Electronic Theory of Solids
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Lecture - 05
Density of States: Fermi Energy, Fermi Velocity, Density of States in 1D, 2D and 3D

So let us now as I said start counting the number of states and we are after something called the density of states and from there we will calculate certain physical properties of the system. For example, we can calculate the Fermi velocity, the Fermi momentum, Fermi energy and number of particles. So, those are number of electrons and so, on density of electrons.

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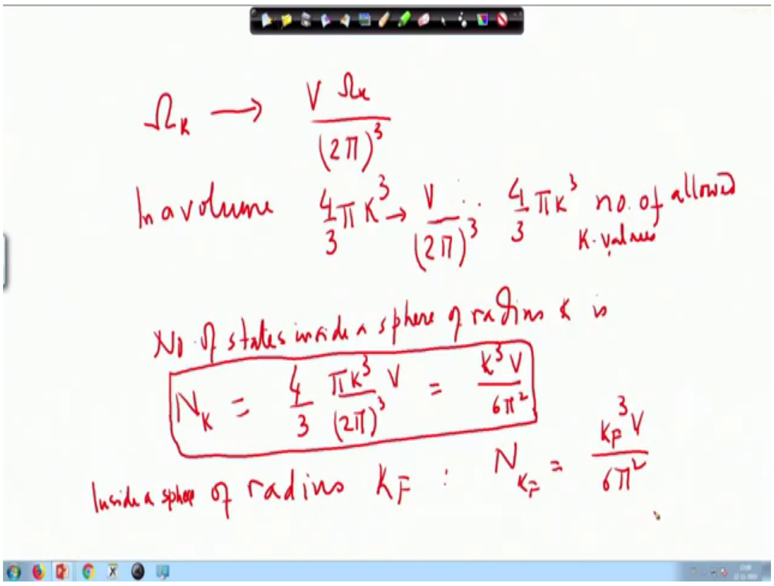

$\Omega_k \rightarrow \frac{V \Omega_k}{(2\pi)^3}$

In a volume $\frac{4}{3}\pi k^3 \rightarrow \frac{V}{(2\pi)^3} \cdot \frac{4}{3}\pi k^3$ no. of allowed k-values

No. of states inside a sphere of radius k is

$$\boxed{N_k = \frac{4}{3}\frac{\pi k^3}{(2\pi)^3} V = \frac{k^3 V}{6\pi^2}}$$

Inside a sphere of radius k_F : $N_{k_F} = \frac{k_F^3 V}{6\pi^2}$

So, let us just start doing in. Now we just showed that in a volume omega k in k space, you have V times omega k times divide by 2 pi cube number of states. So, then in a volume of a sphere which is four-third pi k cube up to a momentum k the number of states is V omega k. So, this omega k I do not required omega k is replace by this by 2 pi cube. So, that is the in a volume four-third pi k cube, the number of states is this into 4 by 3 pi k cube number of states allowed k values which is basically the states k values.

So, this is the number of states inside a sphere of radius k is just this four-third pi. So, number of states. So, let me call number of k states representing by N sub k four-third pi k cube into V by 2 pi cube. So, this gives me k cube into V by 6 pi square. So, that is the number of k values that are allowed into the is 4, 2, 6 yeah, this is k cube V by 6 pi square.

Now, this; So, inside the with the a radius of k_F, then inside a sphere of radius k_F, k_F then the number of states $N_{k\,F}$ is equal to k_F cube into V by 6 pi square. So, these many allowed k values at there in this state. Now, the interesting thing is that the electrons are spin half fermions. So, there are two spin states spin projections allowed in each state, right. So, I can put at most two electrons in each of this k-states. So, each k allowed k value actually accommodates 2 k, 2 spin states two electrons spin. So, if you counting if you also count the spin then let us call these as levels.

