Physics of Nanoscale Devices
Prof. Vishvendra Singh Poonia
Department of Electronics and Communication Engineering
Indian Institute of Technology, Roorkee

Lecture - 13
Density of States – 2D, 1D, 0D

Hello everyone. Today, we are going to discuss Density of States in 2D solids, 1D solids, and 0D solids. Basically, we will try to conclude the density of state discussions today.

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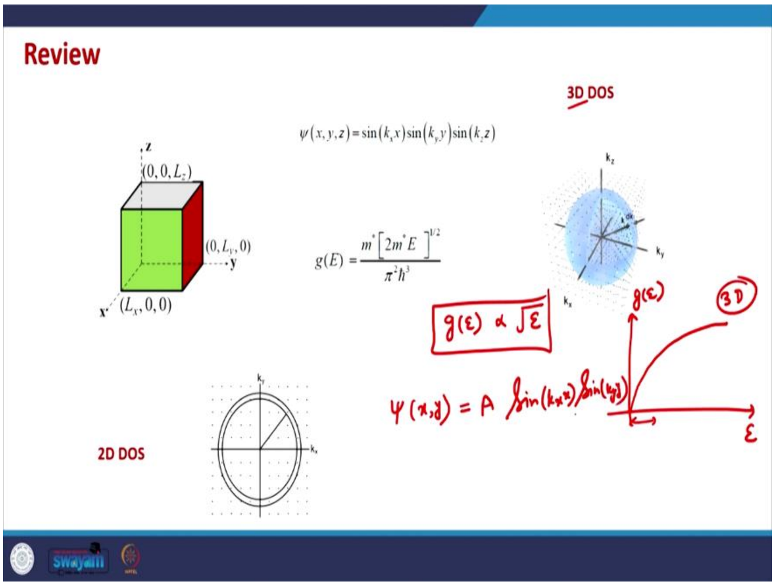

Review

3D DOS

$\psi(x,y,z) = \sin(k_x x)\sin(k_y y)\sin(k_z z)$

$$g(E) = \frac{m^*\left[2m^*E\right]^{1/2}}{\pi^2\hbar^3}$$

$\boxed{g(\varepsilon) \propto \sqrt{\varepsilon}}$

$\psi(x,y) = A \sin(k_x x)\sin(k_y y)$

2D DOS

And before delving into that let me quickly review what we discussed in the last class. We discussed in detail about the density of states in 3D solids. 3D solids mean that the dimension of the solids, the solid is significant in all 3 directions. By significant I mean electron is confined in all 3 directions in the solid in an extent which is larger than the dimension of the electron, generally the dimension of the electron.

So, this is what we concluded about the 3D density of states that the density of states in 3D solids is directly proportional to the energy value. And there are certain approximations that we make and those approximations are not unrealistic approximations. They are fairly reasonable approximations, specially at the top of the valence band and at the bottom of the conduction band.

So, the discussion that we are doing here that is quite aptly suitable for application in our practical devices as well. Specially, in the most important parts of the bands that is the top of the valence band and the bottom of the conduction band. We saw that the density of state of a 3D solid has a pattern like this.

This g(E) as a function of energy for 3D solids is like this. First, for low energy values g(E) is quite low which means that the available electronic states for low energies is less in 3D solids.

Then, we started our discussion of 2D solids as well, and a 2D case is also quite similar to a 3D case to the 3D case. Here even it is more simple, here only we have two directions in which we need to solve the Schrodinger equation and the solution of electronic wave function in 2D solids turns out to be A sin k_xx sin k_yy.

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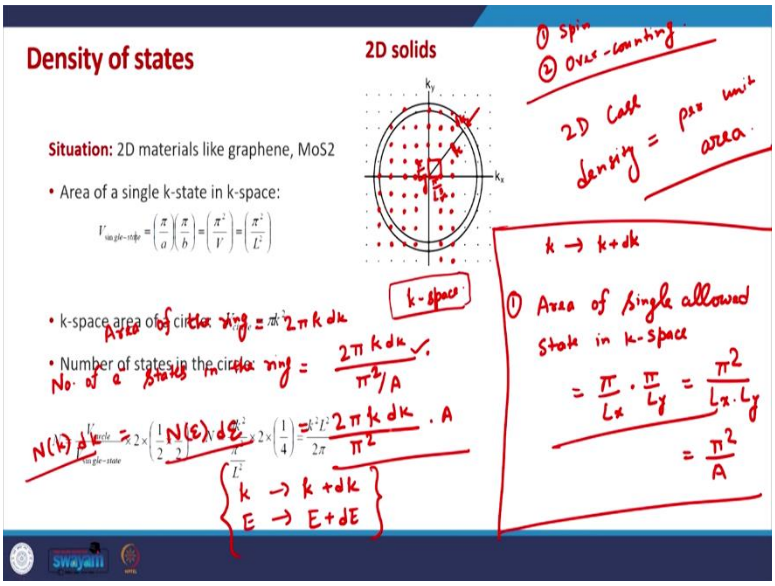

