Optoelectronic Materials and Devices

Prof. Dr Deepak Gupta
Department of Materials Science and Engineering
Indian institute of Technology, Kanpur

Electronic Structure of Materials
Lecture - 02
Free Electron Theory

Now, welcome to lecture number two, we will start from here what we learned in the first lecture, I gave you the Drude's theory. The Drude's theory elegant theory in it is time more than 100 years ago when Drude's proposed this theory it was really elegant theory it was really remarkable that he and the kind assumptions he made. Then, kind of predictions which could be made appeared that the Drude's theory seemed to work except that it was a good fortune that there was any matching with the experimental results with Drude's theory.

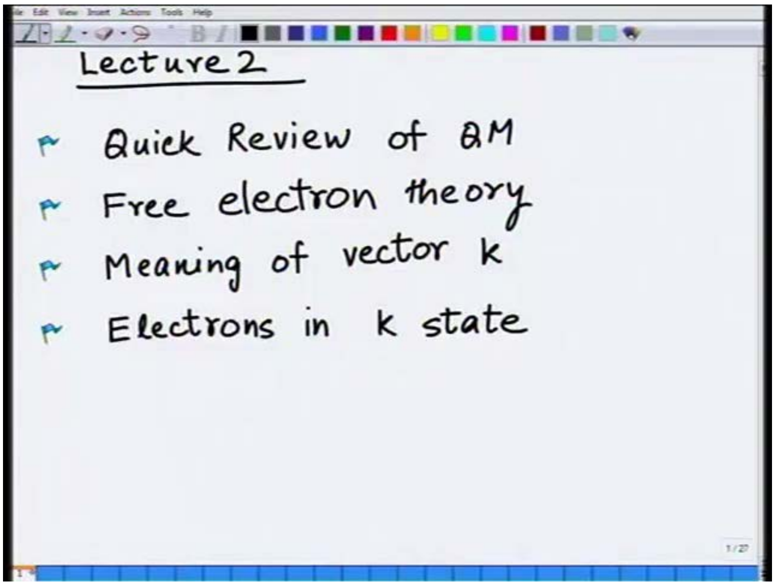
That is just because two has cancelled out then wanted to show that if you do not have those two errors cancelling out, then in cases of ball effect or magnitude resistance. Also, for example, this plasma frequency for transparency of metal and there are many other examples also where you see that group theory seems to work well. For group one element such as lithium, potassium, cesium etcetera, but it begins to fail little for many other metals and many other situations.

So, clearly something is wrong with that theory, so first improvement came by what was done was that you see what Drude assumed based on kinetic theory of gases that when electron collides with the ion it comes out with random velocities. Those velocities are taken through kinetic theory of gases which means they follow Maxwell Boltzmann distribution. Now, we know that electron is electron follows from the direct distribution not Maxwell Boltzmann distribution. Therefore, first improvement which was made was by what is called as Somerfield's theory of metal in which essentially he took Drude's model, but substituted in there a Fermi direct distribution for electron velocities.

Then, he applied that theory also which gave some improvement, but there is a objection to it that in otherwise it what is a classical theory Drude theory that is how could you put a distribution which is whose nature is quantum mechanics. So, that is the second which is the objection for Somerfield theory also which therefore, I have done Drude's theory because of it is historical importance. So, I will not take care of this, I will not cover this Somerfield theory in here, but move on to perfectly quantum mechanical theory based on first attempt.

We will make is free electron theory; I assume that the students are familiar with quantum mechanics.

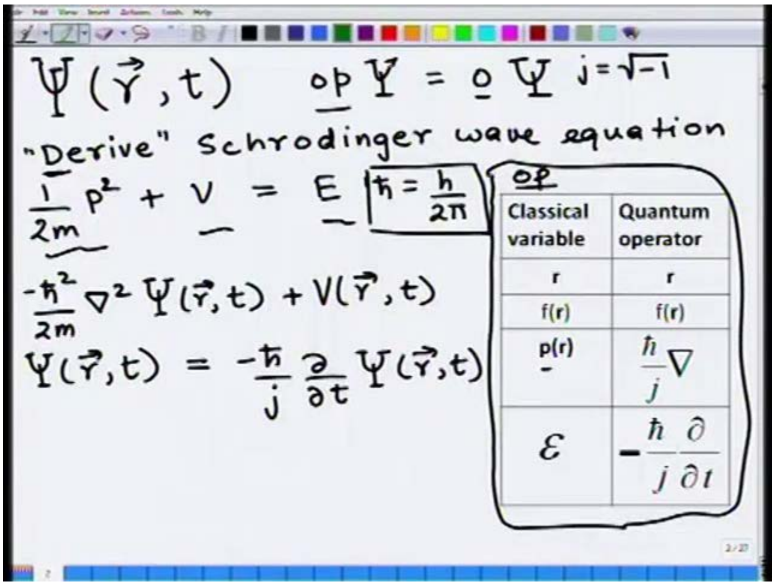
(Refer Slide Time: 02:52)



So, what I will do in this lecture is do a very quick 2 minute, 5 minute review of quantum mechanics the relevant portion for free electron theory thus to just to jog your memory, but I expect you to know already. Then, I will introduce this idea of free electron theory and then in that free electron theory we will see quantum states emerging and we will try to understand the meaning of k vector which is very important. You will see that eventually when we derive properties of materials, we will derive them from an energy versus k type of curve from which all the properties of these metals and semiconductors.

We derive and hence it is important understand to meaning of k vector which will emerge out of this free electron theory. Then, we will start putting since these are; I am saying already k represents a quantum mechanical state in this state. We will start putting electrons which are there in the system, so this is where we will end this lecture midway in the free electron theory and then in third lecture we will continue over this. Let us start with the quick review of quantum mechanics, essentially what I will do is that that just basic thing.

(Refer Slide Time: 04:01)



Remember, recall that we deal with this wave function xi and I am using a notation where I put hat on top of all them this quantity contains all the relevant information about the electron it is a function of position and of time. This is the wave function which has all, which contains all the information of electron, you can derive anything you want through this through this electron through this wave function. Then, of course he says that f corresponding to classical operator, there is a quantum mechanical operator. This operators is let me write these operators are given here that for position, there is a classical operator r corresponding quantum mechanical operator is r.

So, if this is a function f, the classical variable is f there is a quantum operator f for example, the momentum if the momentum is p in classical variable. Then, in case of there is an equivalent quantum operator in quantum mechanics, there is an operator where as in the variable this quantum momentum operator is like here. If there is a quantity called energy in classical variable, then there is a energy operator in here in quantum mechanics. There by, if I take this operator, if we apply this operator on to this operator which ever operator we are talking about here operators applied to this wave function which I have written.

Now, here then it gives you an Eigen value of this particular operators if I apply momentum operator on this wave function. Then, gives me it gives me momentum Eigen values multiplied by this wave function itself that is the basic idea of these operators in quantum mechanics, you will recall. So, what I will do here is that I will sort of derive if you wish derive for Schrodinger's equation wave equation, obviously you can understand that I am writing derive in inverted commas. What that means is obviously you cannot derive, it is basically a postulate, but I will pretend to derive by saying that in classical, you think of 1 over 2 m that means the kinetic energy is the total kinetic energy plus the potential energy is equal to total energy.

