Mathematics for Chemistry
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Module - 01
Lecture - 05
Practice Problems

So, today I will do a couple of practice problems, yeah you should also in addition to these practice problems I also encourage you to look at the textbook suggested for the course to see practice problems in them. In particularly this part is very well discussed in the in the book by Macquarie.

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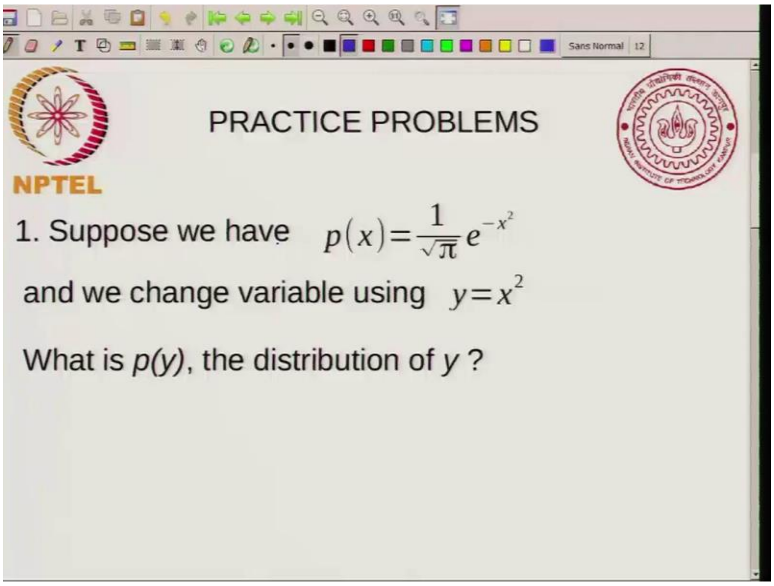

So, let us pick a couple of practice problems. So, the first one I will read out the problem. Suppose we have a distribution p of x given by 1 by root pi e to the minus x square and we change variable using y equal to x square, what is p of y the distribution of y? So, suppose you have a distribution of 1 variable and you change the variable then, how do you look at the distribution of the new variable?

Now, this is in order to solve this, you need to think a little bit more about how this transformation of variables and what it does to the probability distribution. You remember that, you always have the condition that integral p of x d x over the range from minus infinity to plus infinity this should be equal to 1 and so what you would expect is that, if you change the variable y then you would also have integral p of y d y forward whatever the range of y this should be equal to 1, over the range of y since y is x square axis a. So, y has to be positive should be 0 to infinity. So, this should be equal to 1.

So, when we make this transformation you have to satisfy this condition. So, what we do is we choose a transformation that satisfies p of x, d x equal to p of y d y. So, we choose the transformation that satisfies is and so what you will get this, you can show that this works out to be p of y equal to p of x into d x by d y and I can write this as p of x divided by d y by d x.

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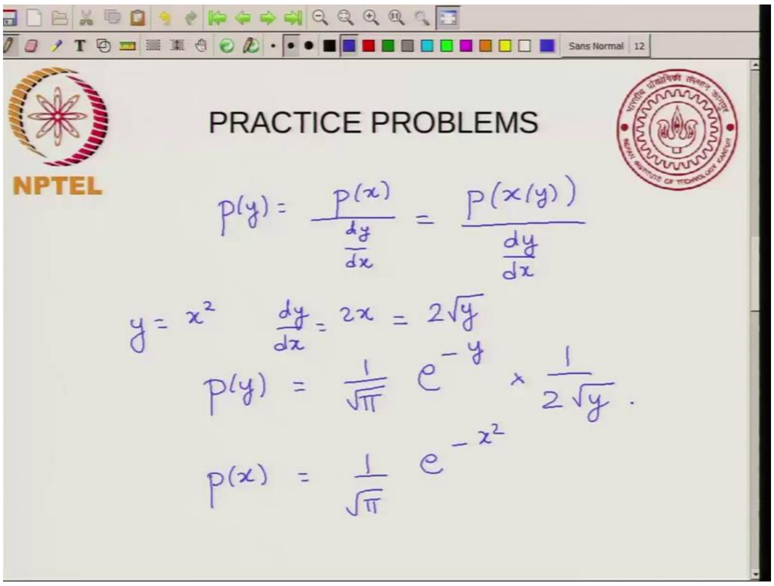

So, what we have is p of y is equal to p of x divided by d y by d x. