Condensed Matter Physics
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Lecture - 09
The Free Electron Theory of Metals-Worked Examples

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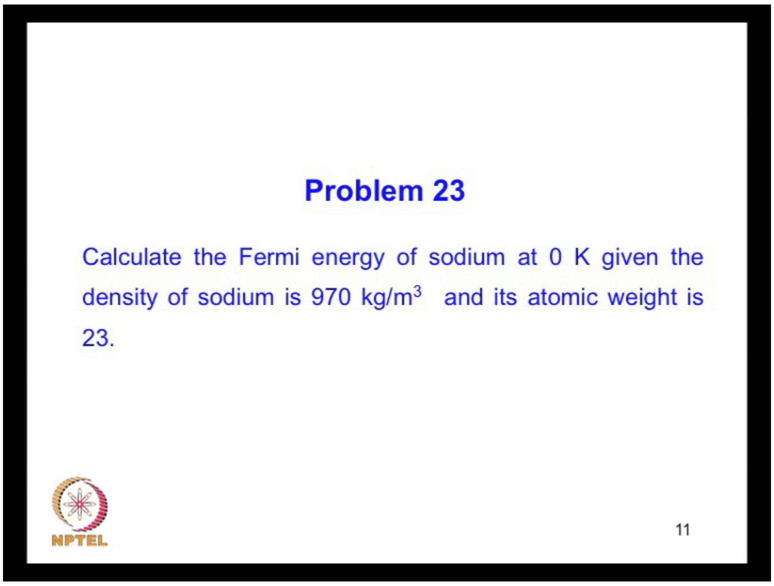

Now, we will move on to some questions relating to electrons in solids, the free electrons in metals in particular.

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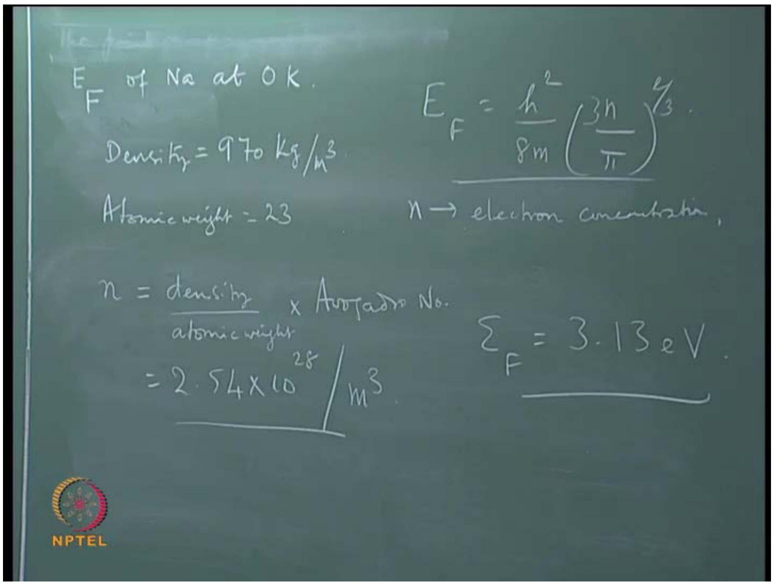

The problem that we will discuss is we are asked to calculate the Fermi energy of sodium at 0 k, where given the density of sodium is 970 kilograms per meter cube, and the atomic weight is 23 as we know. We know that the basic expression for the Fermi energy is h square by 8 m into n by pi to the power 2 by 3, where n is the electron concentration, 3 n by pi.

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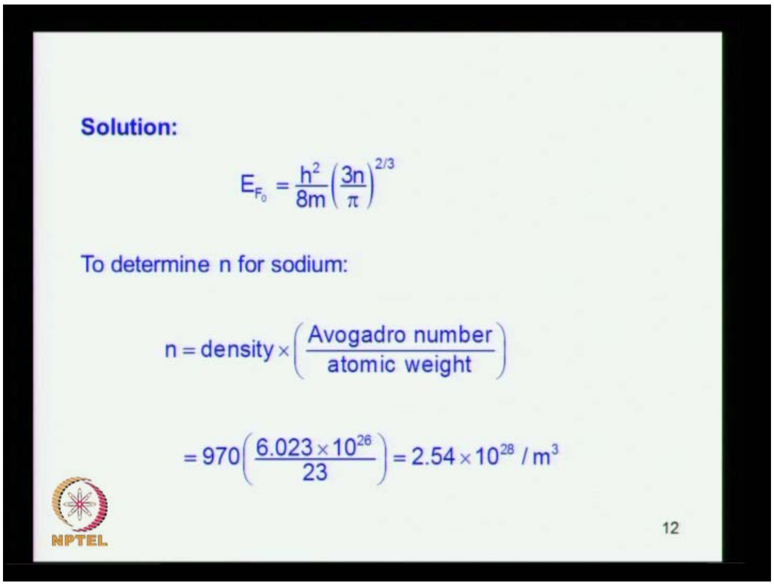

So, we are required to find n for which we take the density and divide by the atomic weight and multiplied by Avogadro number. And that the density and the atomic weight are given here, Avogadro number is known the result of this calculation is 2.54 into 10 to the power 28 electron per meter cube. We are assuming that is in sodium is monovalant that this is really the number of atoms per in unit value and assuming that each atoms donates one conduction electron, we get the number of electrons per unit volume as this.

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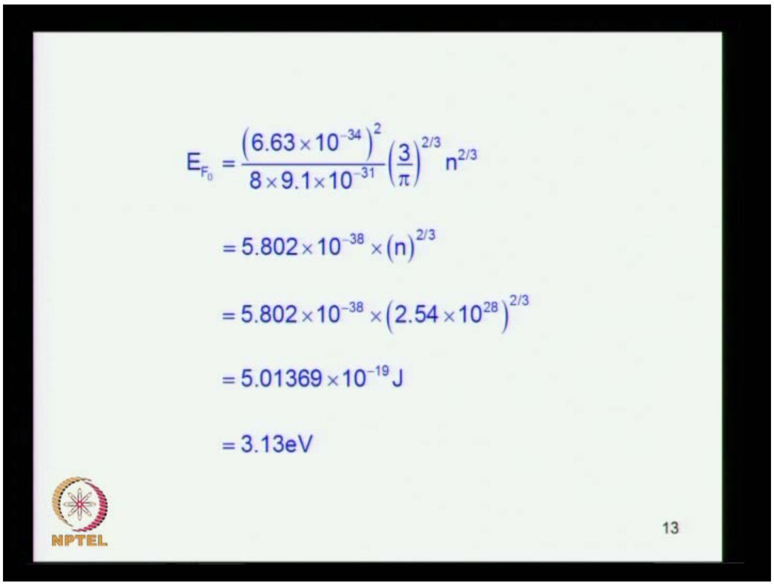

And therefore, substituting this value of n, we get the Fermi energy as 3.13 electron volts this is a just a question of substituting this expression is. So, that is the Fermi energy of sodium at zero Kelvin.

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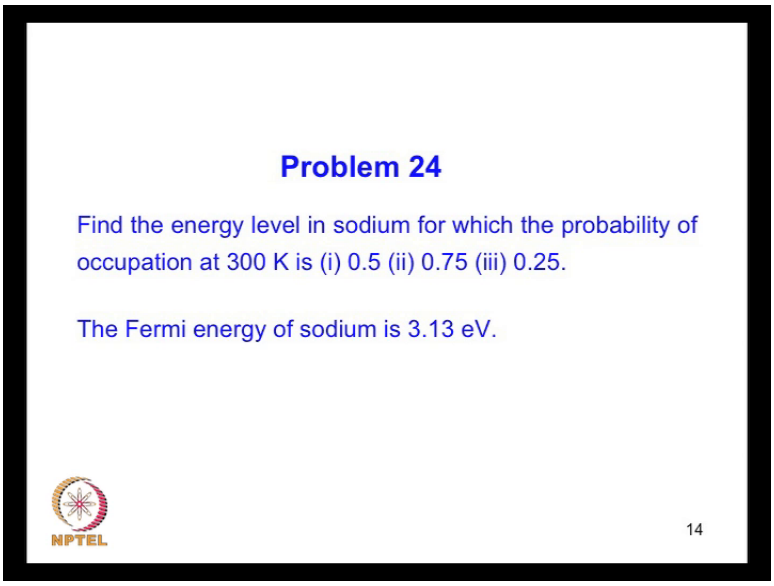

In the next problem, we again deal with sodium we are asked to find the energy level in sodium at absolute zero, no, not at absolute zero.

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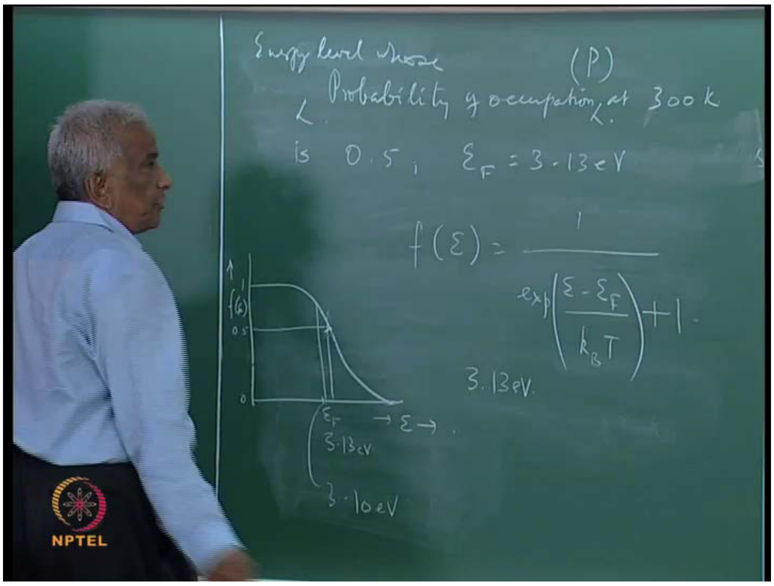

But probability of occupation of this energy level at a temperature of 300 Kelvin is 0.5. Energy level whose probability of occupation since here from given the result of the previous problem that E f the Fermi energy at zero k is at 3.13 electron volts. For this we go back to the Fermi Dirac distribution function which finite temperatures as they form like this, we have discussed all these already. So, that is the shape of Fermi Dirac distribution function and therefore, we know that the probability of occupation at 300 k becomes half exactly at the Fermi level.

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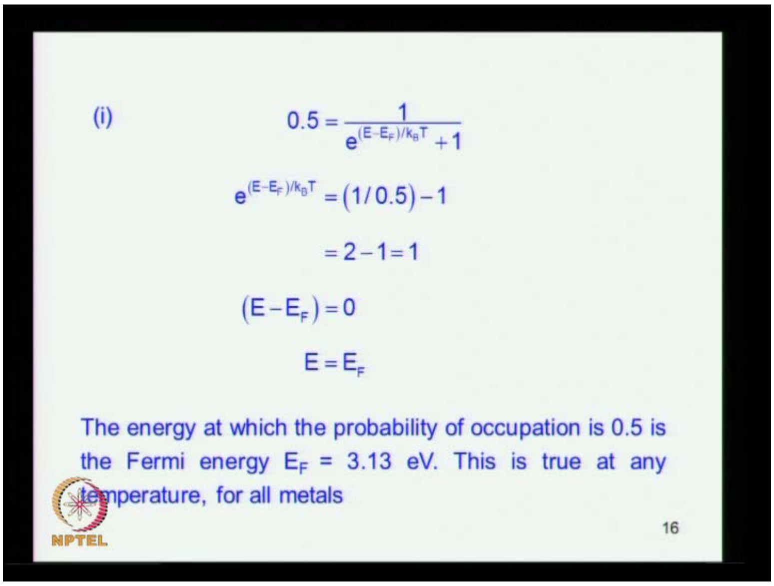

So, we can find this we can readily see that this has to be at an energy of 3.13 electron volts.

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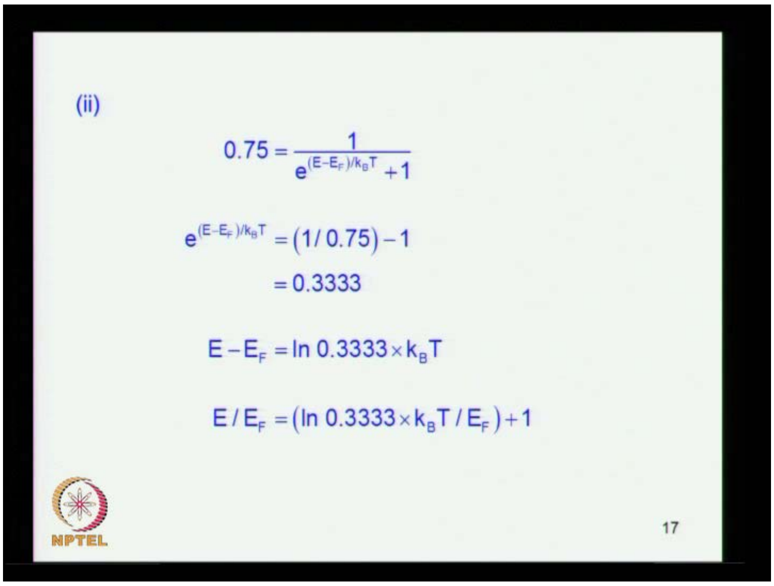

This is true in general of all metals. The value of half for the probability of half occupation occurs at the Fermi energy. In the same way, we can find the values energy at which the probability of occupation becomes for example, 0.75.