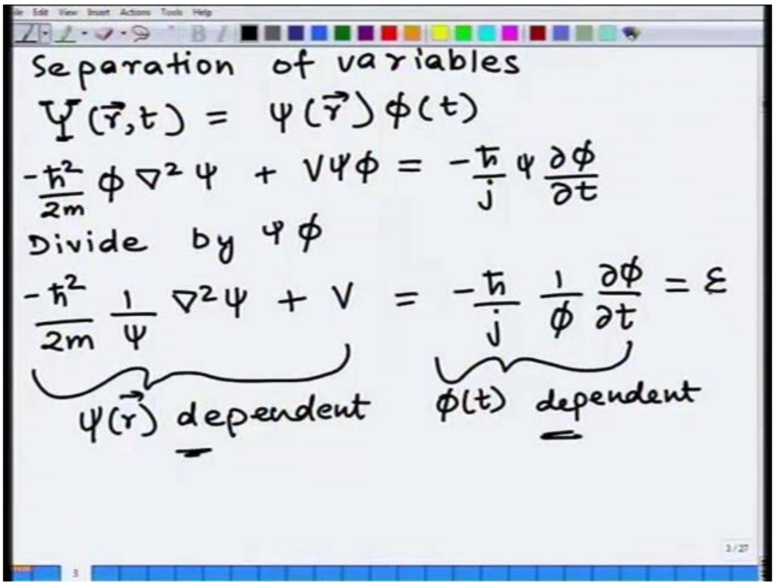
Thus, what you think of in a classical way what I will do is, I will take this momentum operator apply on the wave function to derive this kinetic energy the potential energy and the total energy well as thus use this these operators which I have written down here. There are the operators, all these operators which I have written down, let us use these operators and derive the Schrodinger equation quote and quote derive the Schrodinger equation for the wave. We will write it is as same thing, I will take the momentum operator, so this will become and j indicates by the way this j. I use symbol j, what is j j is equal to square root of minus 1.

So, it is an imaginary quantity something to use, so I am using, I am going to use j in this in here. Therefore, this j is when j square forces is equal to minus 1, so what I am going to write this as minus h square by 2 m and remember let us introduce another symbol, this h bar. I hope you are familiar with this meaning of h bar, h bar is equal to applying constant divided by 2 pi. Therefore, this is written as h bar, so h bar 2 m and radian square and this thing is square of this applied to this wave function xi of r comma t.

This vector r comma t is what I have written here plus this potential of position and times you wish equal to this energy. Now, I am going to write as times xi, sorry since this is the function here and corresponding operator is this of r comma t. This is then equal to this energy this energy, now I am going to use the energy operator minus h bar by j del by del t of this wave function here.

So, here the Schrodinger's wave equation which we have just derived from the classical sense, you noticed that essentially this operator then becomes a postulate. So, I assume that you already know quantum mechanics, this is just a quick review of what we intend to do here and so then then what I am going to do is, I am going to assume separation of valuable variables.

(Refer Slide Time: 08:59)

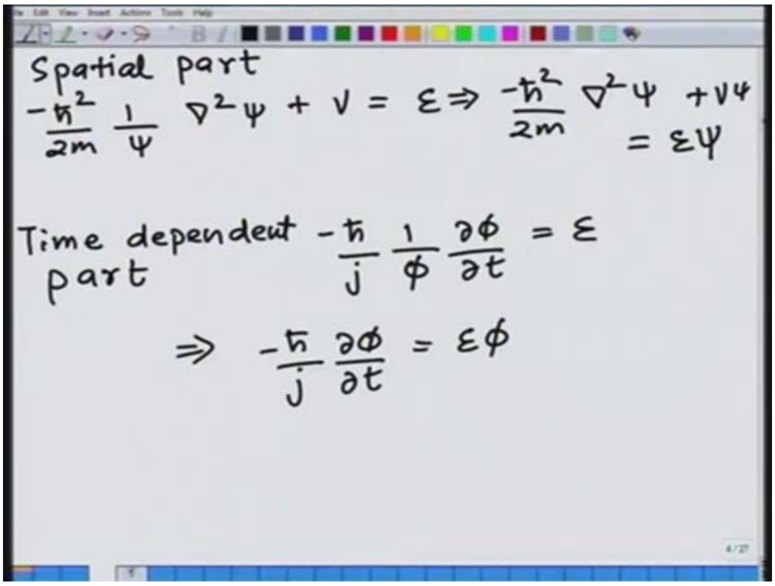


I assume that it is possible to separate this wave functions spatial part and time dependent part it is possible to separate them out. That means write this as xi of position only, the difference in symbol is that I draw these hats, here in case of when it is r comma t, but if it is only this is a different symbol when I do not draw the hats here.

Here is only function of position versus phi which is of time dependent I am assuming that it is possible it may not always be possible, but I am assuming that is possible that to write the wave function as two separate functions one of position and one of time. So, then we can substitute this in into our Schrodinger equation which changes what I wrote down. So, in that case, this becomes h square by 2 m times phi which is time dependent, hence need not take it is and this is only special derivative. So, only phi appears here plus v times phi times phi equal to and then of course only the time dependent part.

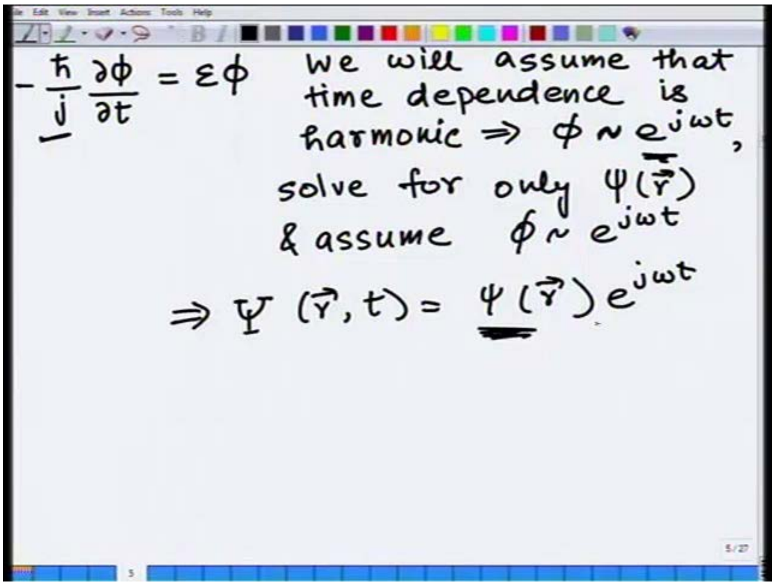
We need to consider here by j and phi comes out and del phi by del t, we separate it now like this divided by what do you get divided by this quantity what you get is minus h square this is the exercise you have seen in past. Also, in point of time if you do not recall today, then you need to brush up whenever you going to introduce to this, what do you notice? What you notice is, this is only phi dependent which is a position dependent if only phi r dependent and this is time dependent and yet they are equal, yet two sides spatial part and the time dependent part are equal. That only means that they both must be equal to same constant they must be both equal to same constant and that constant is that constant we are taking as a energy and, therefore because this spatial part.

