per unit volume of the material and if you have this what you will end up with is if you know the energy you take one unit volume of the semiconductor and you plot the energy versus number of states. You know the distribution of states and this energy. So, let us say you plot the distribution of these states.

So, let us say you have the density of states which we will denote by you know N of E and N as a function of energy or you denote it as G as function of energy or you denote it as D as a function of energy sometimes depending on you know what the mood is feely just use a different variable, but you will get the context of it. So, it is it is the density of states and you have all these states present that are distributed in energy and we want to know as to what this distribution is it that is it going to be uniform or is it that it is going to vary you know as various the square root of E or what is it what is the distribution of the states as a function of energy in a per unit volume of a 3D material ok.

So, let us so, we will do this exercise first for a 3D material and we will see how to go about making this calculation and then we will do the same calculation for a 2D material and for a 1D material and finally, answer questions for a 0D material now what do you mean by a 2D material is like a it is quite large in 2 dimensions, but quite thin in the 3rd dimension. So, you can imagine a 2D semiconductor which says you might have heard of for example, say molybdenum disulphide or grapheme etcetera and a 1D material is probably something that is you know it is just thin and long it is like a little wire. So, any nano wire it could be you know could be approaching a 1D material and a 0D material is something which is in a conceptually a point it is it is got no dimension on x y and z.

So, you will be a quantum dot would probably be approaching a 0D material. So, we will we will look at the density of states for all these examples, but for the time being we are interested in the density of states for a three dimensional material and we want to know we want to perform this calculation of how many states per unit energy per unit volume.

So, that you have the distribution and this tells me the number of chairs. So, the number of places the electrons can occupy and after getting this if I somehow can calculate the probability that an electron occupies a state at a particular energy I can use these two answers to get the count of the number of electrons which I will then use to calculate the current so that is the whole idea ok. So, what we will be doing in this exercise is to find out how the density of states how does N vary with E ok.

What kind how does it vary with is it proportional to E or what is it how does it vary with E with E?

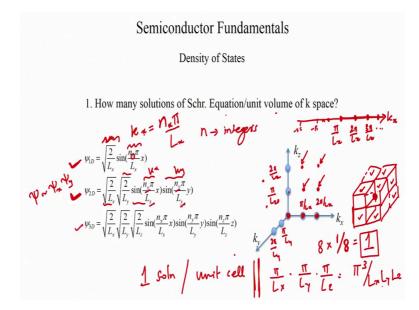
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Semiconductor Fundamentals	
Density of States $-3D$	
1. How many solutions of Schr. Equation/unit volume of k space? $k \sim wave vector$ k space = reciprocal	

So, in order to answer this we are going to just ask ourselves five questions and we will do the same thing for all the cases. Now this is for a 3D material now the first question is how many solutions of Schrodinger's equation that is how many states are there per unit volume in k space ok. So, what does k space k space k is the wave vector in sum and k space is essentially your reciprocal lattice space.

So, we are not going to be looking at the actual material it is in it is spatial coordinates, instead we are looking at the reciprocal lattice space that is the frequency the spatial frequency space if you like and we ask ourselves a question as to how many solutions are Schrodinger's equations are there per unit volume of k space and why is this easy to calculate, because we have already solved for the wave function in these in k space.

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So, if you remember your particle in a box we always will keep going back to that little example. So, we solved the wave function for a particle in a one dimensional box and we found that the wave function was this right. So, we got this by normalizing everything and we got this little term which is nothing, but your k; k of x and we got this to be a quantized value and we had to have a integer n and I have used the subscript x to represent the x direction ok.

So, you have k x is equal to n x pi by L x. So, k could only take integer values of pi by L x and why should that happen? Because it had to meet the boundary condition of the wave function not existing outside the box ok so, that was a boundary condition, but nevertheless k will be quantized no matter what you see you know how you define your potential.

So, k is a quantized parameter so, n is got all n can only be integers and therefore, if I were to draw if I were to draw the k x vector or if I look at the k x space then I see it can only take discrete points right it can have values of pi by L x, 2 pi by L x, 3 pi by L x and so on and so forth and you could also have say minus pi minus 2 pi and so on.