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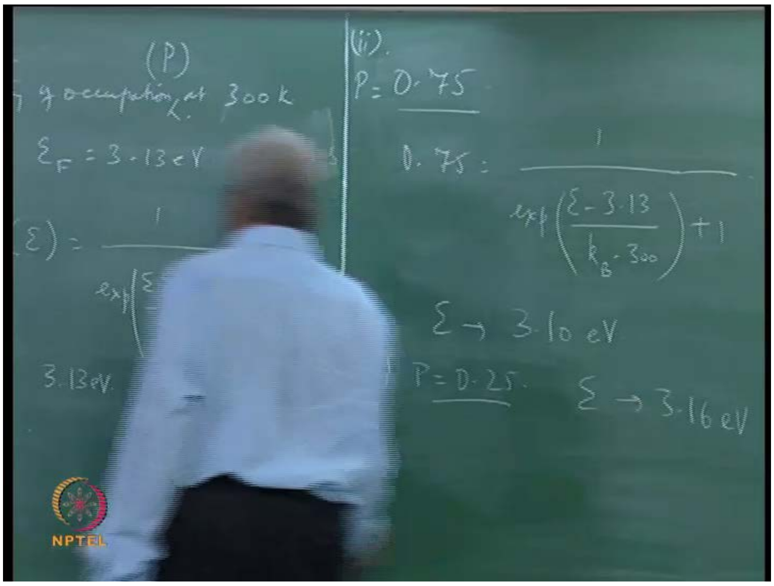

So, that is the second question we have to find. So, substituting 0.75 equal to 1 by exponential e minus 3.13 by k B into 300 plus 1 substituting in this we can readily see that the E happens to be something like 3.10 electron volts.

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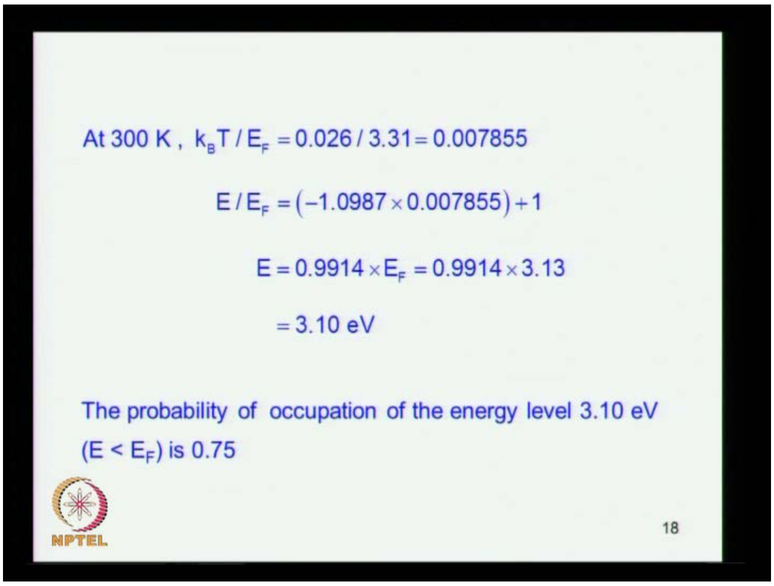

And that would be this is 3.13, and this will be somewhere here 3.10 electron volts in which we have a probability of occupation of 0.75. The next question concerns the same value for energy level for which the probability is 0.25.

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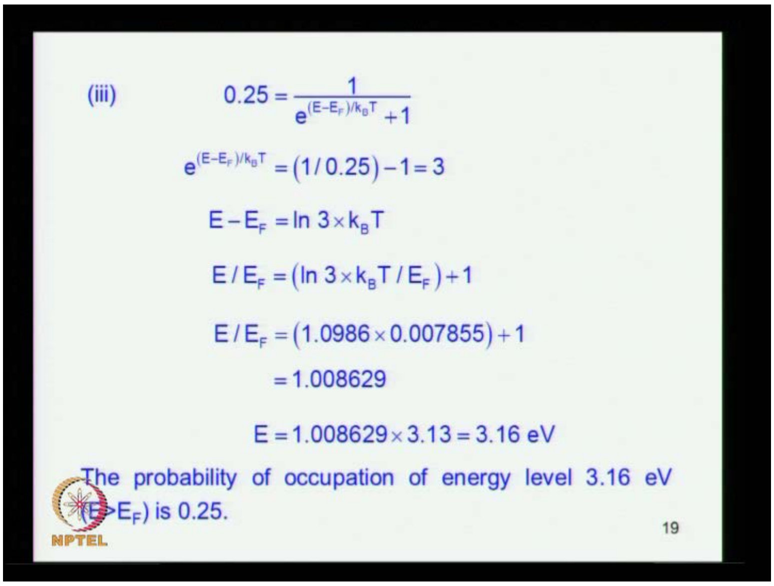

And for following same procedure, we find the corresponding energy is 3.16 electron volts. In other words, we have the Fermi tail here and it is slightly above the Fermi level this is 3.16 electron volts and that is where the probability reduces further from 0.5 to 0.25, but still it is non-zero. So, states here are occupied with a probability of one-fourth.

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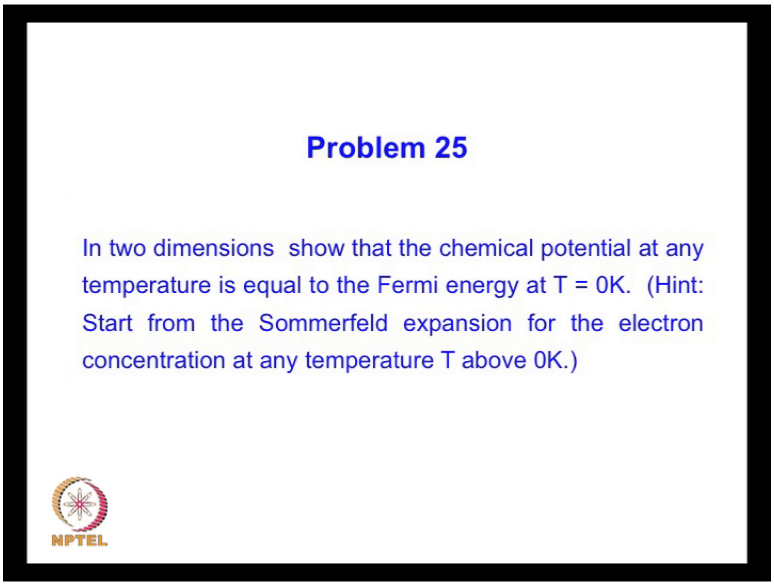

The next problem is about the chemical potential in two dimensions are at any temperature for the electron gas.