(Refer Slide Time: 11:47)



We are going to write minus h square by 2 m, therefore we are going to write this is as one over phi plus v as equal to this energy e implies in more common form as we see it 2 m h into square of phi which is of position only plus v phi equal to energy times phi. This is a spatial part and time dependent part of the wave function, then likewise since this quantity e this energy should be equal to the same quantity here in the same both quantity should be equal. Therefore, minus h by j write this as phi del phi by del t equal to this, this implies that I am going to write this as h by j del phi by del t is equal to which is time dependent only.

(Refer Slide Time: 13:11)

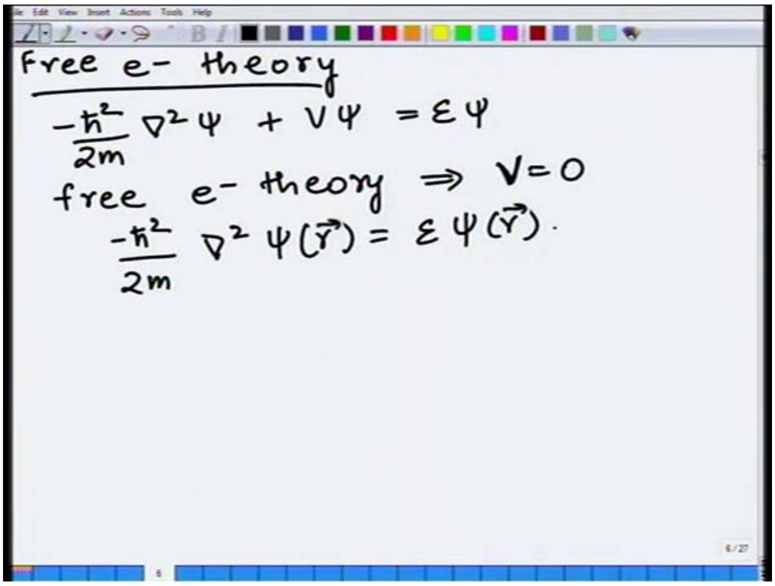


We will assume we will assume, in fact in doing, so maybe I have made a mistake, I go back a little bit in order for this to be true. I have make sure that this v is only function of position, I should move this part and should be only function of position, only then it will be true that this part is only spatial dependent. So, hence we will assume that, so we will assume that time dependence is harmonic, this implies that we will take phi to be e to power some constant times e to power j omega t.

That means rotating in time with the angular speed omega you can clearly see you can substitute this into this equation here and you will see that this is a solution to this equation. So, we are going to assume that whatever we do subsequently, what we will assume is we will solve for only the spatial part of phi solve for only spatial part xi and assume phi to be e to power to j omega t. Then, this whole wave function r comma t to be equal to phi of r times some constant times e to power j omega t time dependent, so this point and this is the part we going to solve.

So, this is all that we going to do in this class, we going to put focus only on this part, you assume that once we have calculated this part of the wave function, it is always possible to multiply this by e to power j omega t and get the whole wave function. So, essentially that was a quick review of that was the quick review of the quantum mechanics which we need to do here. These are operators, we will require energy operator s, we will require these different operators we will require, now let us move on to this free electron theory.

(Refer Slide Time: 15:34)



What do we mean and what are we doing here essentially like I said this Drude's theory and this Drude's theory which was a classical theory Somerfield theory in which a distribution was put in which was quantum mechanical. Otherwise, a classical theory, now we are moving towards something which is purely quantum mechanical. We will keep it simple, we will keep it very simple and we will use the same similar assumptions like Drude did.

For example, this called free electron, we will assume that it is free electron when we say free electron in the same sense as Drude did. We will assume this free electron here to mean as free electron and independent electron meaning thereby neglect any interaction between electron and electron and will neglect interaction any potential arising of electron and ions. That means, we assume that in a metal the ion positive charges well shielded by the valance electrons and sorry the inner shells of the electrons inner shells and because of the screening the valance electrons are very loosely bound to the ions. Since, they are very loosely bound, we will ignore this interaction and we will say this interaction is nearly 0 and that is what is really meant by free electron.

So, then how would we solve for this problem of conductivity, eventually how it is how we would think of conductivity in in a material in metals. If this is a situation in quantum mechanical sense is essentially what we are going to attempt to do. Now, recall so what we going to do we recall that h square by 2 m phi, we derive this as to be equal to this is the Schrodinger equation. The spatial part of the Schrodinger equation what we had derived the free electron theory implies free electron theory, essentially implies v is equal to 0 that means all the potential the potential is 0.

There is no interaction, we have ignored electron which is fairer approximation which is not too terrible though there are systems were electron interactions are very important, but electron ion interaction. Some typically presented material which you cannot ignore, but in some metal if it is possible to ignore them in that case potential is totally 0. There is no interaction and essentially free electron theory, therefore is about solving this equation of position. Of course, let me write it again this time is about solving this Schrodinger equation with some boundary conditions, what boundary conditions? Now, then you are, you can, since if have a material, you can make sure you can confine the electron into the material after all do not allow this electron to leak out of this material.

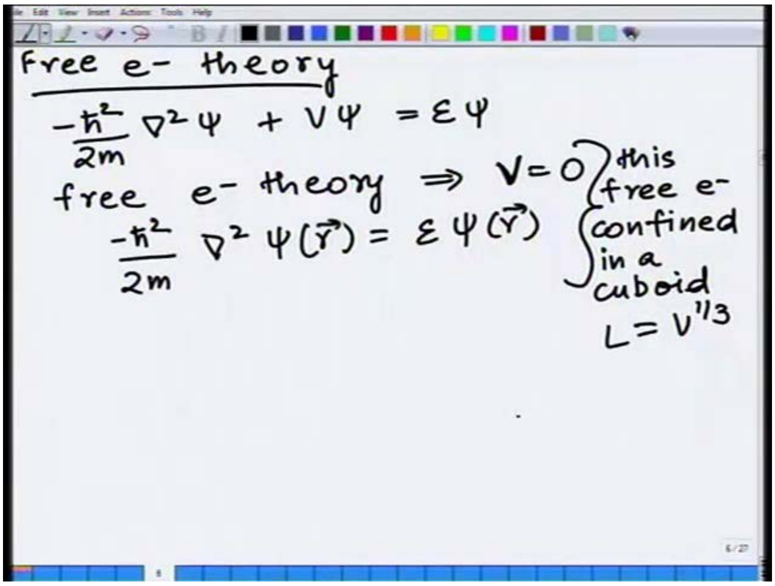
So, it stays in the material that is one way and that you can do by not letting the wave function leak out of leak out of this material that is one way, but when you are and that leads such a solution. If I try to solve it this way, then you will end of it is standing waves in the material. Now, you are interested in when we are interested in transport of energy then it is much better to deal with running waves and in order to obtain a solution which is running wave like solution.

So, not that the other solution is wrong, just that for convenience, if you want to a running wave like solution, then it is possible to write what are called as cyclic boundary conditions. So, I will write down the cyclic boundary conditions mathematically because it can only draw it, I am going do it in three dimensions, but in one dimension, I will show you what it means.

