Lecture - 12
Density of States - 3D, 2D

Hello everyone. In the previous class, we discussed the idea of Density of States qualitatively and why it is important. We started our discussion of 3D density of states in previous class. Today, we will building on that, we will see how mathematically we can derive density of states for 3D materials and for 2D materials as well.

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So, this is what we saw in the previous class. We saw that a 3D material can be approximated by a 3D potential well which means it becomes a 3D particle, particle in a 3D box situation, it becomes a 3D potential box and by using the notion of effective mass. If the E k relationship is parabolic, in that case the electronic wave functions are given as a direct generalization of 1D potential box electronic wave function.

And here, the allowed k_x, k_y, k_z values are as we saw in the previous discussion as well; k_x is essentially $n_x\pi/L_x$; k_y is $n_y\pi/L_y$ and k_z is $n_z\pi/L_z$; where, n_x, n_y and n_z can be any integer, they belong to the set of integers basically. And density of state is essentially the number of allowed electronic states which means we need to calculate number of allowed electronic states in the material.

And the easiest and natural way of doing that is to calculate the number of allowed combinations of k_x, k_y, k_z points and that is why we move to k space, which means we plot the allowed k points on k_x, k_y, k_z axis system and this is how it looks like essentially. Here, there are two points that we need to sort of make clear in the beginning. Each point in this space, each point essentially belong to an allowed electronic state.

So, each of these points is an allowed electronic state. It can be anywhere; but we have not considered the spin degree of freedom of electrons basically. So, this is just the special wave function. This wave function of electrons in space. So, if we consider the electronic degree, so the spin degree of freedom of electrons, each of these point can hold up to two electrons. So, that is why the number of allowed electronic states will be twice of these points in a way. So, each point can hold up to two points.

So, there are two allowed states corresponding to one point. So, that is point number 1. Point number 1 is we need to consider the spin of electrons and as we know electron is a spin half system, which means its spin angular momentum can take 2 values; its quantized and it can take plus half or minus half and that is why each point can correspond to either of the one of the two angular momentum states.

2nd point is in addition to the spin states, if we closely look at various points in the k space what we see is that if we change for example, if we change k_x to $-k_x$, the wave function here will change from $\Psi'(x, y, z)$.

So, now, the wave, so let us say if we make a change from k_x to $-k_x$, in that case, the electronic wave function will change from $\Psi(x)$ to $\Psi'(x)$ and $\Psi'(x)$ will be essentially minus if we put instead of k_x, if we put $-k_x$, it will be sin $-k_x x$ sin $k_y y$ sin $k_z z$ ok.

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So, that will be the wave function which means $\Psi'(x,y,z)$ will be $-\Psi(x,y,z)$. So, the wave function will just have a negative sign outside of all the sins and cosine. So, there will be a global phase in the wave function that is introduced, if we make a change of sign in k_x, k_y and k_z ok. And as we know from our discussion of postulates of quantum mechanics that if there is a global phase, it does not make any difference on the probability density function of the system.

So, this will remain the same. Also, it will not make any difference on the expectation value of the; of any operator so to say. So, this is the expectation value of any operator. This is over the entire volume. This will not change and this will not change. Essentially, a global phase, a global phase factor does not physically mean anything actually. It corresponds to the same electron basically ok. So, what it means is that all wave functions, which are differed from each other just by a global phase.

For example, this wave function psi prime and wave function psi, the only difference between the two is that psi prime is minus psi. So, there is a factor of global phase. It does not physically make any difference. So, they essentially correspond to the same electron. So, all these wave functions, which just have a difference of global phase factor, they are physically the same thing. And what it implies is that, so there are 8 octants in the k_x, k_y, k_z system here.

And a point in first octant and the point in a second octant will have a difference of a global phase. Similarly, the points in all these octants will have a difference of just a global phase.

So, which means that a point in first octant is similar to the points in all 8 octants; so, which essentially mean that the number of; the number of allowed wave functions or number of distinct allowed wave functions need to be divided by 8; So yeah.