So, only those values were allowed and if you solve Schrodinger's equation for a 2D box we could we use the technique of separating the two wave functions a separation of variables which was we split psi as psi x and psi y and we found that it is simply a product of these two wave functions. So, here you have k x and k y and both of them are quantized and I have defined the quantum versus n x and n y and the lengths of the box are L x and L y and similarly for a three dimensional box you will have the prod you will have the wave function be a product of psi x psi y and psi z.

And therefore, you will have three k, k x k y and k z defining your k space. So, here I just drawn it out here. So, you have the solutions the Schrodinger's equation being discrete points. So, this would be pi by L x 2 pi by L x and so on this would be pi by L z 2 pi by L z and so on this would be pi by L y 2 pi by L y and so on. So, you have this three dimensional grid of points. So, I have not completed this grid, but you can imagine this is a three dimensional grid of points and each point is a solution to Schrodinger's equation.

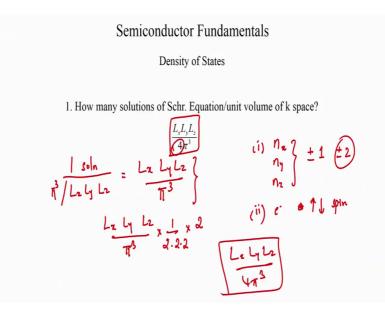
So, it is the electrons can only take these values the electrons can only exist in these states. So, if you were to imagine this three dimensional grid and now each of these are solutions. So, what is the answer to this question you know how many solutions are Schrodinger's equation are there per unit volume of k space. So, let us you know imagine this 3D grid that sort of sits like this. So, you have these little cubes cuboids if you would like now let me just draw it better.

So, you will have these little cuboids and the vertices of these cuboids are essentially the solutions to Schrodinger's equation. So, you will have four of them sitting right in front and you could imagine four at the back you will you will have four at the back. So, you have this little region and if you imagine the point right in the middle of this it is being shared by the four cubes in the front and the four cuboids at the back.

So, one solution each solution is shared by 8 unit cells of k space and each unit cell in k space has got 8 solutions. So, there are 8 solutions each shared by 8 of them. So, that are effectively 8 into 1 by 8 which is equal to 1 solution of Schrodinger's equation per unit volume in case p per unit cell in k space we have not yet calculated the volume. So, this many solution so, we have 1 solution per unit cell now we need to get the answer as to how many solutions per unit volume. So, we need to find out what is the volume of what the volume of each unit cell is.

And the volume is simply this product right it is pi by L x into pi by L y into pi by L z. So, that is the volume. So, let me just write it a little better my apologies so, the volume of a unit cell n k space is pi by L x into pi by L y into pi by L z which is pi cube by L x L y L z. So, there is 1 solution per unit cell and that unit cell has got this volume ok.

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Therefore how many solutions are Schrodinger's equation are there per unit volume? The answer is simply as far as our calculations go so, far the answer is simply 1 solution divided by the volume of L x L y L z say pi cube by L x L y and L z which is L x L y L z by pi cube.

But this answer is your more or less correct here, but we are still not accounted for several things we need to a small correction we need to have a correction factor and the correction factor has got to do with two to read it is got two reasons for it the first is our integers you know the quantum numbers n x n y and n z could have plus or minus values ok. So, you could have plus or minus one plus or minus two and both these are you know the equivalent the same energy.

So, we had double counting for the number of solutions. So, in order to get the correct number of solutions I probably need to take this answer and divided by 1 by 2 into 2 into 2 you know I need to half it for each of the dimensions, but then there is also another point the electrons can have plus or I mean the up or down spin it can have two spins. So, 2 electrons can occupy a state ok.

So, we need to account for that by multiplying a factor of 2 therefore, the corrected answer is essentially this ok it is got it has to have a 4 a term 4 there. So, the correct answer to the number of solutions are Schrodinger's equation per unit volume of k space

So, now let us proceed ok.

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Semiconductor Fundamentals Density of States downs having the same  $\vec{k}$   $(\vec{k})$ :  $\sqrt{k_x^2 + k_y^2 + k_z^2}$ Soln / unit vol =  $\frac{L_x L_y L_2}{4\pi^3} - \frac{J_{unit}w}{4\pi^3}$   $\frac{L_x L_y L_2}{4\pi^3} \cdot \frac{4\pi k^2 \cdot dk}{4\pi^3}$ 2. How many energy states between k and

Now, we want to know how many energy states or how many solutions exist between k and k plus dk ok. So, now, imagine you have taken your k space you have your k z, k x and k y and you have filled it you fill the grid up you have uses zoom out of this. So, we were looking at the grid in a very microscopic sense and we calculated the number of solutions per unit volume, but now I am going to zoom out and I am going to see this massive grid of points right it is just going to be a massive grid of points.