Density of states

2D solids

① spin
② over-counting.

2D case density = per unit area.

Situation: 2D materials like graphene, MoS2

- Area of a single k-state in k-space:

$$V_{single-state} = \left(\frac{\pi}{a}\right)\left(\frac{\pi}{b}\right) = \left(\frac{\pi^2}{V}\right) = \left(\frac{\pi^2}{L^2}\right)$$

k-space

- k-space area of circle = πk^2

Area of ring = $2\pi k\,dk$

- Number of states in the circle:

No. of states in the ring = $\frac{2\pi k\,dk}{\pi^2/A}$ ✓.

$$N = \frac{V_{circle}}{V_{single-state}} \times 2 \times \left(\frac{1}{2}\cdot\frac{1}{2}\right) = \frac{\pi k^2}{\frac{\pi^2}{L^2}} \times 2 \times \left(\frac{1}{4}\right) = \frac{k^2L^2}{2\pi}$$

$$N(k)\,dk = N(E)\,dE = \frac{2\pi k\,dk}{\pi^2}\cdot A$$

$$\left\{\begin{matrix} k \to k + dk \\ E \to E + dE \end{matrix}\right\}$$

$k \to k + dk$

① Area of single allowed state in k-space

$$= \frac{\pi}{L_x}\cdot\frac{\pi}{L_y} = \frac{\pi^2}{L_x \cdot L_y}$$

$$= \frac{\pi^2}{A}$$

And these k_x and k_y values are discrete values. And as we saw that in order to find out the density of states, we need to calculate the allowed electronic states and that we do in k-space. So, we go to the k-space which means we plot k_x and k_y axis, and we put the allowed k points in the k-space.

And each point now corresponds to a wave function of electron. There are two other constraints that we or two other points that we need to keep in mind, one is that we did not consider the spin degree of freedom of electrons.

So, we need to multiply the number of allowed states by 2, but at the same time we saw that points in different quadrants of the k-space, they essentially belong to the same electronic or they essentially describe the same electron because they only have a difference of global phase.

And global phase physically does not make any difference in quantum mechanics, ok. So, two points, one is the spin and second is the over counting of electronic state. These two things we need to keep in mind.

So, here in order to now find out the density of states, we need to calculate the number of k points in k-space and we need to find out the sort of the density of k points, allowed k points in the k-space. In this case, in a 2D case, density will mean per unit area. So, density will essentially mean per unit area. In 3D case, it was per unit volume.

So, in order to find out the number of allowed k points in the range from k to k + dk, we draw a spheric, we draw a circular ring whose inner radius is k and outer radius is k + dk. So, this width of the ring is dk. And area of single allowed state in k-space, this area is $\frac{\pi}{L_x}$ times $\frac{\pi}{L_y}$.

So, this is the area of single allowed electronic state in the k-space and that is essentially $\frac{\pi}{L_x}$ times $\frac{\pi}{L_y}$. So, this is the area of one electronic state, one allowed electronic state in the k-space.

Now, what is the area of the circular ring? So, the area of the ring will be $2\pi kdk$, area of the circle is πk^2, circle of radius k is πk^2e and area of the ring will be $2\pi kdk.$ So, now, a number of electronic states in the ring will be area of the ring $2\pi kdk$ divided by area of the single state. And the area of the single state would be $\frac{\pi^2}{L_x L_y}$, and $L_x L_y$ is also the area of the entire solid, essentially.

So, this number of states number of electronic states in the ring would be the area of the ring which is this divided by area of the single electron, single electronic state or area occupied by a single state, so it would be $\frac{\pi^2}{A}$. So, these are number of electronic states in the ring, essentially. So, these are the total number of electronic states in a range from k to k + dk. And this is denoted by N(E) times dE also by N(k) times dk.