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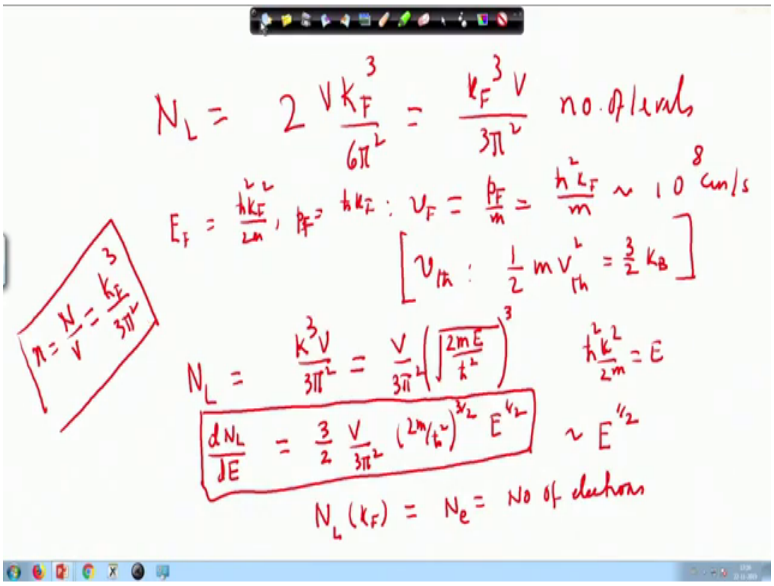

$$N_L = 2\frac{Vk_F^3}{6\pi^2} = \frac{k_F^3 V}{3\pi^2} \text{ no. of levels}$$

$$E_F = \frac{\hbar^2 k_F^2}{2m},\ p_F = \hbar k_F : v_F = \frac{p_F}{m} = \frac{\hbar^2 k_F}{m} \sim 10^8 \text{ cm/s}$$

$$\left[v_{th} : \frac{1}{2} m v_{th}^2 = \frac{3}{2} k_B\right]$$

$$\boxed{n = \frac{N}{V} = \frac{k_F^3}{3\pi^2}}$$

$$N_L = \frac{k^3 V}{3\pi^2} = \frac{V}{3\pi^2}\left(\sqrt{\frac{2mE}{\hbar^2}}\right)^3 \qquad \frac{\hbar^2 k^2}{2m} = E$$

$$\boxed{\frac{dN_L}{dE} = \frac{3}{2}\frac{V}{3\pi^2}(2m/\hbar^2)^{3/2} E^{1/2}} \sim E^{1/2}$$

$$N_L(k_F) = N_e = \text{No of electrons}$$

So, the number of levels then is N equal to 2 times this number that we just calculated k_F cube by 6 pi square into V. So, that is k_F cube V by 3 pi square. So, number of levels in that volume of k space. So, correspondingly this E_F is h cross square k_F square by twice m p_F equal to h cross k_F, then the Fermi velocity v_F is equal to p_F by m which is h cross k_F by m, ok. Now if you remember your classical velocity, this velocity is about 10 to the power 8 centimeter per second typically.

So, if you remember your classical situation, where the corresponding velocity there was the thermal velocity. So, I am just writing it thermal which we obtain from this relation that half mV square thermal is equal to 3 by 2 k B. So, that gives a root over 3 k B by m square root 3 k B by m is the thermal velocity. This much smaller compare to this velocity, this is a fairly high velocity nearly a 100 of the velocity of light speed of light.

So, this velocity is very very large and simply because you have to fill up states from the bottom and you cannot put more than 2 electrons at a lowest energy level lowest at any k value and so, you have to go on up up up up in momentum states and their energies are going up. And you actually can see that if you calculate this E_F in a typical metal, it can be anywhere between half an electron volt to 15 electron volt its so, large.

Now, if you convert that to temperature for example, 15 electron volt will be like 15 each electron volt gives you 10,000 degree Kelvin 11,000 degree Kelvin. So, you can imagine what energy is we are talking about now. So, and that is simply because of the fact that the Pauli principle prevented us from putting electrons as many as electrons as we want at the lowest energy state. We had to go up 2 is the maximum that you could do for spin half fermion, ok. So, let me just calculate something that is very useful.