(Refer Slide Time: 19:27)

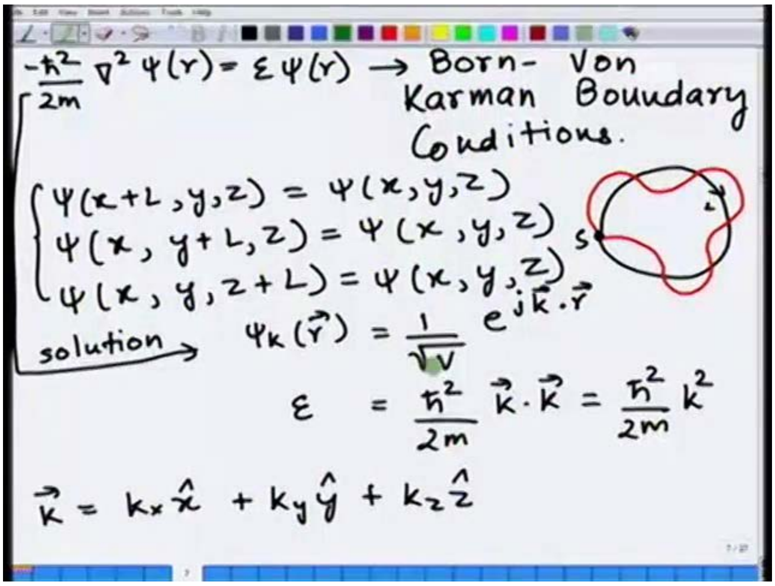
So, I am going to write down this Born Von Karman boundary conditions, what are these boundary conditions?

(Refer Slide Time: 19:42)



I am going to think of free electron, so imagine this free electron confined in a cuboid of edge length l and volume v. So, that means 1 by 3 power of volume is in the edge length, so imagine that this electron confined in all three directions in imagine, this is confined in a cube.

(Refer Slide Time: 20:12)



In that case phi, you can write at position x plus l comma y comma z is same as phi of x comma y comma z. I am going to write phi of x comma y plus l slowly y plus l comma z is equal to phi x comma y comma z. Similarly, x comma y comma z plus l is equal to phi x comma y comma z this is a mathematical written down in three dimension if you wish to see it in one dimension you can think like this. If this is starting point and in one dimension, let us consider the dimension one dimension to follow a circular path a closed loop imagine this to be the starting point and imagine this to be the terminating point.

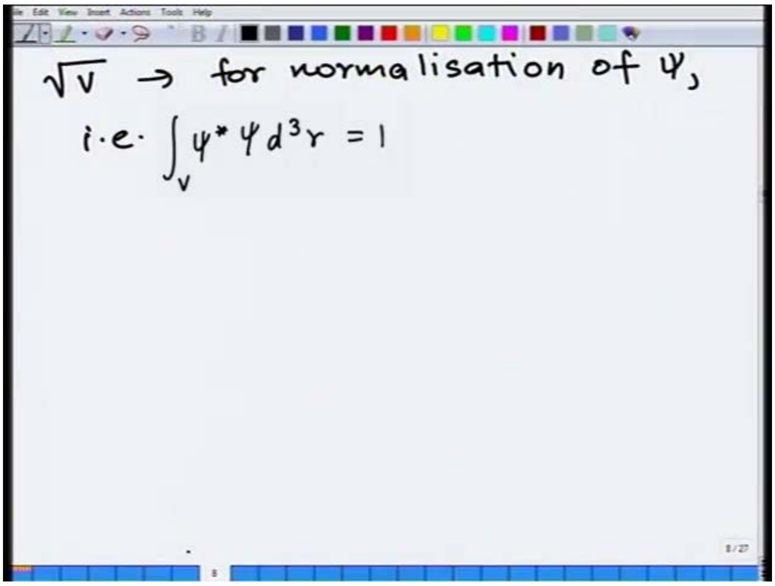
So, imagine a wave function which goes something maybe we use a different pen, so we draw a closed loop and we using the color here and we say draw the wave function. Then, it goes something like this, let us say wave function is like this this wave so that it terminates like this, it is a starting point imagine this that x equal to l is viewed back on 2 x. So, this is the starting point let us say and that is this is the finishing point x plus l is the total length here total length here, this is the length this is the length l we are talking about this is we are going around this and this is of length l.

So, we going around x, we start from x and go x plus l the whole start from x go round the length l you end up the same point. Therefore, wave function is the same essentially we are going to saying is what comes in from this boundary leaves from this boundary in case running in case of this this kind of boundary condition come in come out, energy comes in, energy goes out. So, this point is considered a basically collapsed onto that starting point and this in order to write, I cannot one cannot draw that in three dimension.

So, in three dimension, therefore we are writing it mathematically, so these are the boundary conditions we will apply for this running wave like solution. So, then notice without regard to this boundary condition solution to this particular equation is of form you can see that phi of k a symbol I am giving this r is equal to 1 by square root V e to power j k dot r this k is the wave number. You can take this and substitute in there substitute this into this equation which is right here, up here into this equation you substitute this solution.

We can substitute there and check whether this satisfies or not, if this you find that this solution will satisfy there with definition that k of course k vector is equal to k of x, x hat k of y, y hat. Let us write this explicitly and that this energy then in that cases h square by two m k dot k this is the same k, k dot k or equal to h square by 2 m k square. Thus, the energy, so this is a solution and this square root v basically appears for normalization that is you must make sure that should be 1.

(Refer Slide Time: 24:03)

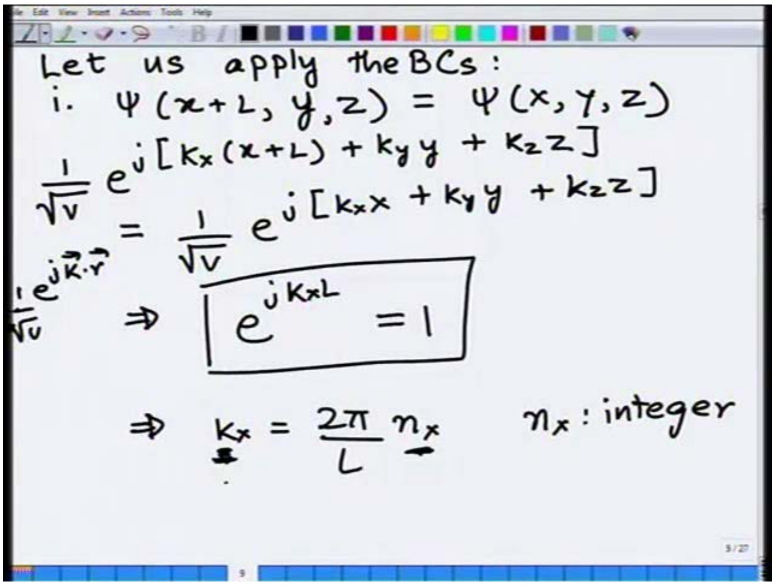


So, essentially in to make sure that this wave function is normalized this square root of v is appearing there thus about it, but the form of solution is this here, let us use a different pen here now. So, this is a form of solution essentially which you can substitute into this equation right here into this equation you can substitute in there. So, these two together then constitute the solution to this particular equation which we are trying to solve as a Eigen value problem.

Now, we going to go and apply the boundary conditions in there and see how the quantization starts appearing in this except or even before I do that notice we have introduced k which clearly is this solution is plain wave like solution. So, if you look at this vector k then you can see I had mentioned that wave k vector has a meaning. So, obviously it is a wave vector first of all, first of all it is a wave vector that is fairly obvious from the solution itself, but what else it means eventually we will see and this is you can see that this k vector automatically started becoming related to energy starts.