And if you ask yourselves; what is the locus of points having the same k now this k is essentially you know it is essentially the combination of k x, k y and k z ok. So, if you ask yourself as to what is the locus of points that have the same value of k in a 3D space ok. So, you have got this mass of grid of points and what is the locus of keeping the k constant; the answer is quite obvious it has to be a spherical shell it or it has to be a sphere. So, if you were to keep k the same and look at all the points that have got the same value of k the answer is it is going to be a sphere in 3D space ok.

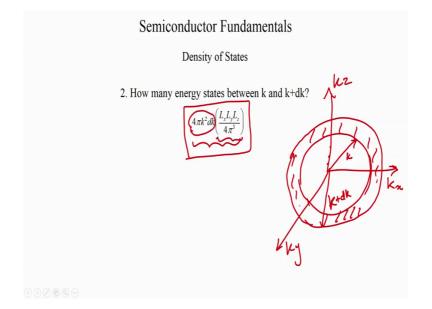
And what is the region between k and k plus dk. So, this is k you could have another sphere which has got a radius of k plus dk right and we are interested in the number of

energy states that exists between k and k plus dk ok. So, we are interested in the number of energy states or number of solutions to Schrodinger's equation that exist in this region here we are still in reciprocal lattice plane we are still in k space and we are looking at the number of solutions that exist in this region.

So, how do we calculate this? Well I need just need to know how many unit volumes are there in this space. I know the number of solutions per unit volume which is equal to my L x L y L z by 4 pi cube and I just need to know what is the volume ok so, if this is the number of solutions in 1 volume let us say 1 unit volume how many unit volumes are there in this region I am interested in ok.

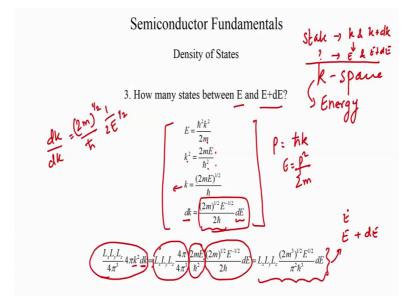
So, what is the volume of the space the volume of that space is the surface of the sphere into dk so which is 4 pi k square dk. So, that is the volume of the space which I am interested in. And how many solutions are there in this volume? The answer is simply L x, L y, L z by 4 pi cube into 4 pi k square dk ok which is very neatly written out here.

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So, there are this many energy states in the region between k and k plus dk so, which is where k. So, we are looking at the reciprocal lattice space once more where k where you have k x, k y and k z and you have all the points that have got the same k to be sphere because this is this is a massive grid of points and all the points that I have got a radius of k plus dk is another sphere that is very concentric to this and this region has got a volume of this much and there are this many solutions per unit volume and therefore, there are so many solutions of Schrodinger's equation in this region of interest just to repeat everything ok.

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So, what is the next question the next question is how many states exist between E and E plus d E ok. So, so far we have been making all our arguments in k space now we want to convert this information in k space to energy because we are trying to estimate the density of states which is the number of states per unit volume per unit energy. So, I know the number of solution number of solutions to Schrodinger's equations or the number of states existing between k and k plus dk. I know that now can I translate this to the number of states between E and E plus d E ok. So, that is the question ok.

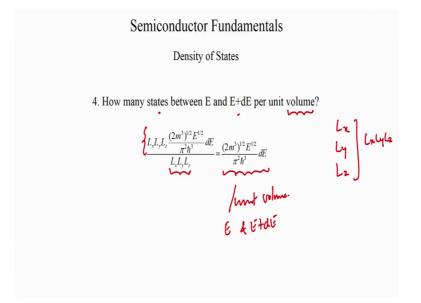
So, if I know this can I calculate that? So, how is k connected to E, k is nothing but your wave vector so, h bar k is my momentum and E is p square by 2 m therefore, E is h bar square k square by 2 m and therefore, k square is 2 m E by h bar square and k is a square root of this whole thing which is 2 m in the square root by h bar and what is d k, b y d E; d k by d E is obtained by differentiating this right.