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So, if we calculate all k points, we need to multiply by a factor of 2 because we need to incorporate electronic spin. But we also need to divide by 8 because all k point combinations in all octants are essentially similar to each other. They are essentially corresponding to same electrons ok.

So, all the distinct electronic state are just present in one octane of this k_x, k_y, k_z plane. So, with these two points in mind, now we are in a situation to calculate the distinct number of electronic states in a 3D system.
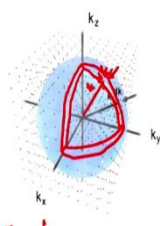
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So, we need to calculate the density of these points which means we need to calculate number of electronic states per unit volume per unit energy source. So, in order to calculate the density of state, we plot a spherical shell in this k_x, k_y, k_z plane. So, we plot a spherical shell of thickness dk. So, the inner radius of the spherical shell is k and the outer radius is k + d k.

So, now, the number of states in the spherical shell, which means in an energy range from k to k + d k will correspond to electronic states in energy range from E to E + d E ok. So, the number of electronic states which have value or which lie in the spherical shell will correspond to the electronic states in this energy range energy from E to E + d E basically ok.
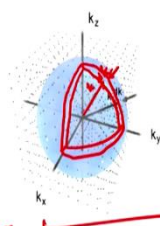
So, now, let us do a simple calculation. The volume of a single allowed electronic state is essentially it will be a small cube in the reciprocal space, in the k space and this the volume of single state will be π/L_x times π/L_y times π/L_z.

So, this will be $\pi^3/L_x L_y L_z$ equals π^3/V; where, V is the volume of the entire solid which is just a 3D solid essentially. So, this is the volume of allowed electronic state, a single allowed electronic state in k space. Now, the volume of the spherical shell is we are trying to find out the number of electronic state in the spherical shell.

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The volume of spherical shell will be $4\pi k^2 dk$; just this ok. So, we know the volume of a single state, we know the volume of the spherical shell, we can easily find out the number of electronic states in the spherical shell by just by dividing the volume of the spherical shell by the volume of the single electronic state. So, that is what we will do volume of the single electronic state is π^3/V.
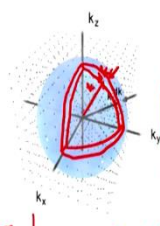
So, number of electronic states in the energy range from E to E + dE will be $4\pi k^2 dk$ divided by π^3/V. So, these are the number of electronic states in this energy range from E to E + dE essentially. So, this is the number of electronic states in the energy range is denoted as N(E)dE; in the energy range from E to E + dE will be denoted as N(E)dE and this will be $4\pi k^2 dk$V/π^3.

So, any in that sense becomes the number of electronic states per unit energy, which is also a function of energy. Now, we need to convert or we need to change the variable on the right hand side from k to E basically and that is here that is where here we will use the E k relationship, which is a parabolic relationship, if we use the idea of effective mass.

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So, please keep in mind that we are making an approximation that the E k relationship is parabolic and we can make or we can use the notion of effective mass like this. So, in this case, k will be given as $\frac{\sqrt{2m^*E}}{\hbar}$ just by rearranging the terms and from here itself, k^2 is $2m^*E$ divided by $\hbar^2$.

And if we take a derivative of this, it becomes 2kdk is essentially $2m^*dE$ divided by $\hbar^2$. 2 and 2 goes away, so kdk is equal to m^*dE divided by $\hbar^2$. So, this we will put here in this expression. So, by using this relationship and this E relationship k value, N(E)dE is 4 by here π, π and π^3 becomes π^2.
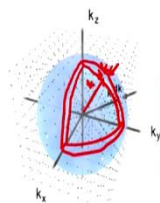
This k^2dkV can be written as k times kdk times V. So, this k value is just $\frac{\sqrt{2m^*E}}{\hbar}$; $4/\pi \frac{\sqrt{2m^*E}}{\hbar}$ and kdk is m^*dE divided by $\hbar^2$ times volume. So, this is the total number of electronic states in the system ok, in the energy range from E to E + dE. Now, the dE, dE go away and as we discussed there are two other factors that we need to consider.