So, these are the total number of electronic states for values of wave vector from k to k + dk or for energy range of E to E + dE. So, for these this is the number of electronic total number of electronic states in this energy range. Now, the density of state calculation is straight forward. Density of states essentially means number of electronic states per unit volume, in this case it will be per unit area at a given energy which means we need to also divide by dE.

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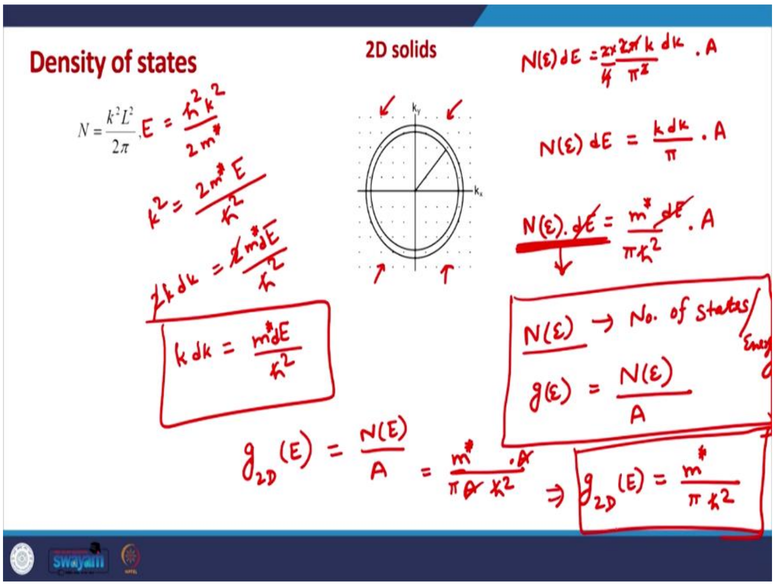

Density of states

2D solids

$N = \frac{k^2L^2}{2\pi}$, $E = \frac{\hbar^2 k^2}{2m^*}$

$k^2 = \frac{2m^*E}{\hbar^2}$

$\cancel{2}k\,dk = \frac{\cancel{2}m^*dE}{\hbar^2}$

$\boxed{k\,dk = \frac{m^*dE}{\hbar^2}}$

$N(E)\,dE = \frac{\cancel{2}\times 2\cancel{\pi}k\,dk}{\cancel{4}\,\pi^{\cancel{2}}}\cdot A$

$N(E)\,dE = \frac{k\,dk}{\pi}\cdot A$

$N(E)\cdot\cancel{dE} = \frac{m^*\cancel{dE}}{\pi\hbar^2}\cdot A$

N(E) → No. of states/

$g(E) = \frac{N(E)}{A}$

$g_{2D}(E) = \frac{N(E)}{A} = \frac{m^*\cdot\cancel{A}}{\pi\cancel{A}\hbar^2} \Rightarrow \boxed{g_{2D}(E) = \frac{m^*}{\pi\hbar^2}}$

So, this is a total number of electronic states is $2\pi kdk$ A times, so N(E)dE is $2\pi kdk$ divided by π^2 $into\ A$. Now, the two points that we discussed is we need to consider the electronic spin as well. So, we need to multiply by 2. Also, we need to avoid over counting of allowed electronic states, and k points belonging to different quadrants, they essentially correspond to the same electronic wave function.

So, we need to divide by 4 because these 4 set of k points they correspond to the same electron, so we need to divide by 4 as well, ok. So, this becomes, total number of electronic states in the range from E to E + d E, this becomes kdk divided by π times area.

Now, we go back to our E k relationship and the E k relationship looks like this, E=$\frac{\hbar^2k^2}{2m^*}$, so which means k^2 is like our earlier calculations $\frac{2m^*E}{\hbar^2}$. And if we take a derivative on both sides, it is 2kdk equals $\frac{2m^*dE}{\hbar^2}$.

We can remove 2 from each side, so it becomes k.dk is equal to $\frac{m^* dE}{\hbar^2}$. So, if we put this value there, total number of electronic states in the energy range as a function of energy would be, so this is dE here, we need to take derivative on the right side as well, $\frac{m^* dE}{\hbar^2} A$. So, this number on the left hand side this is the total number of electronic states in the system.