So, you have 2 m to the power half by h bar and the differential of E to the power half which is 1 by 2 E power half and therefore, you have d k is equal to this term into d E. So, we have these four relations with us now what we are going to do is we know that the number of solutions in this region between k and k plus d k is this. Now we are going to substitute for k square and d k with these expressions in terms of E and d E.

So, what is k square k square is 2 m E by h bar square so instead of so let us keep these terms separate and instead of k square I am going to substitute 2 m E by h bar square and instead of d k I am going to substitute this particular expression and after a bit of simplification you cancel off say common terms you will end up with the number of states between E and E plus d E is given by this quantity here ok.

So, we now know the number of solutions to Schrodinger's equation sitting between two energy levels E and E plus d E ok. So, now, let us see how to get to the density of states.

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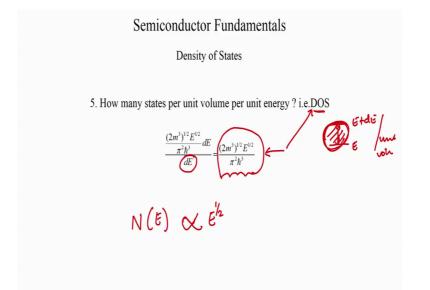


Now we ask our fourth question which is how many states exist between E and E plus d E per unit volume now this is the real volume of the material? So, we are no longer in reciprocal space. So, what is the volume?

Now, the box had lens L x, L y and L z therefore, the volume of the box is L x, L y, L z and therefore, this numerator here is the number of solutions to Schrodinger's equation or the number of states between E and E plus d E and this is the volume of the box and therefore, the number of states between E and E plus d E per unit volume is simply that divided by the volume of the box and that gets rid of the L x, L y, L z terms and you have these many states sitting per unit volume and between E and E plus d E.

Now, in order to get the density of states I need to know the number of states per unit volume per unit energy. So, I also need to divided by the; I also need to get a per unit energy term ok.

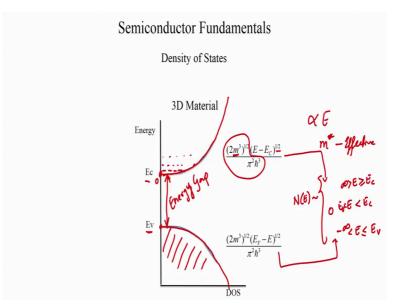
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And how do I do that you simply divided by d E ok. So, you are looking at all the states between here and between E and E plus d E per unit volume and you get your divided by d E which is the energy gap with the energy region you are looking at this. Now I know the that the length of the energy region you are looking at and you end up with the number of states per unit volume per unit energy to be given as this which is nothing but the definition of the density of states.

So, this is the density of states for a 3D material ok. So, most importantly you must be looking at is how does the density of states vary with energy? So, this density of states for 3D material scales as the square root of energy it is proportional to the square root of energy. Now since we will be using 3D silicon as the model material in our course here it is useful to draw this out. So, forgive this very rough sketch which is drawn here.

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So, for a perfectly crystalline material you have your valence band edge and your conduction band edge and in between this is something which we defined as the energy gap. Now for a perfectly crystalline material the energy gap will have absolutely no states it is only when defects start to appear that the energy gap will start getting filled up with states. But as far as most of the course is concerned there are no states in the energy gap. It is only when we talk about disordered material later towards the end of the course we will we start worrying about states in the gap or even when we talk about doping for example, but for now there are no states in the gap.

So, your density of states which is proportional to E basically implies this, that there are states above the conduction band edge which is the bottom of the conduction band and the valence band edge which is the top of the valence band there are states in these regions and the way the states vary with energy is as E minus E c to the power half.

So, you have states varying like this in the conduction band and you have states varying in proportion to E v minus E to the power half. You have states varying like this and the valence band so that is what it implies. So, this is how the states in so, if you look at the number of solutions to Schrodinger's equation right at this point there are 0 states and just immediately after that you have a little bit and then after that you have a little bit more.