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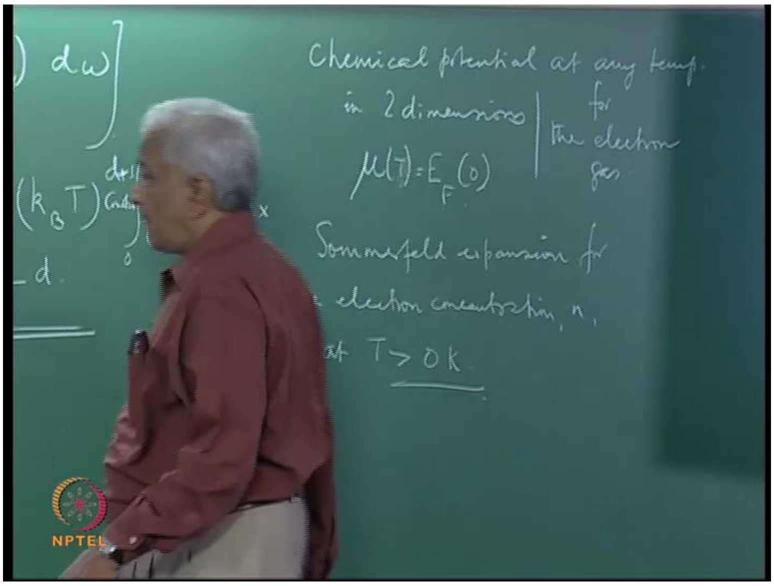

And we are required to prove this is the standard symbol, for this is mu and this is we are required to prove that this is equal to E f zero at this is the Fermi energy at T equal to zero k this is mu of t mu at any temperature. So, in order to prove this, we have to start from the slope called Sommerfeld expansion for the electron concentration in at any temperature T.

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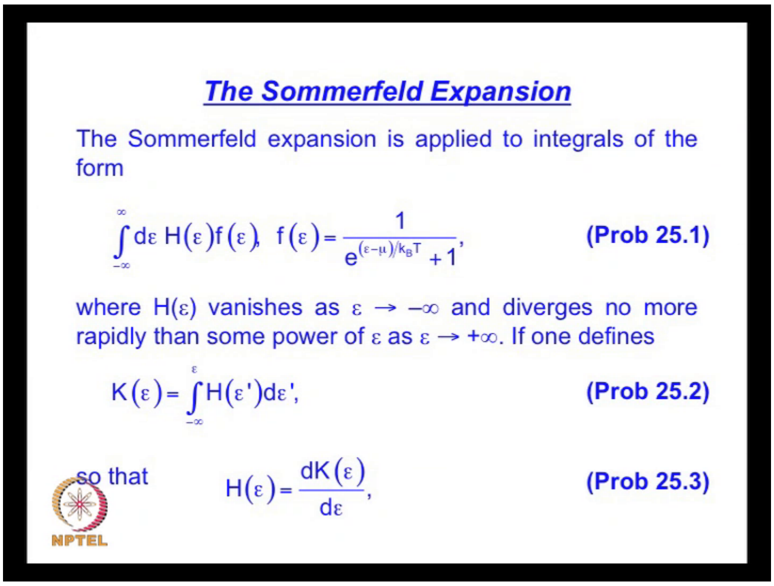

So, what is the Sommerfeld expansion?

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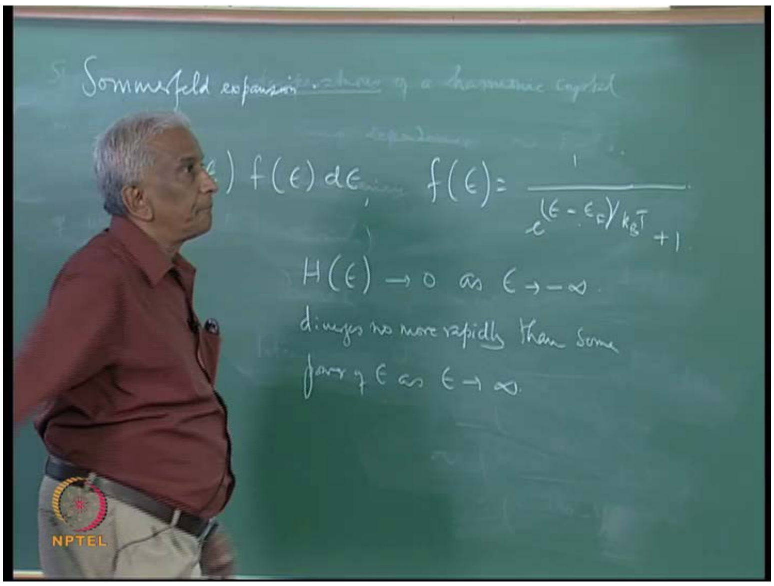

Let us consider this before answering the question. So, let us discuss the Sommerfeld expansion. In order to use this the concerned integrals of the form H of E F of E d E from minus infinity to plus infinity, where F of E is the Fermi derived distribution function and the function F of E tends to zero or vanishes as E tends to minus infinity, and diverges no more rapidly than some power of epsilon as epsilon tends to infinity.

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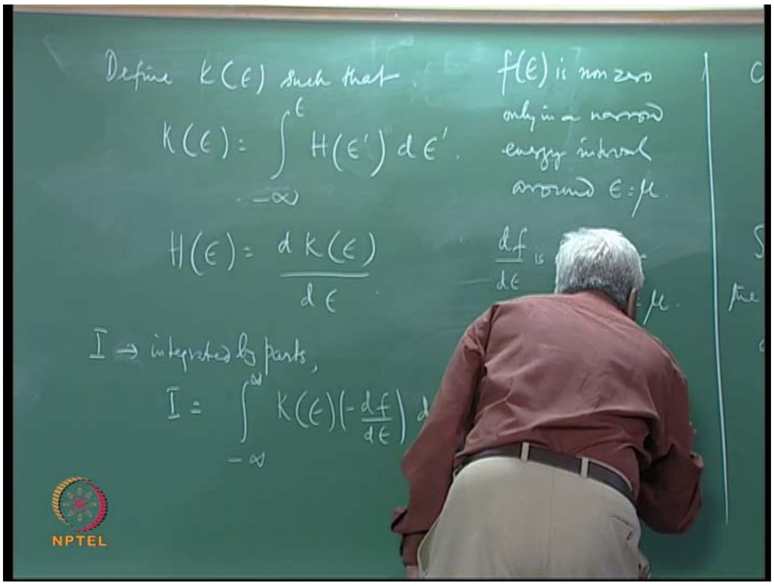

So, if it is so then let us define another function k of function epsilon define function k of epsilon such that k of epsilon equals integral zero to epsilon H of epsilon prime d epsilon prime. In other words, H of epsilon is just d k of epsilon by d epsilon. With this definition, now let us go back to let us call this integral I, then this integral maybe integrated by parts, and get we get I equal to the first term will go to zero. So, we will have integral minus infinity two plus infinity k of e into minus d f by d e times d e. Therefore, the d f by d e is large only around e equal to mu.