We need to consider the electronic spin first, so which means that we need to multiply this expression by 2 in order to consider the electronic spin. And second, we saw that various k points in different octants or k points in different octants, just introduce a global phase which will not change, which will not make any physical sense, which will essentially be the same electron. So, we just need to count the number of electronic states in 1 octant; here, we have done we have done the calculation for all 8 octants.

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So, we need to multiply by 2 in order to consider a factor of spin and we need to divide by 8 in order to not over count the distinct allowed electronic states. So, we need to multiply by 2 for spin and divide by 8 for distinct k values and rest of the expression looks like this; 4 by $\pi^2 \hbar^3$ times $m^*\sqrt{2m^*E}$ times V. So, 4, twice, 8; so, they go away.

So, which means the total number of electronic states per unit energy is just $m^*\sqrt{2m^*E}$ divided by $\pi^2 \hbar^3$ times V and the density of state now is so here, we have considered the spin; we have considered the over counting of electrons. Now, the density of state will simply be the total number of electronic states per unit energy per unit volume.

We need to divide by the volume. So, it becomes $m^*\sqrt{2m^*E}$ divided by $\pi^2 \hbar^3$ ok. So, this is the number of electronics density of states in a 3D material. So, there are some interesting observations that we can make from this expression actually.

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So, finally, the number of electronic states in a 3D material will be 3D solid will be this g(E) is $m^*\sqrt{2m^*E}$ divided by $\pi^2\,\hbar^3$ ok. So, m^* is a is constant, if we assume that the E k relationship is parabolic, in that case a m^* is constant π^1 and $\hbar^1$ are other constants. So, essentially, g(E) is directly proportional to $E^{\frac{1}{2}}$; square root of E basically.

And if we plot g(E) as a function of energy, just to see how electronic states are distributed, this will be a square root function. So, it will be a sub-linear kind of function, not exactly like this. It will be something like this. This is not the exact quantitative sort of plot, just to see how qualitatively g(E) depends on E. This is how it depends on E essentially and what it implies is that. So, g(E) is essentially the density of states, which means these are the allowed electronic states in a material.

So, in 3D materials, it turns out that for low energy values, for these energy values, this g(E) is very small. So, the density of states in 3D materials is very small for small energy values; but as we go as we increase the energy value, as we go to higher energies, this g(E) becomes more and ultimately, it becomes a saturation, a saturating kind of function; not exactly saturating, but the rate of increase lessens.

It does not increase with the same rate as it increases in the beginning. So, the number of allowed states for low energies in 3D materials is small and they become large as we increase the energy. So, this is the key takeaway and this will be quite important, when we discuss the discuss a 3D channel, where we will be using this kind of channel in a device.

So, there number of states available in a certain energy range will be very important because that will govern the conduction from the source to the drain. So, that is why understanding this is important. So, that is about the density of states in 3D materials and we have seen that the density of state g(E) is directly proportional to square root of E. Now, let us see how it sort of varies in 2D solids.

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So, like a 3D solid, a 2D solid can be like a graphene material or MoS$_2$. So, a 2D solid is essentially a solid which is extended only in two directions. So, the dimensions of the solid are like this. It has L$_x$ length, L$_y$ width.

This is the solid, 2D solid. By using the same principles as we used in 3D materials, 3D by using the same approximations, if we sort of have this E k relationship, this kind of E k relationship, E is directly proportional to k square or a function of k minus a constant square parabolic relationship between E and k.