So, N(E) would be number of states total number of states per unit energy. This is the number of states, this entire left hand side expression, N(E) times dE, this is the number of states in the energy range from E to E + dE, basically. So, this number any would be number of states per unit energy and the density of state as we; so, for 3D case will be number of states per unit area per unit energy. So, this will be N(E) divided by area, ok.

So, now, we are in a position to sort of calculate the density of states for the 2D case. So, for 2D case if we represent, the density of state by g_{2D}(E), this would be N(E) by area and it becomes $m^* dE$ by times A, A and A cancels which means g_{2D}(E) is you know even m star goes sorry, this dE also goes away because N(E) is $\frac{m^* A}{\hbar^2}$, so this dE also goes away. So, what we are left with is $\frac{m^*}{\hbar^2}$.

So, here we also had π, so k.dk.A/ π and k dk is $\frac{m^* dE}{\hbar^2}$. So, we will also have a π here, so essentially it would be $\frac{m^*}{\pi \hbar^2}$ So, this is the density of states in a 2D solid as a function of energy. This is the expression for the density of states in a 2D solid.

And as you might have already guessed here that on the right hand side everything is a constant, essentially. So, we are assuming a parabolic band structure. So, this m^* is a constant, π is a constant, $\hbar$ is also a constant, so this g_{2D}(E) expression is essentially a constant.

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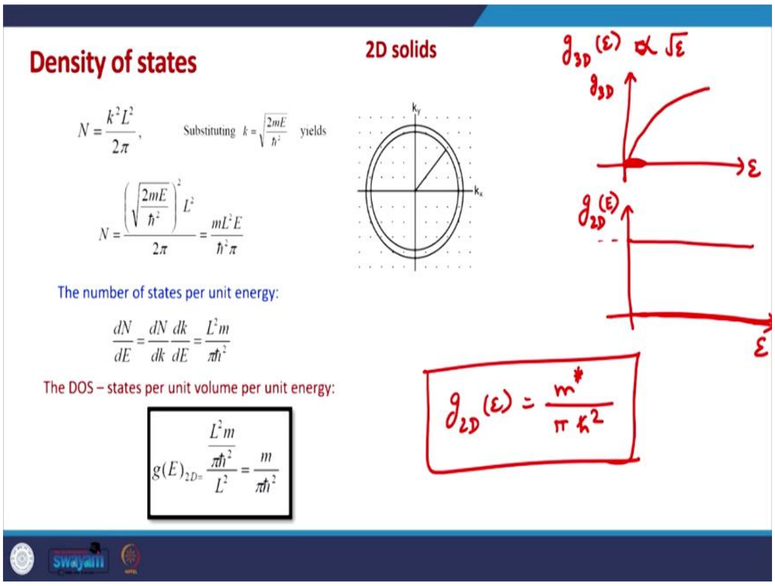

Density of states

2D solids

$$N = \frac{k^2 L^2}{2\pi},$$

Substituting $k = \sqrt{\frac{2mE}{\hbar^2}}$ yields

$$N = \frac{\left(\sqrt{\frac{2mE}{\hbar^2}}\right)^2 L^2}{2\pi} = \frac{mL^2E}{\hbar^2\pi}$$

The number of states per unit energy:

$$\frac{dN}{dE} = \frac{dN}{dk}\frac{dk}{dE} = \frac{L^2 m}{\pi\hbar^2}$$

The DOS – states per unit volume per unit energy:

$$\boxed{g(E)_{2D} = \frac{\frac{L^2 m}{\pi\hbar^2}}{L^2} = \frac{m}{\pi\hbar^2}}$$

$g_{3D}(\varepsilon) \propto \sqrt{\varepsilon}$

$$\boxed{g_{2D}(\varepsilon) = \frac{m^*}{\pi\hbar^2}}$$

So, g$_{2D}$(E) is $\frac{m^*}{\pi\hbar^2}$. And this is an interesting result if we compare this to the 3D case, because in 3D case we saw that the density of state for 3D case is directly proportional to square root of E and that is why if we plot density of state for a 3D case as a function of energy, it is a function like this, but for a 2D case the density of state is constant.