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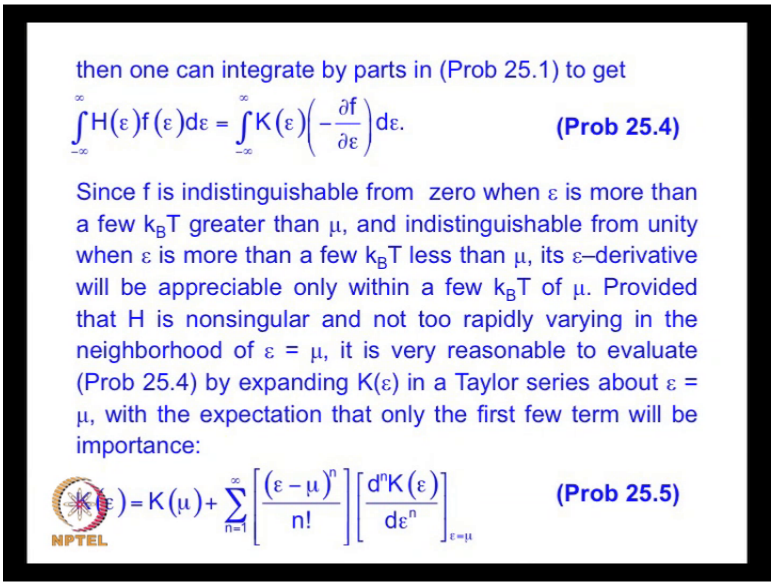

Therefore what do we do, we expand therefore, expand k of e as in a Taylor series at epsilon equal to mu in this integral I.

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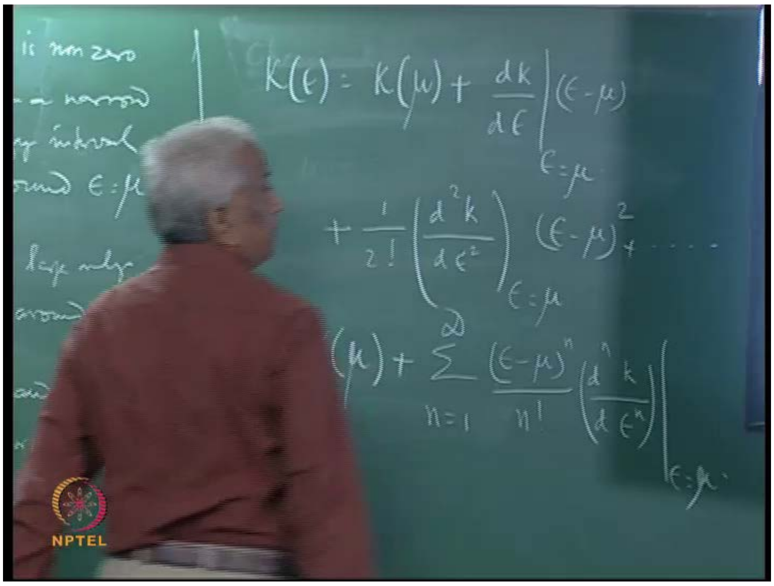

So if we do this, we get things like K of e equals K of mu plus d K by d epsilon e equal to mu times epsilon minus mu plus 1 by 2 factorial d square k like d epsilon square at epsilon equal to mu times epsilon minus mu hole square plus terms like this. So, in general, we can write this as k of mu plus the sum from over n equal to one to infinity of epsilon mu minus mu to the power l by n factorial into d n k by d epsilon n evaluated at epsilon equal to mu.

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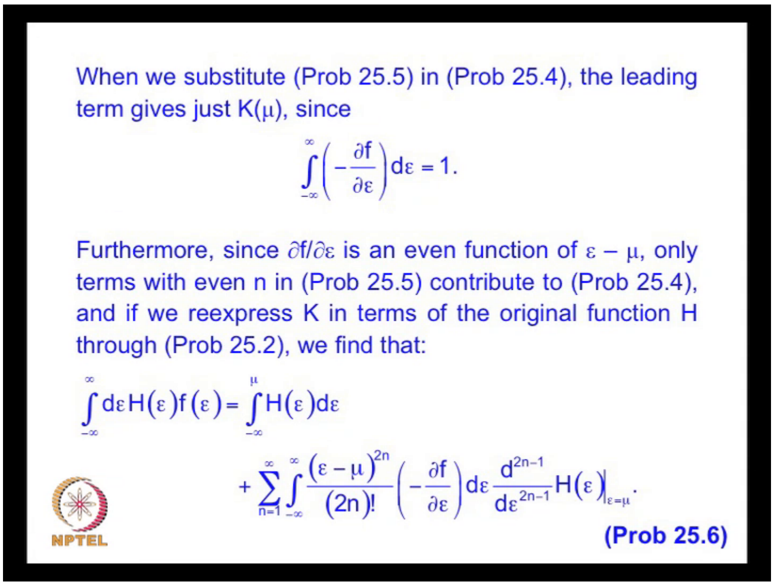

So, this is what we are going to substitute here.