Now, since N within a volume within a radius of k in sphere of radius k, there are k cube V by 3 pi square number of states, I can write this as 3 pi square into k is h now we know that h cross square k square by twice m equal to E. So, this basically 2 mE by h cross square. So, that is the, to the power. So, that is cube. So, I have to take a cube of that ok. So, now what I can calculate easily is this number dN_L dE and this will give me a number which is 3 by 2 V by 3 pi square into 2 m by h cross square to the power 3 by 2 into E to the power half.

So, that is the number of you can simplify it and, but the important thing is that the density of this the; so, this is the number of levels available between 2 energy is E and E plus dE and this goes as E to the power half. So, that is a very important relation that in three-dimension for a quadratic spectrum, the density of state goes as E to the power half root over of E.

Now, the interesting thing is that if you look at this. So, the number of if I take my k up to or E up to E_F, then this N L up to k_F is actually the same as the number of electrons; number of electrons. Because I have put in 2 electrons in each of this occupied k states, each of these case states that them going to occupy and then that is the total number of electrons. So, the number of levels gives me the number of electrons. This factor of 2 comes when you count the number of levels, number of states you do not count the two, but then you multiply by 2 to get the number of levels which is the same as the number of electrons.

So, from that you can actually figure out that the density is N by V is equal to k_F cube by 3 pi square that V is gone ok.

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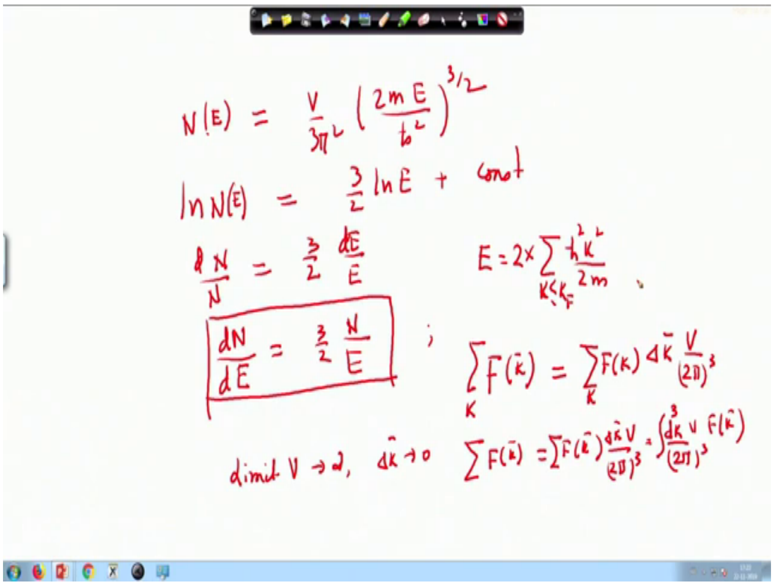

$$N(E) = \frac{V}{3\pi^2}\left(\frac{2mE}{\hbar^2}\right)^{3/2}$$

$$\ln N(E) = \frac{3}{2}\ln E + \text{const}$$

$$\frac{dN}{N} = \frac{3}{2}\frac{dE}{E}$$

$$\boxed{\frac{dN}{dE} = \frac{3}{2}\frac{N}{E}}\ ;$$

$$E = 2\times\sum_{k<k_F}\frac{\hbar^2 k^2}{2m}$$

$$\sum_{k} F(\bar{k}) = \sum_{k} F(k)\,\Delta\bar{k}\,\frac{V}{(2\pi)^3}$$

dimit $V \to \infty$, $\Delta\bar{k} \to 0$ $\sum F(\bar{k}) = \sum F(\bar{k})\frac{d\bar{k}\,V}{(2\pi)^3} = \int\frac{d^3k\,V}{(2\pi)^3}F(\bar{k})$

Now the other another interesting relation you can find out is that N up to an energy E; N up to an energy E is as we just mentioned is V by 3 pi square into 2 m E by h cross square to the power 3 by 2. So, they are you are feeling you have to highest field level is at E, your counting the number of electrons up to an energy E. So, that is basically the this and then what you can do is the take log on both sides, log of N of E equal to whatever comes here you do not bother is 3 by 2 log of E plus constant, these are all constant terms h cross square m V 3 pi square.