And if we plot g$_{2D}$ versus E, it will essentially be a straight line parallel to the energy axis. So, it will not change with energy. And this is an interesting difference between 3D materials and 2D materials, between a 3D channel and a 2D channel. In 3D channels, at low energy values, the density of states or number of allowed electronic states is very less.

But in a 3D channel, the density of states or number of allowed electronic states that can exist in a material is the same irrespective of the energy or it is the same basically, same for all energy values. So, if we change our channel from if we make our channel 2D the density of state changes and it will change the conduction in a major way.

So, this is why understanding density of states is quite important, ok. So, now, we will see how the density of states look like for 1D solids, ok. 2D case was easy.

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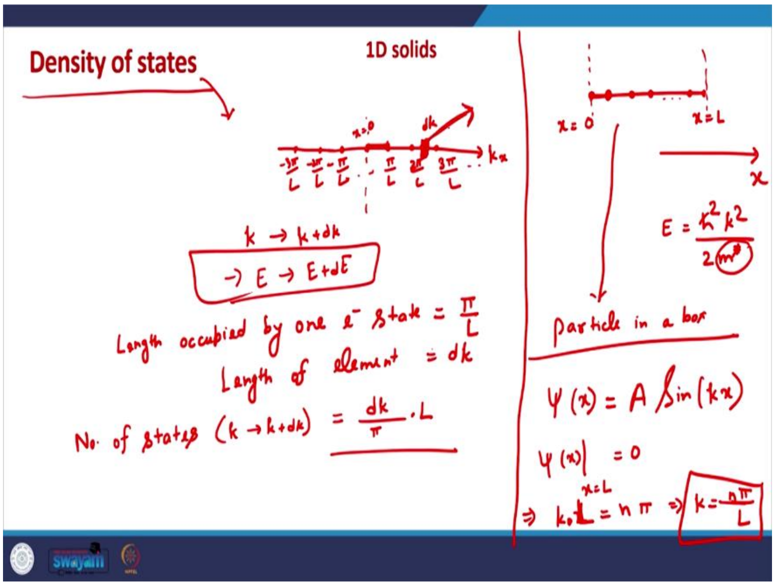

Density of states

1D solids

$k \to k+dk$

$\boxed{\to E \to E+dE}$

Length occupied by one e^- state $= \frac{\pi}{L}$

Length of element $= dk$

No. of states $(k \to k+dk) = \frac{dk}{\pi} \cdot L$

$E = \frac{\hbar^2 k^2}{2 m^*}$

particle in a box

$\psi(x) = A \sin(kx)$

$\psi(x)\Big|_{x=L} = 0$

$\Rightarrow k \cdot L = n\pi \Rightarrow \boxed{k = \frac{n\pi}{L}}$

Now, a 1D solid means that the solid is now like a nano wire. So, the electron is confined between x equal to 0 to x equals to L let us say and this is the x axis. There might be atoms between x equal to 0 to x equal to L, but as we previously discussed in KP, after KP model that by effective mass we can sort of in incorporate the impact of the crystalline potential of the lattice.

So, the E k relationship is h bar square k square divided by 2 m star, m star is the effective mass of the electron in the solid. And by considering the effective mass, we can assume that the electron is independent of the lattice interaction and electron is just confined in the boundaries of the solid. It is just confined between x equal to 0 to x equal to L. And this is essentially the particle in a box situation.

And the solution of Schrodinger equation of particle in a box we have already done. In fact, we have repeatedly done it in 3D and 2D cases, repeatedly discussed it. So, for density of states, please remember this please sort of make yourself understand this that in order to calculate the density of states which is the number of allowed electronic states in a material, we need to first solve the Schrodinger equation for that material.

And the Schrodinger equation solution for 1D solid would be essentially same as the Schrodinger equation solution for particle in a box. And because of the boundary conditions the wave function at x equal to L should be 0, so which means k times x should be nπ.

So, the k values $n\pi/L$, where n is any integer, n belongs to the set of integers. And in density of states, not only do we need to solve the Schrodinger equation for electron, we also need to count the number of allowed electronic states in the material.

And in order to count the number of states we make a shift to k-space. So, the k-space for 1D solid will also be a one-dimensional k-space, only one axis, and the allowed k values will be $n\pi/L$. So, the values will be these. So, this is π/L, $2\pi/L$, $3\pi/L$, and so on. Let us say, this is the x equal to 0 point; $-\pi/L$, $-2\pi/L$, $-3\pi/L$ will also be valid solutions of the Schrodinger equation, ok.