If already this starts, this k is related to energy we will see that this k also has implication has some meaning to it relates to the momentum also. Therefore, meaning of k becomes very important which we will try to understand subsequently as we go along in here.

(Refer Slide Time: 25:53)

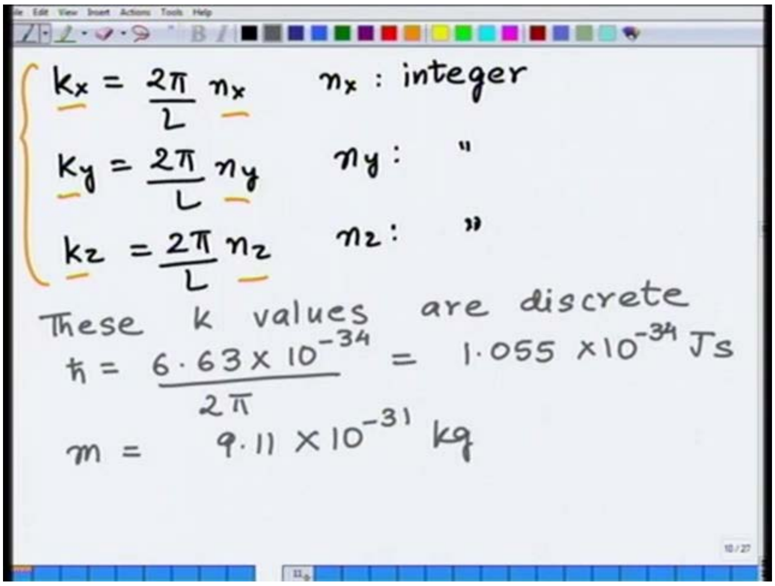


So, let us apply the boundary conditions now the boundary conditions one of the boundary conditions is that we call let me repeat this again let us apply this one that x plus l comma y comma z is equal to phi x comma y comma z, let us apply this. so, what we will do let us substitute that into the solution, so we have one over square root of v which is the solution here e to power j. We are going to write this k x times x plus l plus k y times y plus k z times z as the equal to one over square root of v which is basically this wave function.

This we know over j k x x plus x k y y plus k z z k dot r basically e to power remember the solution is of form j k dot r. Essentially, that is what we are writing here essentially that is what we are writing 1 over square root of v was our solution form for substituting in there what does that imply?

That implies that from this two equations implies e to power j k x l is equal to 1 that is what it means boundary condition. This essentially that is what implies with this boundary condition this forces the k x cannot be any value, but k x can only be k x can only be 2 pi multiple of l n x where n x is integer where n x can only be integer. So, n x value can be essentially, now notice that my value of k x is our value of k x is quantized. So, n x is a quantum number in that sense k x is a quantum number, since n x is only be integer k can take only definite values fix values and recall since k is related to energy. So, energy can therefore only discrete values essentially thus a common feature which you see in quantum mechanics, so similarly, by same token.

(Refer Slide Time: 28:36)



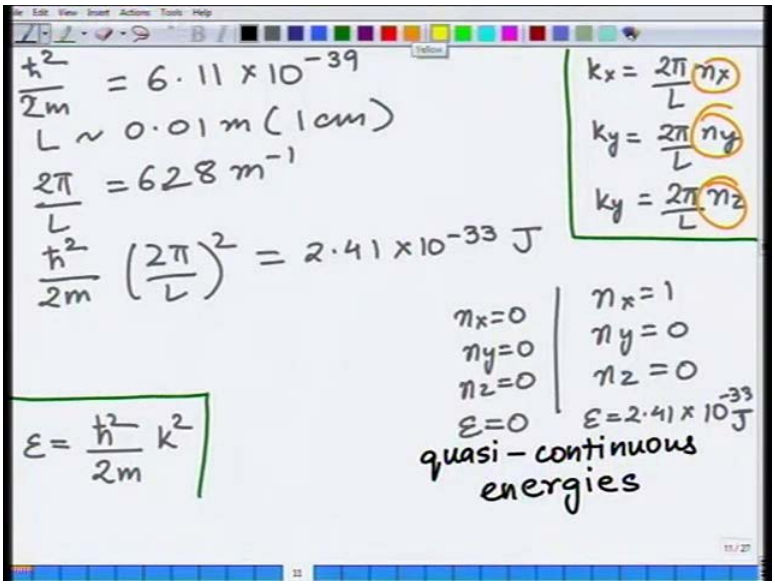
If I use the other two boundary conditions you will find, then two by l n y would become for the second boundary condition and a third boundary condition we will find k z is equal to two pi by l n z these are the only allowed of course n y n z are all integers. Also, these are also integers, so this is what we get out of this that, let us summarize of the more time that here is the wave function which satisfies the Schrodinger equation together with the Eigen value of energy right here, let us use another color.

So, here is the wave function which satisfies the Schrodinger equation and correspondingly the Eigen value of energy which is dependent on this quantity called k there this quantity k here. Then, if you move on, then we find that if you apply the boundary condition to it than the k can only take definite values and since k can take only definite values than energy is also discrete. Therefore, also what do you see, therefore we are now have three quantum number n x, n y, n z.

Loosely speaking, we can think of three quantum numbers to be k x, k y, k z along with than the fourth one which is the spin of the electron. We can now think of we call that I have written the wave function as only that of spatial and time. In addition to that, we should also consider the spin state which I have ignored we can assume that spin state is plus half minus half up spin or down spin. So, two spins are possible so along with these three quantum numbers plus the spin quantum number then completely describes my system.

Now, this k values are discrete let us see what it means let us do some calculation h bar is equal to 6.63 into 10 to power ten to 34 minus joules second divided by 2 pi which is equal to 1.055 into 10 to power minus 34 joules second. Mass of electron of course is 9.11 into 10 to power minus 31 kg, so let us than therefore calculate this quantity h square h bar square by 2 m.

(Refer Slide Time: 31:21)

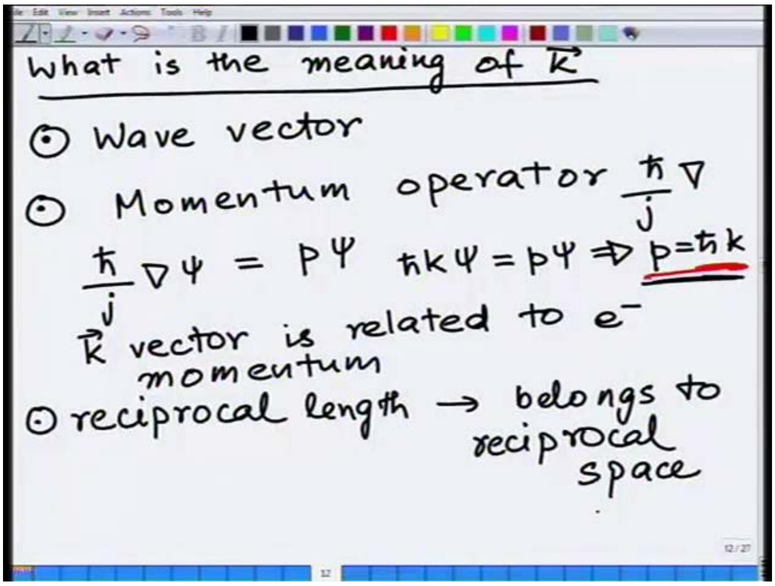


I have calculated this to be 6.11 into 10 to power minus 39 in appropriate units and if you take l to be 0.01 meter that means 1 centimeter. If we take the l to be that dimension then two pi by l is 628 meter inverse and then in that case if you look at this remember 2 pi by l of some integer multiple. So, let us look at this quantity h square by 2 m 2 pi by L square this quantity, then becomes 2.41 into 10 to power minus 33 joules now notice that as n x changes or n x y changes and n z changes by integer one integer k x changes by this much amount.