And how does it all how does this envelope scale? It scales as E minus E c to the power half into this particular term and all this m which you have seen throughout is all the

effective mass should all be in m star it is all the effective mass which we discussed earlier. And similarly the states below the valence band edge so, these are the this is the distribution if you ask what is N of E what is the density of state distribution and 3D material perfectly crystalline 3D material.

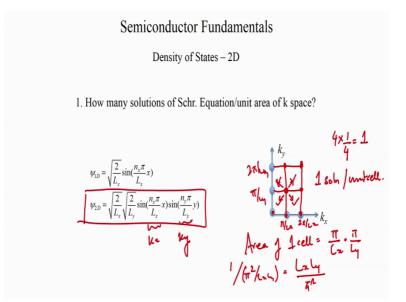
The answer is it is this when E is greater than equal to E c that is from infinite to E c it is this when E is less than sorry E is less than equal to E v ok, but greater than minus infinity and it is 0 when E is between E c and E v ok which is the energy gap. So, that is the distribution of the states in a 3D material; now what about a 2D material.

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Semiconductor Fundam	entals
Density of States (DoS)	
2D Material	
How many states/unit energy/un	nit area?

We ask ourselves the same questions, but the only thing is we need to ask ourselves how many states per unit energy per unit area is in the material, because we are now looking at a 2D material we just go through the same process again ok. Let's see what it gives us.

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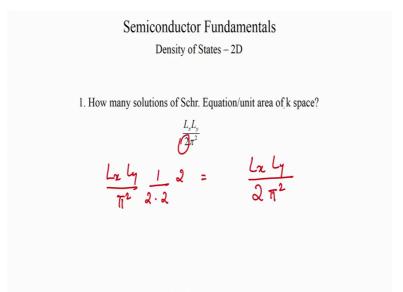


So, first question is how many solutions of Schrodinger's equation at that per unit area in k space. So, in now your wave function is just you know you are just looking at a 2D box you are just looking at a two dimensional box. So, therefore, there are only k x and k y to worry about in the k space ok. So, you have this grid of 2D points 2D grid and if you were to draw if you let us say let us take let us draw these connect these lattice.

If you look at the unit cells you have one unit cell here, one unit cell here, one here and one here. Now per unit cell how many solutions do you have? You have four solutions which mark the vertices of this of this rectangle ok, but each solution is shared by 4 unit cells this solution for example, is shared by this cell by this by this and by this. So, each solution is shared by 4 unit cells. So, you have 1 solution for unit cell ok. So, that is the number of solutions per unit cell in k space.

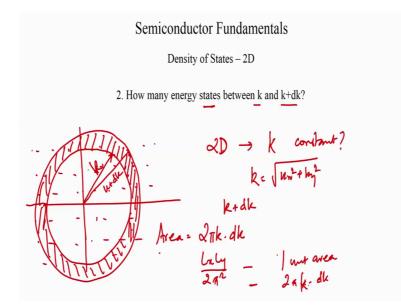
And what is the area of 1 unit cell? Area of 1 unit cell is simply your pi by L x. So, these points are all pi by L x 2 pi by L x and so on and that is pi by L y 2 pi by L y and so on so, it is pi by L x into pi by L y. So, that is the area of one cell and therefore, the number of solutions per unit area is going to be simply one divided by pi square by L x, L y which is L x, L y by pi square.

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But once again just like the last time we need to make a correction ok. Now we have to be a double counting for the plus and minus. So, you have L x L y by pi square the plus and minus with double counting there are two dimensions. So, we divide by 1 to be half it for each dimension and there are two spins and therefore, you have a corrected or the correction factor of 2 pi square which defines the number of solutions for Schrodinger's equation per unit area and k space.

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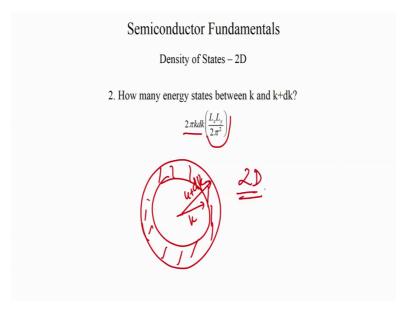


And now we ask ourselves next question you know how many energy states between k and k plus dk so, what is the locus of point. So, now, let us take our k space which is a two dimensional space and fill it up ok. So, you have this massive grid of points if you can imagine a graph paper that you might have used in school you have this massive grid of points discrete points and these are all the solutions of Schrodinger's equation and we want to know how many states between k and k plus dk ok.