Now, take a just derivative. So, dN by N is equal to 3 by 2 dE by E so; that means, dN by dE equal to 3 by 2 N by E. This is a very useful relation; I mean, this is a same this relation is also this tells you the number of electrons up to an so, the act. So, in this is basically again the density of states; number of states between E and E plus d E and that is now express in terms of N and E. Now you can bring your N and E from the previous expression and E by N can be calculated using other quantities like E_F k_F and so on, ok.

So, let me see what we want to do now is that, if once we have the volume of the in the case space and the density of states, we can calculate the certain quantities. For example, we can calculate the total energy how much is the total energy? It is basically h cross square k square by twice m, sum over k up to k F right and then of course, multiply by the spin degeneracy..

So, that is what we want to calculate and then I will show you where this density of states can become useful. So, let us just take any function of k, F of k and we want a summation, right. So, this is basically the same as F k into delta k. If delta k is a volume in the k space, then what. So, this is an identity because the number of states inside the volume delta k is basically are basically this. Delta k divided by 2 pi by l cube which is V by 2 pi cube.

So, now, take limit V going to very large, which means delta k is very small. So, delta k in going to 0 limit and then you can just write this as sum over F k equal to F k delta k V by 2 pi cube equal to dk; so, d 3 k by 2 pi cube into v to F of k.

So, this can be converted to an integral. So, to calculate this, now I can use this one in instead of summation overall the k states I have to keep counting the k values. All these, I will not do that because that is a 2 tedious and that is not possible at in some at some in some situations. And so, I will just take the density of states and I know how many density of states lie in a interval k and k plus d k and that is what we just do.

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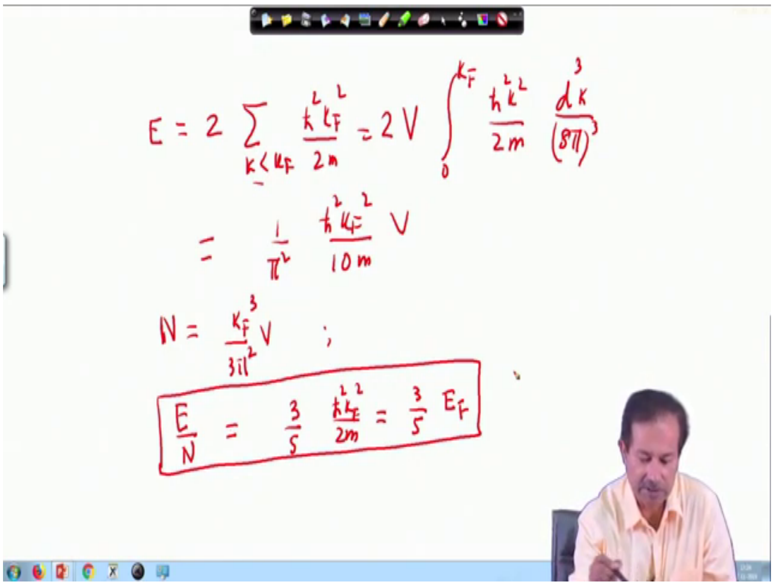

$$E = 2\sum_{k<k_F} \frac{\hbar^2 k_F^2}{2m} = 2V\int_0^{k_F} \frac{\hbar^2 k^2}{2m}\,\frac{d^3k}{(8\pi)^3}$$