So, now, we need to calculate the number of electronic states in a range of k to k + dk. So, for that we take a linear element on the k axis. So, we take a strip of dk width only, and we will try to see how many electronic states exist in this dk length, then this will also be equal to the number of electronic states in energy range from E to E + dE and from this number we can calculate the density of states as we have done for 3D and 2D cases, ok.

So, the here the density of states will mean number of electronic states per unit length per unit energy basically. So, length occupied by one electronic state is, so the length in which one allowed electronic state exist in k-space is essentially π/L and length of the linear element that we have taken is essentially dk, the length of this is dk.

So, the number of states in the energy for k range of k to k + dk will be the length of the linear element, number of states in this linear element would be the length of the linear element divided by the length of the single allowed electronic state.

So, this will be the number of electronic states in the in this linear element of k-space in 1D solids. So, with this, now we can see that the number of states in the energy range from E to E + dE is essentially the number of electronic states in the k range from k to k + dk.

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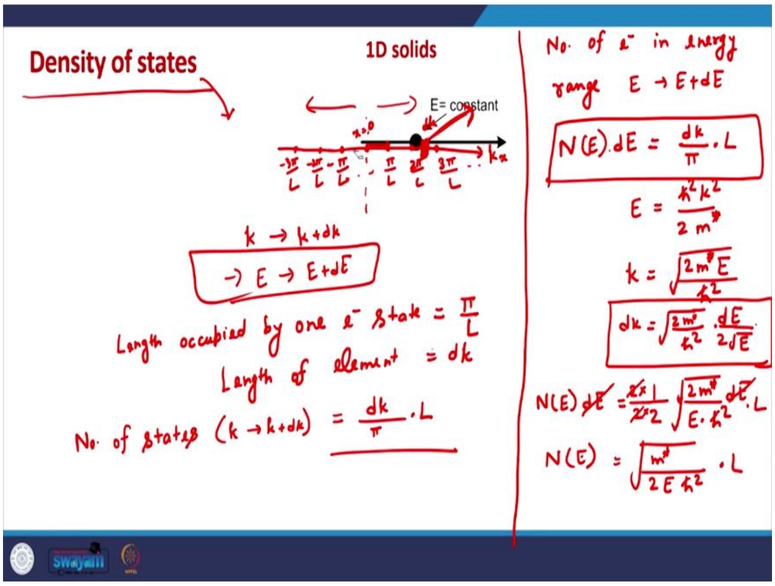

Density of states

1D solids

$k \to k+dk$

$\boxed{\to E \to E+dE}$

Length occupied by one e^- state $= \frac{\pi}{L}$

Length of element $= dk$

No. of states $(k \to k+dk) = \frac{dk}{\pi}\cdot L$

No. of e^- in energy range $E \to E+dE$

$$\boxed{N(E).dE = \frac{dk}{\pi}\cdot L}$$

$$E = \frac{\hbar^2 k^2}{2m^*}$$

$$k = \sqrt{\frac{2m^* E}{\hbar^2}}$$

$$\boxed{dk = \sqrt{\frac{2m^*}{\hbar^2}}\cdot\frac{dE}{2\sqrt{E}}}$$

$$N(E)\cancel{dE} = \frac{\cancel{2}\times 1}{\cancel{2}\times 2}\sqrt{\frac{2m^*}{E\cdot\hbar^2}}\cancel{dE}\cdot L$$

$$N(E) = \sqrt{\frac{m^*}{2E\hbar^2}}\cdot L$$

So, the number of electrons from number of electrons in energy range from E to E + dE is which is described as N(E) times dE. This will be equal to dk.L$/\pi$ and the E k relationship as we have seen is $\frac{\hbar^2 k^2}{2m^*}$ which means that k is $\sqrt{\frac{2m^*E}{\hbar^2}}$.

So, dk will $\sqrt{\frac{2m^*}{\hbar^2}}$; if we take a derivative of square root of E that will be essentially $\frac{1}{2\sqrt{E}}$ in denominator and in numerator, we will have dE. So, if we put this value of dk from here into this expression, ok. So, this number N(E).dE would be $\frac{1}{2}\sqrt{\frac{2m^*}{E\hbar^2}}\,dE$.