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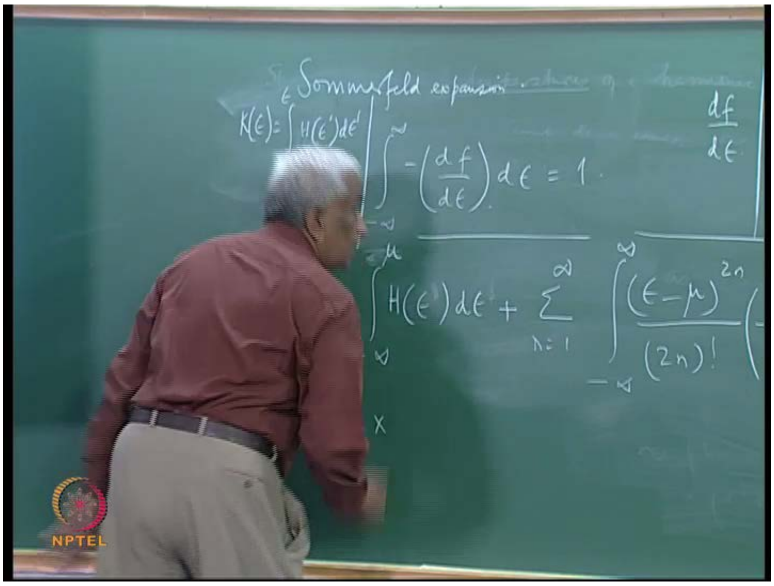

In integral has we also take into account, in fact, this is the delta function with a value one from minus infinity to plus infinity, this is an even function.

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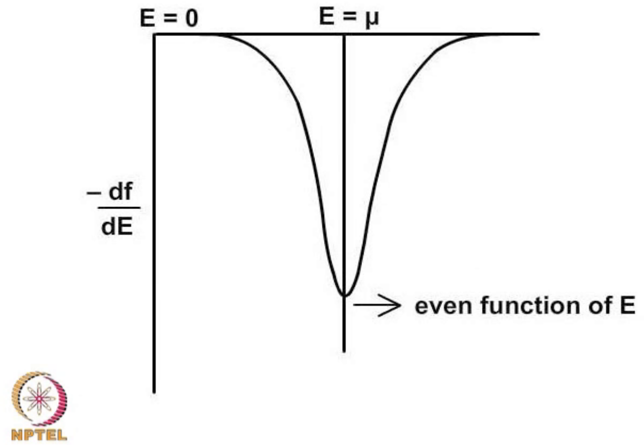

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So it is look like this, so that would be d f by strictly it becomes in the related becomes delta function. So, we use this property therefore, it is a even function of epsilon. Therefore, in this integration over E, we have only left with terms, which are even n. So, taking only those terms we can write the integral required integral as we have the definition that k of E is integral using that. So, the first term will be k of mu. So, this will be a minus infinity to mu that will be the first term plus sigma n equal to 1 to infinity of the integral minus infinity to plus infinity epsilon minus mu, we considered only even terms. So, with the power 2 n and 2 n factorial here into minus d f by d E into d 2 n minus 1 by d epsilon 2 n minus 1 of k evaluated at epsilon equal to mu, times and this is H because I have written 2 n minus one here. So, this is the final result which we can now integrate.

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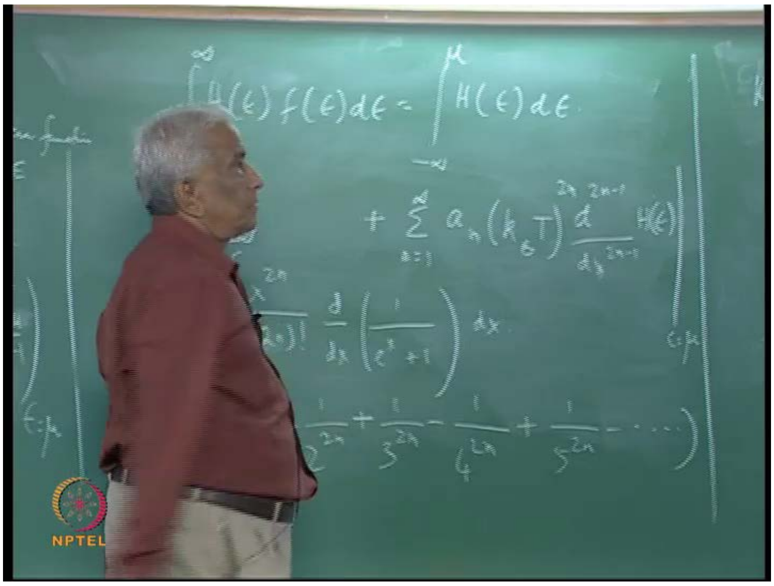

So, we finally, make the substitution epsilon minus mu by k b t as x because that is what is occurring in the derivative of the Fermi Dirac function.

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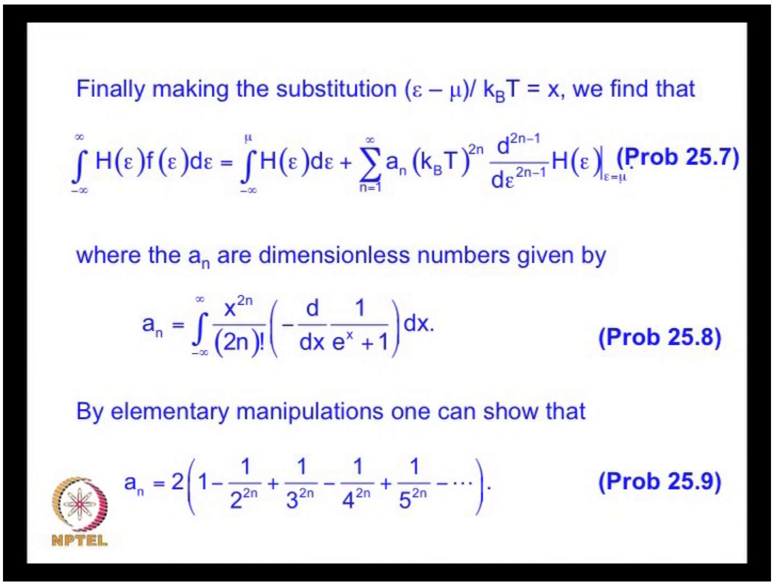

Therefore, we get the integral finally as integral minus infinity H of e F of e d e equals plus sigma n equal to 1 to infinity of a n times k B T to the power 2 n into d to the power 2 n minus 1 by d x to the power 2 n minus 1 of H of e epsilon evaluated at epsilon equal to mu. Where a n as the integral of the form x to the power 2 n by 2 n factorial into d by d x of 1 by e to the power x plus 1 d x . So, one can show that this this integral can be evaluated and we arrive at 2 into 1 minus 1 by 2 to the power n 2 n plus 1 by 3 to the power 2 n minus 1 by 4 to the power 2 plus 1 by 5 to the power 2 n and so on. This is a standard result, which we will assume here.