$$= \frac{1}{\pi^2}\,\frac{\hbar^2 k_F^2}{10m}\,V$$

$$N = \frac{k_F^3}{3\pi^2}V \;;$$

$$\boxed{\frac{E}{N} = \frac{3}{5}\,\frac{\hbar^2 k_F^2}{2m} = \frac{3}{5}E_F}$$

So, exactly what I just did. So, then; that means, 2 times k less than k F h cross square k F square by twice m equal to V integral 0 to k F h cross square k square by twice m into that that volume element divided by 8 pi cube. So, counting states is actually quite useful, now I am what I have done is that, I have just replace the sum by an integral at over a volume in k space and that volume contains how many k values I know. So, that is what I have just done and this basically is the result.

And now d 3 k is k square dk, so, 4 pi k square dk I will put that in and at the end of the day we will find there is this factor of 2 for spin degeneracies. So, I will calculate this, you can go ahead and calculate it and you will find that this is 1 by pi square h cross square k F square by 10 m into V.

Now, we also know that N is equal to k F cube by 3 pi square into V, then it is easy to show that E by N from this 2 relations is equal to 3 by 5 h cross square k_F square by twice m equal to 3 by 5 E $_F$. So, this is a very useful relation, this tells you the energy per particle on an average, energy per particle is like three fifth of the Fermi energy of the system. So, let me recap what I did. So, what I did is that I calculated the first let me just go back to some slides and look at this slide.

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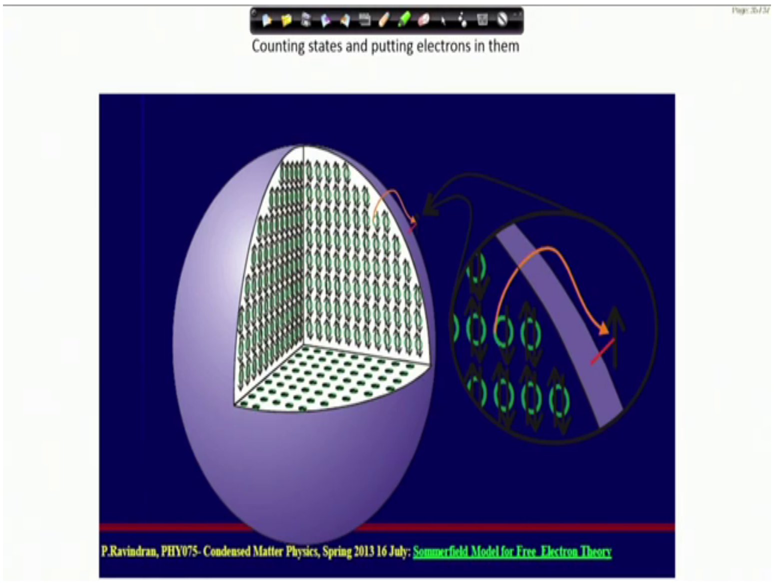

Counting states and putting electrons in them

P.Ravindran, PHY075- Condensed Matter Physics, Spring 2013 16 July: Sommerfield Model for Free Electron Theory

So, this is what I actually did. I this is this k space, ok. Now, in this k space the occupied states look like a sphere as I said. So, this is the sphere that you can see the sphere, this sphere is now opened to this sphere has been opened up and a one-eighth of it is shown and you can see that this dots these green dots are your k states and this circles, small green circles or this dots are the allowed k values. Each of these allowed k values are filled up by 2 electrons they are occupied by 2 electrons.

So, you keep on increasing it, keep on increasing it similar and then you just complete your feeling n all the n electrons are now occupying some k state starting from the lowest one and then these sphere that you are obtained is the Fermi sphere. So, this is the sphere in the case space that is the last occupied surface and that is as I said is called the Fermi surface.