So, dE dE go away. Now, what we are left with is, now we need to again consider those two points as well that each point can correspond to up to 2 states corresponding to 2 different spins of the electron. So, we need to multiply by 2 and we need to divide by 2 as well, because the states for positive values of n and the states for positive negative values of n in k-space, they essentially represent the same electron, because the wave function is differed just by a global phase in these 2 states.

So, in order to avoid over counting, we need to divide by 2. So, 2 and 2 go away. So, what we are left now is with and there is a factor of L as well there, $\sqrt{\frac{m^*}{2E\hbar^2}}$L, ok. So, this N(E) parameter is the number of electronic states per unit energy, ok. So, the density of state would be number of electronic states per unit energy per unit length.

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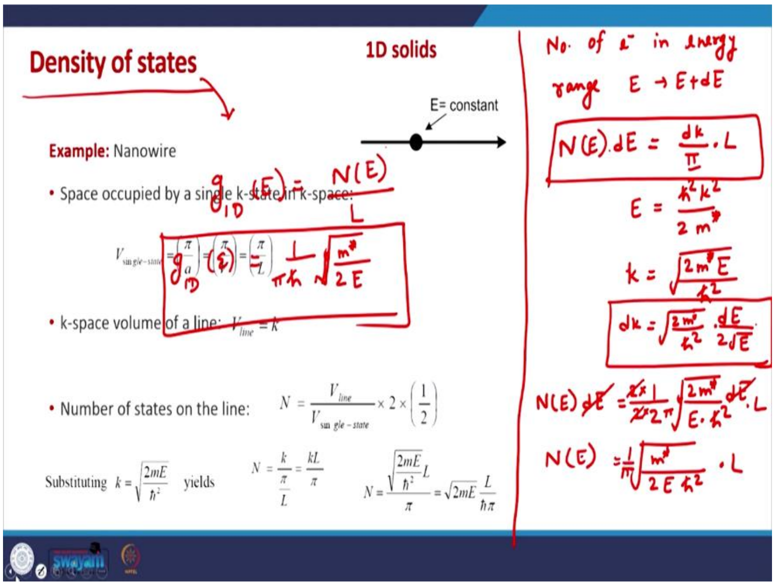

Density of states

1D solids

Example: Nanowire

- Space occupied by a single k-state in k-space: $V_{single-state} = \left(\frac{\pi}{a}\right) = \left(\frac{\pi}{\varepsilon}\right) = \left(\frac{\pi}{L}\right)$

$g_{1D}(E) = \frac{N(E)}{L}$

$\boxed{g_{1D}(E) = \frac{1}{\pi\hbar}\sqrt{\frac{m^*}{2E}}}$

- k-space volume of a line: $V_{line} = k$
- Number of states on the line: $N = \frac{V_{line}}{V_{single-state}} \times 2 \times \left(\frac{1}{2}\right)$

Substituting $k = \sqrt{\frac{2mE}{\hbar^2}}$ yields $N = \frac{k}{\frac{\pi}{L}} = \frac{kL}{\pi}$

$N = \frac{\sqrt{\frac{2mE}{\hbar^2}}L}{\pi} = \sqrt{2mE}\frac{L}{\hbar\pi}$

No. of e^- in energy range $E \rightarrow E+dE$

$\boxed{N(E).dE = \frac{dk}{\pi}.L}$

$E = \frac{\hbar^2 k^2}{2m^*}$

$k = \sqrt{\frac{2m^*E}{\hbar^2}}$

$\boxed{dk = \sqrt{\frac{2m^*}{\hbar^2}}.\frac{dE}{2\sqrt{E}}}$

$N(E)\cancel{dE} = \frac{\cancel{2}\times 1}{\cancel{2}\times 2\pi}\sqrt{\frac{2m^*}{E.\hbar^2}}\cancel{dE}.L$

$N(E) = \frac{1}{\pi}\sqrt{\frac{m^*}{2E\hbar^2}}.L$

So, we just need to divide by, in order to calculate density of states for 1D material we just need to divide N(E) by the length, ok. So, which means density of states for 1D solids is square root of $\frac{1}{\hbar}\sqrt{\frac{m^*}{2E}}$. So, this is the final expression for the density of states for 1D solids, ok.