So, imagine if one state to be at n x equal to zero and then in that case we will see the energy to be 0 k to be in x, x direction. Let us assume this big assumption, so let us assume n x is equal to 0 n y equal to 0 and n z to be equal to be 0 and then in next case let us assume n x to be equal to 1 n y to be 0 and n z to be 0. Then, next state next accessible state for electron, so if you look at this for this case energy is equal to 0 as we see in k square depends on k square h square by 2 m h square by 2 m k square. That means energy is 0, in next case this k value will be equal to 2 pi by l, so in this case n x is equal to 1.

So, n x is equal to 1 that means k x will be equal to 2 pi by l, so that is why I have done h square by 2 m 2 pi by L whole square. This gives me the idea of energy, next energy, so energy will be 2.41 into 10 to power minus 33 joules, but this gap in terms of electron volts you can divide this number by 1.6 into 10 to power minus 19 only minus 19 and minus 33. So, that means in electron volts also the two energy levels there is one energy level and then next level is only separated by very small energy.

(Refer Slide Time: 34:57)



So, it is always possible though this energies are discrete this because this n x because this n x n y and n z are all discrete, yet we can think them to be quasi continuous. We can think of quasi continuous energies meaning there by that as n x n y n z integers change k x k y k z change very small amount. Therefore, the energies though discrete are changing by very small amount. So, it will appear that as if it is a quasi continuous energy, we can think that energy almost continuous though in principle they are discrete as they should be in quantum mechanical system.

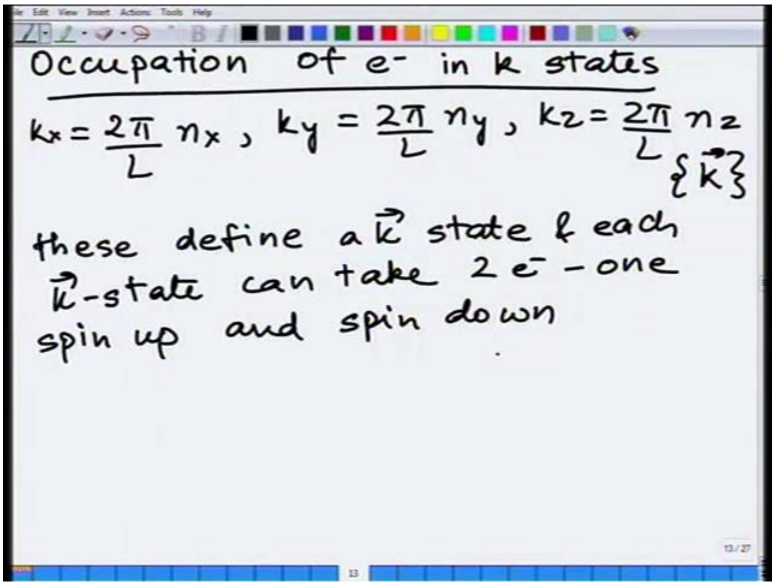
So, let us go further now what is meaning vector k what of course we know it is a wave vector that we know second what we know momentum operator is we will recall before the momentum operator. So, let us find the momentum Eigen value, so what happens let us do this, therefore we will take this operator and apply on the wave function. So, we will take this operator apply on the wave function and should give me my momentum Eigen value times wave function since I already know my wave function.

So, I substitute in there what do we get we are going to get is essentially you substitute in there. You would you would get is, therefore h k times phi as p phi implies this momentum as be equal to h bar k very interesting which says is that k vector is related to electron momentum k vector is related to electron momentum. What that means is that actually, but, I will at this point of time I will also do a clarification that indeed in free electron k vector is exactly giving you electron momentum, but it was not free electron theory. Then, in that case also though not done, here k vector is related to the momentum in sense that change of this quantity h k.

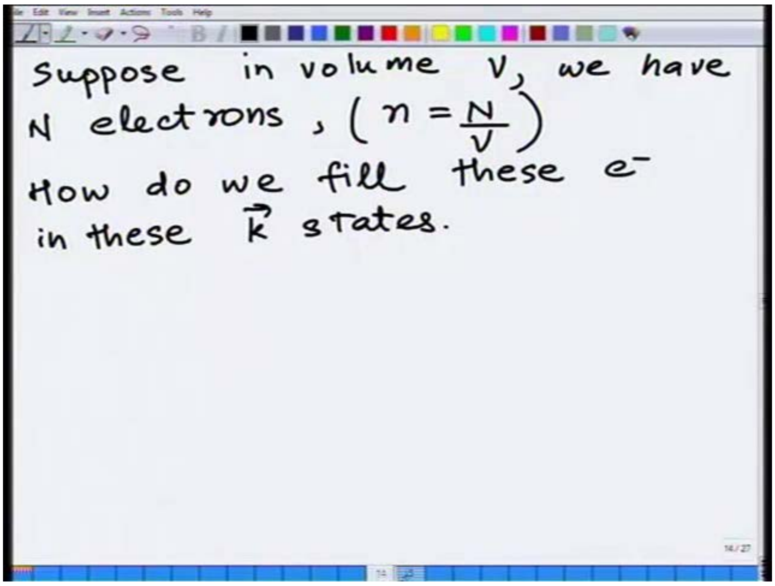
This quantity h k rate of change of this quantity h k is still gives you what is the external force that if you apply the external electric field to that force how does electron respond that to that force change in this momentum is still. This still appears as momentum fluid in external force, what I mean is external force when external force rate of change of this quantity h k is still is effected by this electric field which is applied from outside. Hence, we think of this also as crystal momentum that means that it is not actually an electron momentum the electrons, if it is not free electron in free electron case, this quantity h k is precisely momentum of the electron in case.

If it is not free electron still h k behaves like momentum to the external source though it is not actual momentum. This is then third thing we can notice essentially having defined the momentum and the crystal momentum though in free electron theory. I mention again that this is electron momentum, now let us see what dimensions of k are k is k as dimension of reciprocal length belongs to reciprocal as written down here. It is dimension is reciprocal of length and belongs to reciprocal space it is consequence, we will see as we go along in this course, so these are three points which you should remember.