It separates the on the unoccupied states are outside this sphere, occupied states are inside this sphere. So, that is the sphere of last occupancy it separates the unoccupied from the unoccupied. And it is now this on the side is a bigger picture, this one shows that this one for example, these are shown how you actually put each of this greens circles contain this.

So, example this green circles contain 2 electrons each and if you want to excite an electron from this state, this ground state. The ground state was where everyone was filled up every state was allowed k values where filled up by 2 electrons each to excite now all you have to do is take an electron outside this surface. Because inside the surface every state is filled up outside the surface there are states which as same thing.

So, to generate an excitation of this system, you have to take an electron and then take it outside the sphere. As you can see there the last electrons which are at E_F, they are at the Fermi surface for them the amount of energy required to excite is excitingly small. But the once which are deep down somewhere sorry, somewhere in the down here, for them you have to give this much of energy to pull them out of the Fermi surface.

So, this from here to here that much of an energy is required if you want to pull out an electron from here, but for an electron close to the Fermi level or at the Fermi level, you require almost 0 energy to excite, that is a very important concept in the for theory of electrons. And so, this kind of pictures will emerge at every stage for example, if I want to calculate the specific heat, what do I do? I give some heat energy and then try to see, which are the electrons which take the energy and how much energy is take it taken? Suppose, I give a small amount of energy, then only these states will be excited.

If I want to excite a state from here I have to give huge amount of energy. So, that is the kind of physics that we will discuss in the next class. But, this is a beautiful illustration of how to count the states and put the electrons in the respective states starting from 0 from the lowest energy state and fill up a so, called Fermi surface. So, Fermi volume and fill up all the states below the Fermi surface to get the ground state and then the excitations are just almost zero energy is required to excite an electron, sitting at the Fermi surface to go to a state which is just higher then the Fermi surface which is unoccupied.

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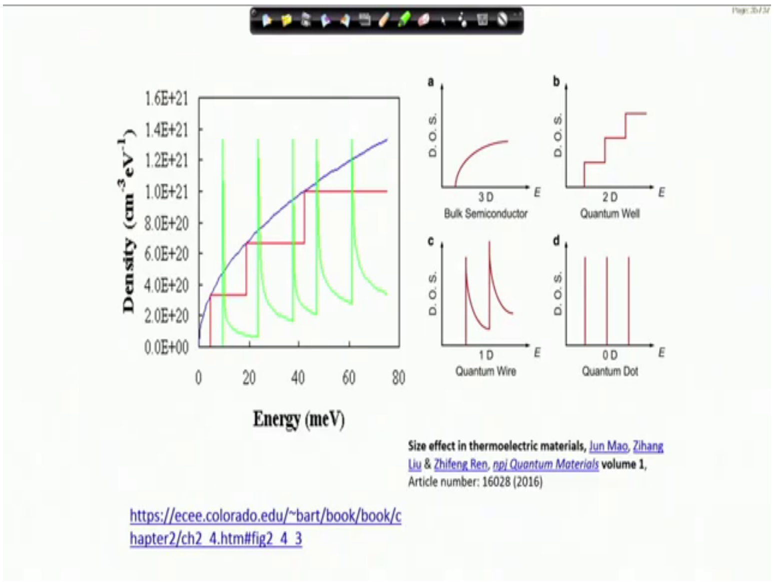

Size effect in thermoelectric materials, Jun Mao, Zihang Liu & Zhifeng Ren, *npj Quantum Materials* **volume 1**, Article number: 16028 (2016)

https://ecee.colorado.edu/~bart/book/book/chapter2/ch2_4.htm#fig2_4_3

So, for example, if you look at this few graph then there are density of states shown here in for different real systems different systems. For example, this as I said this blue curve as you can see is this square root; it goes as square root of energy. So, this is for the three-dimensional case I just worked out. Now, I leave it as a problem for you to work for what happens when you have a two-dimensional system? You will see that in two-dimension the density of states will become independent of energy.