And you might have quickly noticed it that the dependence of density of states on, yeah. So, there is I guess a factor of π as well there which we missed here, so dk, yes. So, there is a factor of π in denominator which would come from here, so $1/\pi$ and it would be ultimately $1/\pi$. So, yeah, I am sorry for missing this factor. So, there is a factor of π.

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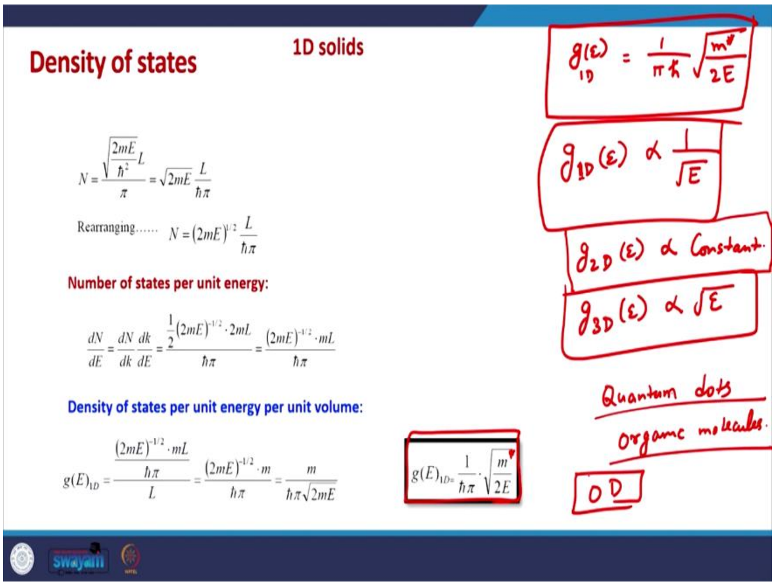

Density of states

1D solids

$$N = \frac{\sqrt{\frac{2mE}{\hbar^2}}L}{\pi} = \sqrt{2mE}\,\frac{L}{\hbar\pi}$$

Rearranging…… $N = (2mE)^{1/2}\frac{L}{\hbar\pi}$

Number of states per unit energy:

$$\frac{dN}{dE} = \frac{dN}{dk}\frac{dk}{dE} = \frac{\frac{1}{2}(2mE)^{-1/2}\cdot 2mL}{\hbar\pi} = \frac{(2mE)^{-1/2}\cdot mL}{\hbar\pi}$$

Density of states per unit energy per unit volume:

$$g(E)_{1D} = \frac{\frac{(2mE)^{-1/2}\cdot mL}{\hbar\pi}}{L} = \frac{(2mE)^{-1/2}\cdot m}{\hbar\pi} = \frac{m}{\hbar\pi\sqrt{2mE}}$$

$$\boxed{g(E)_{1D} = \frac{1}{\hbar\pi}\cdot\sqrt{\frac{m^{*}}{2E}}}$$

$$\boxed{g_{1D}(\varepsilon) = \frac{1}{\pi\hbar}\sqrt{\frac{m^{*}}{2E}}}$$

$$\boxed{g_{1D}(\varepsilon) \propto \frac{1}{\sqrt{E}}}$$

$$\boxed{g_{2D}(\varepsilon) \propto \text{Constant.}}$$

$$\boxed{g_{3D}(\varepsilon) \propto \sqrt{E}}$$

Quantum dots

organic molecules.

$\boxed{0D}$

And ultimately, the final expression for the density of states in 1D solid cells will be this. So, g(E) for 1D solids is $\frac{1}{\pi\hbar}\sqrt{\frac{m^*}{2E}}$. It should be m^* here. And you might have readily noticed that 1D density of states is inversely proportional to the square root of E, ok.

So, as the E value will increase, this g 1D will decrease essentially. And if you compare this with 2D case, in 2D case this was constant essentially. In 3D case, it was directly proportional to the square root of E. So, as you are seeing as we change the dimension, the number of states that the electrons can occupy in the material, they change, their behavior change fundamentally.

Now, the last thing that is left in density of states discussion is the density of states in 0D solids. 0D solids mean quantum dots or organic molecules. So, these solids have very small dimension in all directions which mean that electrons are now confined in a nanoscopic regime in all the directions. They are not free to move in any dimension, any direction basically.

So, for 0D solids I will let you think about this what would be the density of states for 0D solids. Please think about this, and we will discuss this in the next class.

Yeah, thank you for your attention. See you in the next class.