In that case, we can precisely define the effective mass becomes constant because and in that case, all the effect of crystalline potential and the interaction of atomic cores or crystal with the electrons can be encapsulated in effective mass and we can consider this 2D material as a large 2D potential box; exactly the same way as we did in the case of 3D solids.
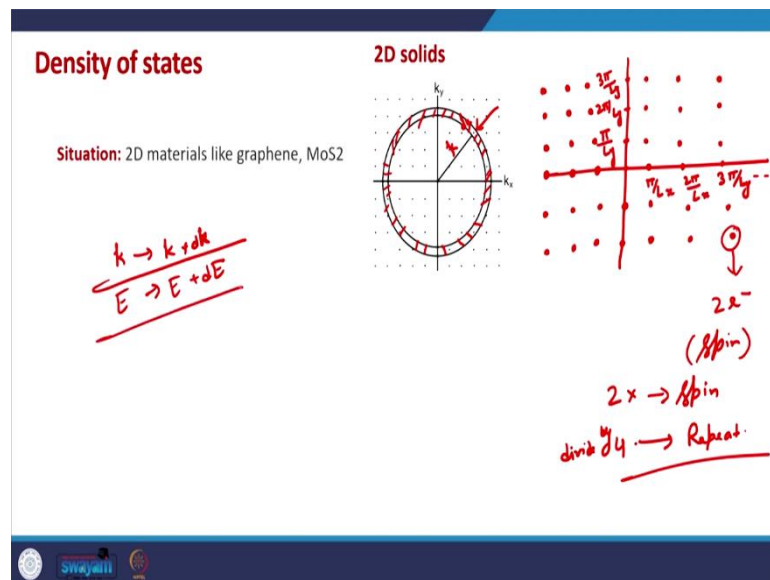
And now, we just need to see now since the effect of crystalline potential has been encapsulated in the idea of effective mass, we just need to solve the Schrodinger equation for the entire solid and this becomes a very large or as at least as large as the solid is that large potential box, but a 2D potential box and the solution of wave function in 1D potential box was A sin k_xx.

So, here also by the same, by generalizing this wave function in 2D case, this will be A sin k_xx times sin k_yy and as we saw in the 3D case because of the boundary conditions, we need to have sin $k_x L_x$ to be 0 and similarly, sin $k_y L_y$ to be 0. This is from the derivation of the particle in a box case and from here, we deduce that the allowed sin k_x values are $\frac{n\pi}{L_x}$ or since there are two possible n here.

So, we will write $\frac{n_x\pi}{L_x}$ is k_x and k_y would be $\frac{n_y\pi}{L_y}$; where, n_x and n_y are integers essentially. And we are trying to see what is the density of states for a 2D material for a 2D solid, so we just need to calculate the distinct allowed electronic states in the solid and for that, we will move to the k space because in k space the counting becomes easier.

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So, in k space, the allowed k points will be essentially. Now, the allowed k points will be $\frac{\pi}{L_x}$, $\frac{2\pi}{L_x}$, $\frac{3\pi}{L_x}$ similarly and so on and on the y axis $\frac{\pi}{L_y}$, $\frac{2\pi}{L_y}$, $\frac{3\pi}{L_y}$ and so on and apart from these points, combination of these points will also be valid solution of Schrodinger equation in

2D case. So, these points will be the finally, these points drawn which are drawn on the screen, these will be the allowed solutions of electronic wave function.

And here also, we need to keep two things in mind; one is the spin of the electrons. So, each point can host up to 2 electrons because of the spin, since electron is a spin half particle. So, each point can host up to 2 electrons. So, the number of states will be twice the number of allowed points. Also, the each point, so the points in different quadrants will essentially correspond to the same wave function because there will be just a difference of a global phase.

So, a factor of 2 will come because of the spin and we need to divide by a factor of 4 because of the repetition of the k values essential corresponding to the same electron. So, now, in this case in order to calculate the number of electronic states from the range from k to k + dk, we will make a circular ring here of inner radius k and outer radius k + dk.

So, we will make a circular radius of width dk; inner radius will be k and outer radius will be k + dk and in this radius, in this ring in k plane, we will try to see how many distinct electronic states exist, that will give us the number of electronic states in the energy range E to E + dE.

So, the electronic states corresponding to a range k to k + dk will also correspond to energy range from E to E + dE and that is how we will do this calculation. I will let you do this on your own. So, please do this on your own and we will discuss this in the next class.

Thank you.