So, it has no dependence on energy and that is something that you should be able to calculate, because now you have a surface rather than a rather than a volume. And, in this volume you will be able to calculate the density of states which will turn out to be energy independent it is just a constant the basically m by pi h cross square.

In one dimension something happens a in one-dimension as you can seen that the these are like spikes and so, these are. So, these are these spikes are like the comedown as this is the density of states. So, this spikes are different energy states at each energy states between 2 energy states, the energy dependence of the density of states is 1 over root omega. So, e to the power minus half and that is interesting because that has a singularity at energy going to 0.

So, it diverges as E goes to 0 and that has a strong effect in many one-dimensional systems many physical phenomena in one-dimension reflect this strong singularity of the in this singularity of the is not a strong singularity, but it is a say singularity in the density of state. So, that is reflected in many of the properties.

The this is quantum dot basically zero-dimensional object here of course, there are only energy levels and these energy levels are basically represented by this kind of delta function, kind of line just a single line at a particular energy. So, that is the density of states for zero-dimensional object which is basically quantum dot.

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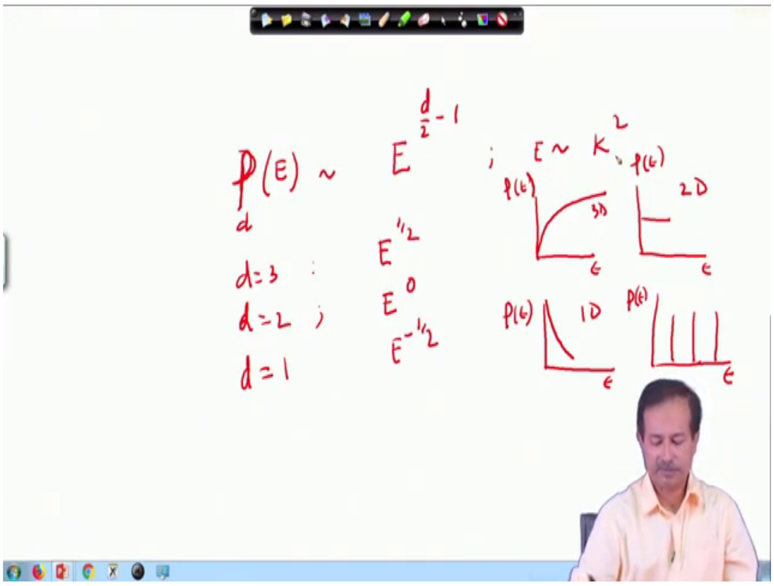

In general the density of states if you calculate the way I just did, you will find that the calculation will give you the density of states as, suppose I write this is as a rho of E which is basically dN d E in a dimension d, typically goes as E to the power d by 2 minus 1 when E goes as k square.

So, this relation basically is what I just showed you that in 3 d, d equal to 3 this is E to the power half, d equal to 2 this is E to the power 0; that means, independent of energy d equal to 1 it is E to the power half minus 1. So, 1 by 2 minus 1 which is minus half; so, this is like square root, the 3 D. 2 D is constant and that step like structure I was showing was basically for different bands, the different steps, the different this straight regions. So, this is 2 D, this rho E versus E rho E versus E and in 1D of course, there is a huge pileup of density of states at E equal to 0 and it goes as 1 by square root of E.

So, this density of states; see the three-dimensional is the most well behaved density of states as you go up in the energy its order of the comes nearly constant. Two-dimension is just constant nothing happens here, but one-dimension has this 1 over E to the power half dependence which causes important effect, which will discuss at some point in the future. Zero-dimension of course, is so, this is 1D and zero-dimension is of course, the levels there just levels at those energies corresponding allowed energies and that is how the density of state looks like, ok.

So, we will discuss the consequences of all of these at suitable point. We will stick to 3 dimension systems for the time being and when time comes we will discuss 3 D, 2 D or lower dimensional systems. For now as a home work you can work out for the 2 D with this kind of a spectrum E versus k square, ok.

Thank you so much.