(Refer Slide Time: 38:49)



(Refer Slide Time: 40:29)



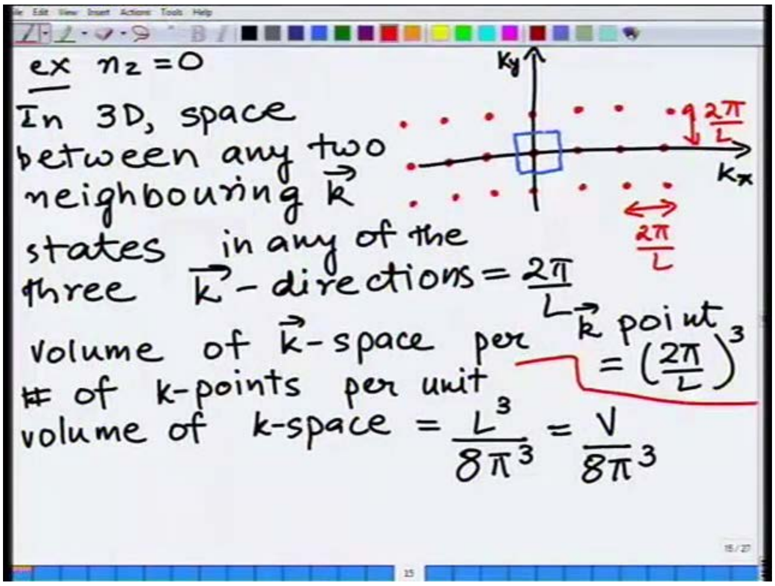
Now, so what do we have we have states so let us look at occupation, next topic the last topic for this lecture, so what have we derived we have derived k x as equal to 2 pi by L n x k y equal to 2 pi by L n y k z equal to 2 pi by L n z. We said that these are the three quantum numbers n x n y n z these, therefore define the k state that means they together define a k state k they define a k state and each k state can take 2 electrons 1 1 spin up and 1 spin down.

That means the four quantum numbers essentially k x k y k z in a spin quantum number that means I take consider one combination of k k x value k y k z value corresponding to 1.

Then, that defines my k state and in this case state, I can put two electrons, now I have defined what the states are now. Suppose, in volume v a volume v we have we have n electrons and small n be equal, therefore N divided by v which is number of electrons per unit volume. So, I have n electrons in volume v question we ask is how do we fill these electrons in these k states remember n x n y n z can take any integer values up to infinity in that sense I have an great number of k states never ends is continuous continuously.

They are pointed to n x n y different integers the k x k y k z values these are states on which I can put electrons on each of these states. I can put two electrons question is, but I have only n electrons, so when I start putting n electrons on these k states how far do I go? I go in n x n y n z or k x k y k z after which I run out of electrons and therefore, it will tell me what is the maximum energy those electrons can have and up to how far they go. Those are the issues we want solve now address though the states continue to exist ad nauseam which is continue to exist. Now, let us look at the filling part, so let us see let us assume a example let me show you example.

(Refer Slide Time: 42:07)



For example, let us assume n z is equal to zero and if I draw this axis like this this is k x this is k y axis k y axis then corresponding to n x equal to 0 n y 0. I have a k x, I have state right here, so here we have a n this is corresponding to n x equal to 0, therefore k x is equal to 0 corresponding n y is equal to 0, therefore k y equal to 0, I have one point. Now, corresponding to when n x is equal to 1 n, n y continues to be 0, I will have another state right here corresponding to n x equal to 2 while k y is still 0.

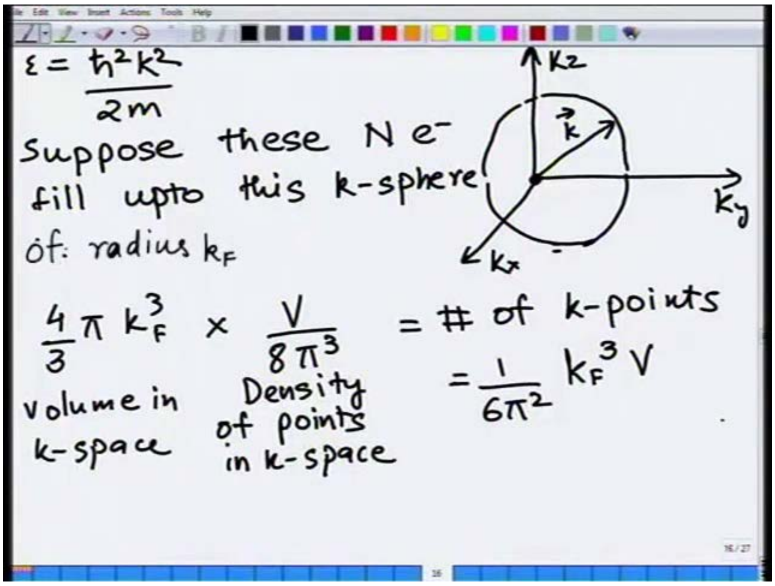
I will have another state right here corresponding to n x equal to 2 while k y is still zero I will have another state here another state here. Therefore, n x equal to minus 1 n x equal to minus 2 n x equal to minus 2 where k y equal to 0. Similarly, for n y equal to plus 1 and n x equal to 0, I have a state here and so on, I will have all the states corresponding to different combination of n x and n y. I will have all the states which are I am denoting here and what is the spacing between these state this between this and this it is 2 pi by l, they are separated by 2 pi by L and what is this spacing 2 pi by L of course.

You can see that even in three dimension in 3D also space between any two k states in any of the three directions k directions is equal to 2 pi by L space between any two neighboring k states. In any of the three direction in the k x direction k y direction k z direction, the space is between 2 pi what do, What does that mean, I can think like this that what is the space what is the volume associated with a k state this the this this in two dimension, I have shown as a square each as length being 2 pi by l.

So, now what I am going to do is, I am going to write this as follows, since the periodicity is 2 pi by L all these points in all the in the three dimensions. Then, volume and watch out the words here carefully volume of k space volume in k space not real volume in this k space this is k space. I have drawn a k x, k y space consisting of k x, k y and k z, then in also any volume in that space is the volume of the k space volume of k space per k point. We take one k point, then that obviously is 2 pi by L whole cube that is the volume associated with each k point because the periodicity in k space is 2 pi by l. That implies that number of therefore, number of k points per unit volume of k space is just inverse of this this.

I am writing inverse of this that will be l cube divided by this inverse of this relationship which I have just written here inverse of this is l cube 8 pi cube which is equal to volume V real volume in the real space eight pi cube. So, that is what this quantity is now what have we done, therefore now have density of k points in k space we have density. Once I have a density of points. Then, if I take large number of volume right in the k space and sample over them, then I am all I have to do is basically multiply with this density as we go along we will see what we are talking about.

(Refer Slide Time: 47:37)

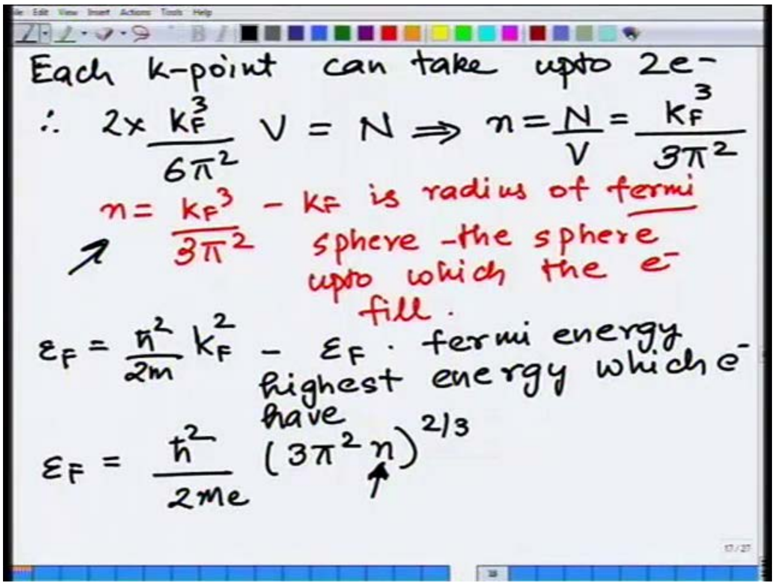


Now, what we are saying is we are saying that if I take notice that energy depends as goes as h square by 2 m k square. So, all points of constant k have same energy, so what surface what if I think of this k space consisting of k x axis. So, if I think of k x axis k x k y and a k z axis, so I think of a sphere in this, I think of a sphere in this about this point and this has a constant k some value k. According to this value on the surface of the sphere all points have same energy, but if think that they are Avogadro, since I have to fill Avogadro number of electrons n will be very large Avogadro number.