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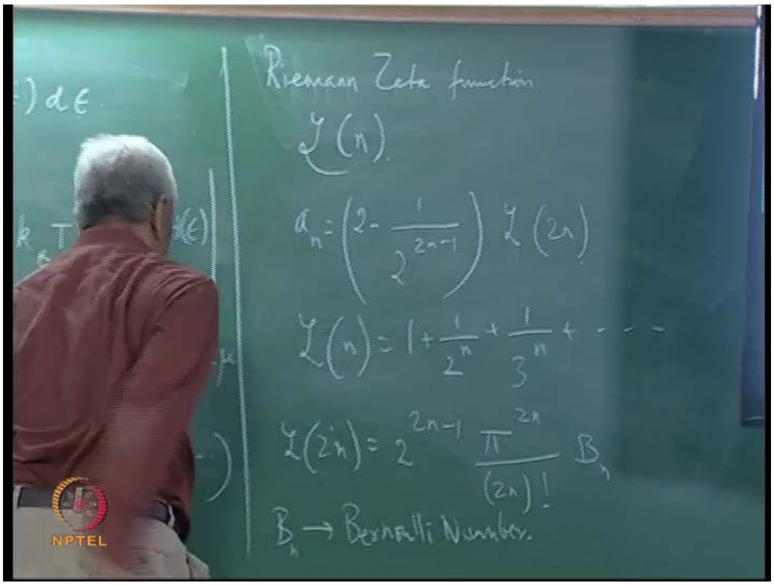

So, this is written usually in terms Riemann zeta function.

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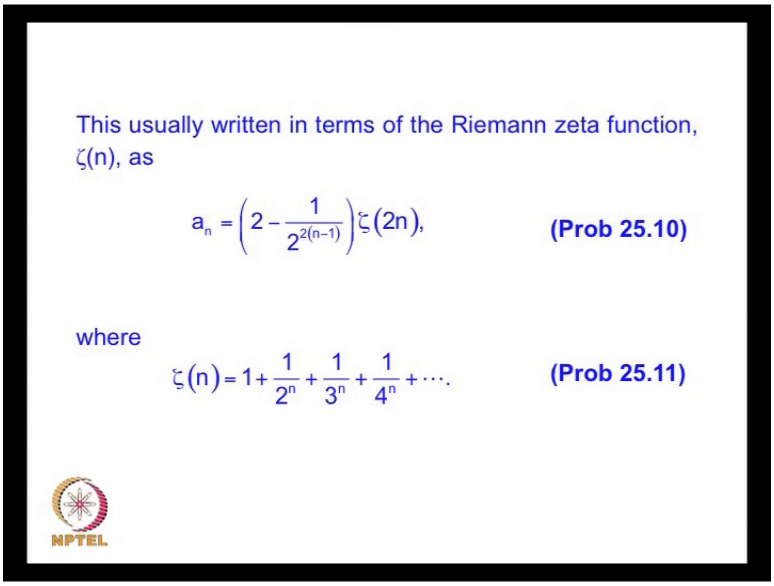

Zeta of n, so we write a n as 2 minus 1 by 2 to power 2 n minus 1 into zeta of 2 n. Where zeta n is 1 plus 1 by 2 to the power n plus 1 by 3 to the power n plus etcetera.

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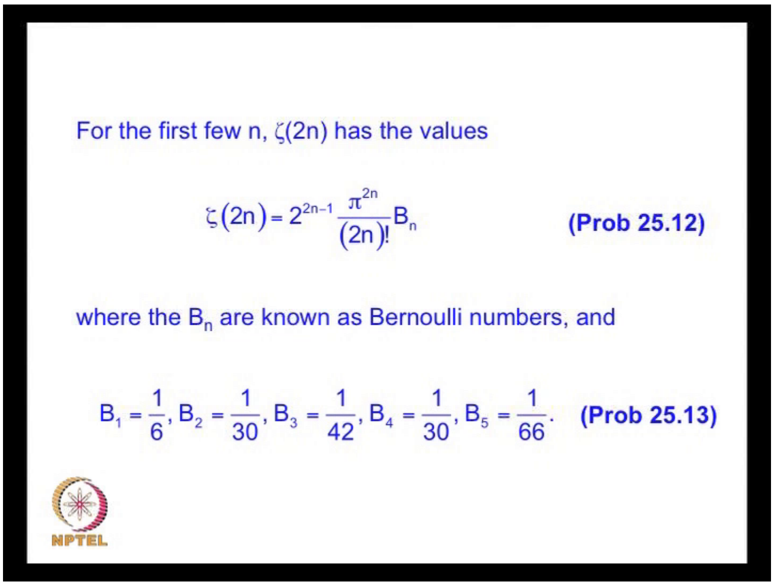

So, this can be evaluated, so zeta 2 n in general as the form 2 to the power 2 n minus 2 times pi to the power 2 n by 2 n factorial into B n, where B n is known as the Bernoulli number.

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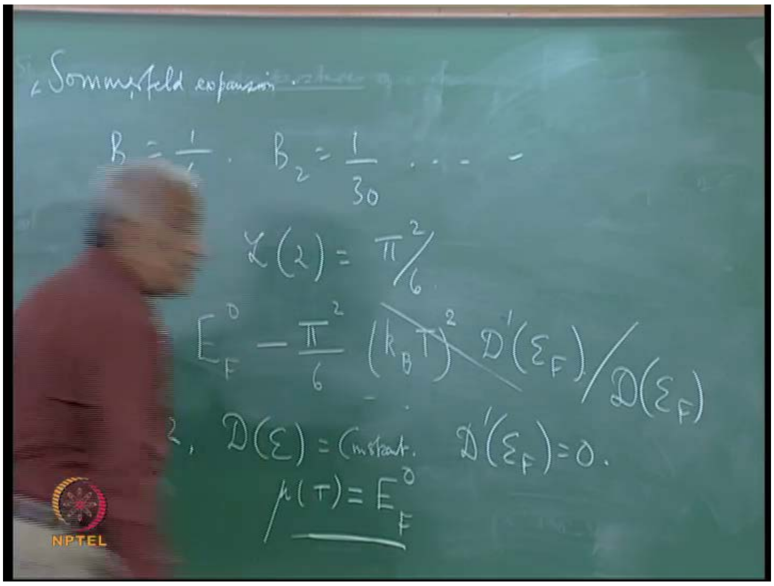

So, this Bernoulli number as the following values B 1 for n equal to 1 is just 1 6; B 2 is 1 by 30 and so on. So, these are known standard results. So, in most practical calculations in metal physics, we need to know rarely more than zeta two zeta 2 the Riemann's zeta function is just pi square by 6.