So, what is the locus of points on a 2D map in a 2D map in 2D space what is the locus of points which keeps k constant. Ok the k will now be square root of k x square plus k y square. So, what is the locus of points the answer is it is a circle you want to keep the radius constant. So, if I keep the radius as k and I draw and I connect all the points that have a constant radius k it is a circle and what about k plus dk, it is another circle which has got a slightly larger radius and it is this, these are two concentric circles and we want to know how many states are there between k and k plus dk.

So, we are interested in the number of states in this little ring here if you remember the 3D case we had spheres because these are three dimensional and we had the spherical shell that was that was the region of interest, but now since it is 2D space you have this little ring. So, what is the area of this ring the area of this ring is the perimeter of a circle into dk. So, that is the area of the ring.

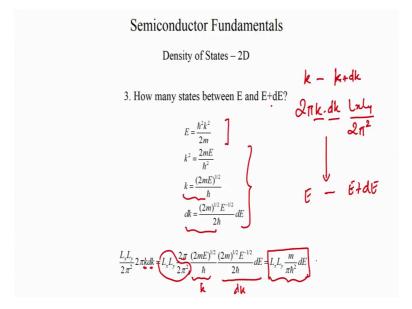
Now, I know that there is L x L y by 2 pi square solutions in 1 per unit area one unit area so how many solutions exist in 2 pi k d k in an area of 2 pi k d k ok.



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So, the answer is simply 2 pi k d k into L x L y by 2 pi square. So, this is the number of states existing in this ring in this region here between k and k plus dk for a 2D material. So, what is the next step next step is to convert this all to energy ok.

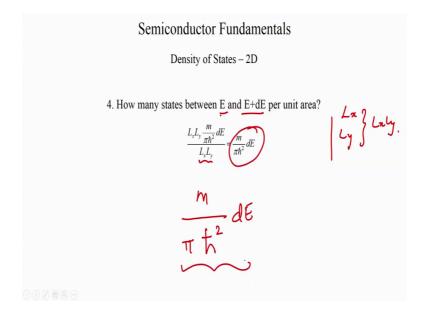
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So, the next question is how many states exist between E and E plus d E right. So, we know that between k and k plus dk we have these many states, that is 2 pi k dk L x L y by 2 pi square states. Now how do I convert all this to the number of states between E and E plus d E we go through the same process again. So, we know E is p square by 2 m which is h bar square k square by 2 m and therefore, all these relations follow and now we substitute for k and d k.

So, these are the number of solutions in terms of E. So, we use this expression and we use this expression. So, that is my k and that is my d k ok. So, it is 2 pi k d k into L x L y by 2 pi square the number of solutions. So, it is this many so when you simplify all this you get this little neat little answer here and this is the number of solutions or the number of states present between E and E plus d E ok.

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And now the next question is; obviously, how many states between E and E plus dE per unit area?

And now the box now we are looking at a 2D box and the area of the box is it is got dimensions of L x and L y and therefore, the area is simply the product which is an L x L y there are these many solutions to Schrodinger's equation in the region between E and E plus d E. And the number of solutions of Schrodinger's equation between E and E plus d per unit area is simply that divided by L x, L y and that gives you this it is m by pi h bar square d E.

So, there are these many states present between E and E plus d E per unit area.

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Semiconductor Fundamentals	
Density of States – 2D	
5. How many states per unit area per unit energy ? i.e. DOS 21	)?
$3D \rightarrow \alpha' E''^{2} \qquad \overbrace{dE}{m \atop dE} = \overbrace{\pi h^{2}}{m}$	
N(E) ~ E° JDOS	

And how many states between how many states in the 2D material per unit area per unit energy which is the density of states for a 2D material the answer is m by pi h bar square d E divided by d which is m by pi h bar square. So, there are these many states per unit energy per unit area in a 2D material you have follow the same process as in the case of 3D.

The only thing is we have adjusted terms for the 2D case, but what is fascinating here is that the density of states does not depend on the energy you do not see an energy term in the 3D case we saw that the density of states was proportional to E to the power half, but here there is no it is proportional to E to the power 0 it is not dependent on energy at all ok so, that is interesting. So, you will find that for a 2D material the density of states is constant with energy.