Then, if I am going to that means I will be accessing all most 10 to 23 k states if i accessing k that mean k state and I ask what is the radius of the sphere in which I will filling all the n since this number of sample space. So, large we can forget that this is a cuboid like arrangement; we can once you calculated this density right here in the k space I can take any volume in k space multiply that by this density number of k points per unit k space volume. So, I can take the volume of the k space multiply with this density and what I can get is therefore, number of k states in that volume essentially that is why we have calculated this density in here.

So, what I am going to do is now as follows, so suppose this these n electrons fill up to radius of this k sphere which I have just drawn here k f. Thus, the radius of that sphere then the volume of that sphere is of course, 4 by 3 pi k f cube, remember volume in the k space is the volume in the k space in k space multiplied by v by 8 pi cube density of points in k points in k space. Then, that gives me total number of k points, then that gives me number of number of k points and since each k point, so that is let us write this quantity as equal to let us see 1 by 6 pi square k f cube multiplied by v, that is what this quantity.

(Refer Slide Time: 49:28)



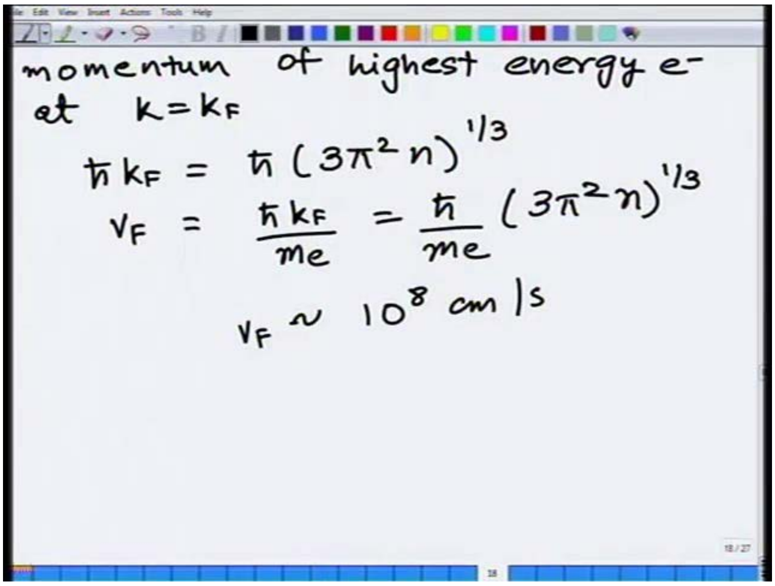
Now, each of this each of this this is number of k points, each k point can take up to two electrons, therefore two times number of k points k f cube divided by 6 pi square multiplied v should therefore be equal to total number of electrons that I have. Total number of electrons that I have what that implies is that we can write n which is equal to n divided by v as be equal to k f cube by 3 pi square. So, my relationship important relationship is k f is radius of what we call as Fermi sphere the sphere up to which the electrons fill.

So, if I have n electrons per unit volume in a system small n number of electrons per unit volume then they fill up k states up to that radius k f and that is called the Fermi sphere. Now, since you already we already know that energy depends on since energy, now if you ask the question up to the why where the Fermi sphere is what is the energy. We know that this energy Fermi energy we will call as Fermi energy be equal to h square by 2 m k f square. Thus, by same definition e f is Fermi energy is the highest energy which electrons have because why the k f is the radius which is the largest radius since k f is the largest radius, so the electron energy is highest there all other electrons imagine like this.

If I have a k x k y k z space in that, there is a sphere in this sphere if I put electrons, I start putting electrons at the lowest energy, I put one on each k state, I start putting two and keep doing this keep doing this keep doing this. We reach up to k f a sphere were we put our last electron and they are done all k states after that radius are, therefore unoccupied all electron and all states below this k f up to k f rather are all occupied each having two electrons on them. So, what is the energy of the electron energy of electron is this e f and that energy is called the Fermi energy and which, now we can write as e f.

We can write also as substitute value of k f in terms of n is from this equation here, take this equation and substitute in there. So, what you get is this comes out as h square by 2 m e 3 pi square n to power 2 by 3, now you know that if you take, remember if we take a metal, we know it is density you have seen in first lecture. If we know it is density, if we know it is molecular weight which we do, if we assume how many electrons per atom it conducts, then we can calculate what the value of n is. If we can calculate the value of n, then we can calculate the Fermi energy up to which these electrons completely fail. That is one thing we can calculate, second thing what we can calculate of that electron that highest energy electron momentum of highest energy electron at k equal to k f.

(Refer Slide Time: 53:20)



What is that quantity equal to, of course we know that momentum is h k f in this case and that therefore will be the h times we substitute k f in there, we know that what k f is, so 3 pi square n to the power 1 by 3 in terms of n. So, if I know number of electrons, though I can predict what the momentum will be once I know the momentum, then I can divide it by mass of I can say what the velocity of this highest velocity of this electrons is which is h k f divided by mass of electron. Then, it can be calculated as h bar by m e three pi square n to power 1 by 3, if you now remember what we did in Drude's theory we calculated estimate of velocity v 0 by classical equi partition of energy in context in context of kinetic theory of gases.

We wrote that as 3 by 2 Boltzmann constant multiplied by temperature and that we equated to half m v square and we calculated velocity. Now, we count that velocity to 10 to power 7 per centimeter per second, now as we calculate this velocity, you will find that this v f is on order of 10 to power 8 centimeters per second. Then, at that time I had mentioned that we have underestimated velocity by a order of magnitude that is what this is that the quantum mechanics is of actual velocity is only 0.01.

The Fermi velocity is almost one percent within 1 percent of the velocity of light, so that is why I will stop at this lecture here on free electron theory. We have built the bases what we have done is that we have built the bases defined what free electron is, then we have built the bases and we have calculated that we have k states quantized k states, but very narrow narrowly packed. Therefore, you can almost think of them as quasi continuous on these states we start putting two electrons and we see how far we can fill this up.

We can fill this up to the energy what is called as Fermi sphere k f and corresponding to that k f is Fermi energy. That is the highest energy electron can have corresponding to that what is the momentum of the electron what is the velocity of an electron. We have derived all those expressions and explained to you next time, I will start with density of electron states and then from that on, I will give it quick view of how we can think of conduction in thick stuffs.

Thank you.