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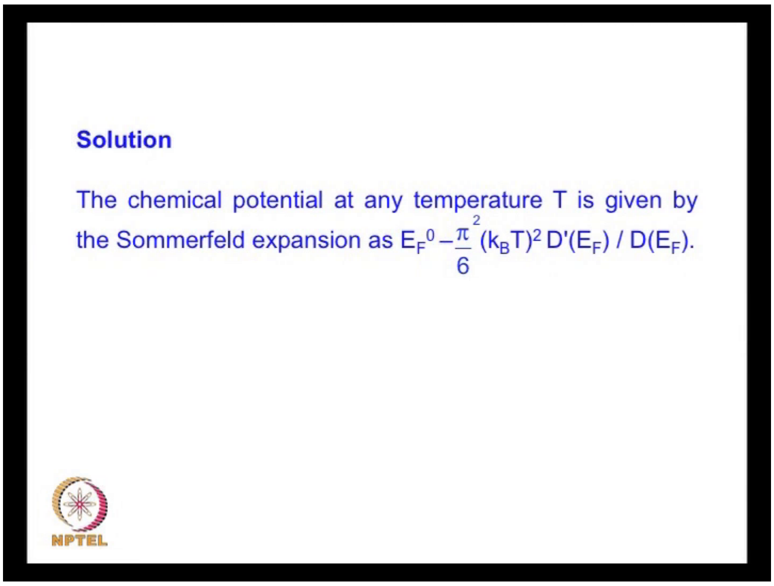

So, using this result we get the chemical potential mu at any temperature T as E F 0, the chemical potential or the Fermi energy and absolute zero minus using the expansion Sommerfeld expansion and truncating it in the first term pi square by 6 k B T whole square into D of E F where D of E F is the density of states D dash by D E F. Where D dash D E F is derivative with respect to the energy.

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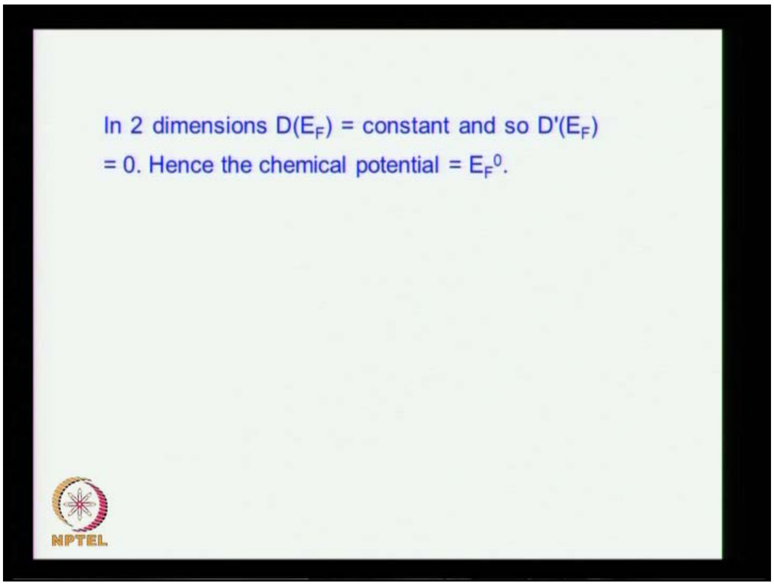

So, we arrive at this result for the chemical potential in two dimensions, the question was about chemical potential in two dimensions, for D equal to 2, we know that the density of states d of e is constant this is the reason which we have considered already. Therefore, D dash E F is zero. Therefore, mu of t the chemical potential at any temperature T above zero k is just the Fermi energy at T equal to zero k, because this term vanishes, so that is the result that we are required to prove.

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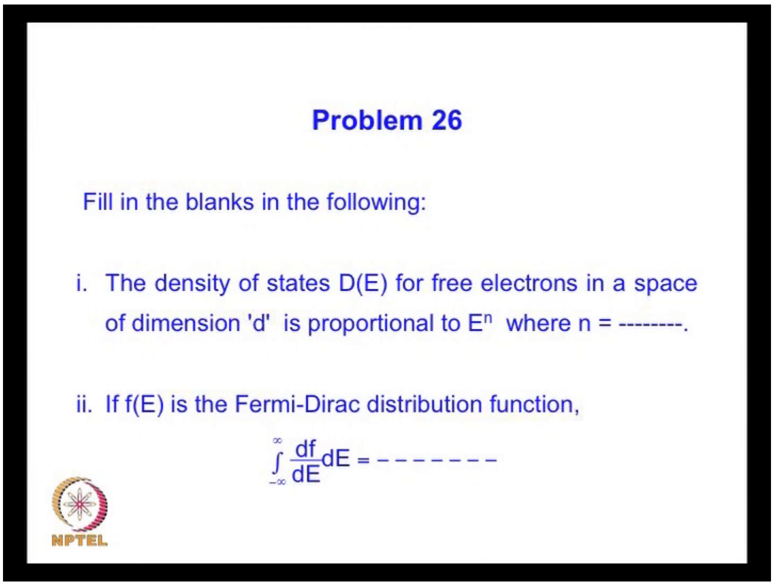

The next question is given in the form of a fill in the blanks, fill in the blanks are straightforward.

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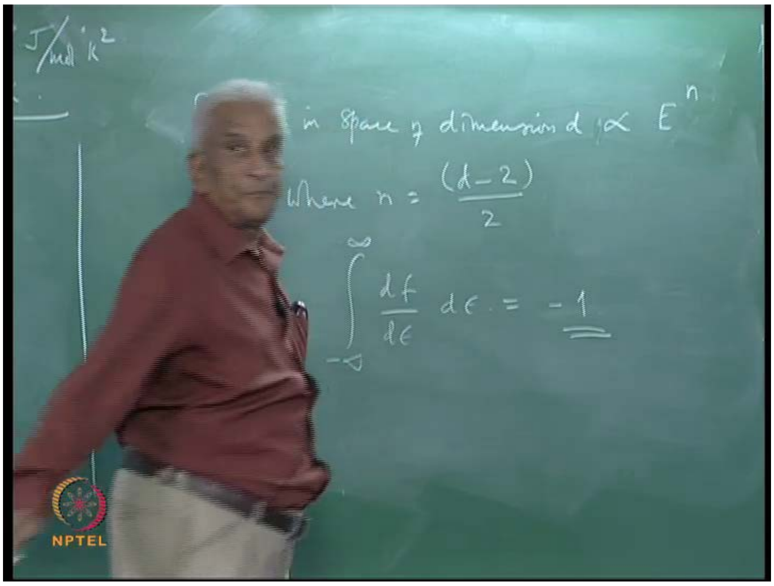

The density of states d of e for free electrons in the space of dimension d in space of dimension d is proportional to the energy to the power n where n is the answer; obviously, we have considered this already the answer is; obviously, d minus 2 by 2. And the next question is about Fermi Dirac distribution function, if the f of e is the Fermi Dirac distribution function integral d f by d e time d e over minus infinity to plus infinity is the answer obviously, minus 1.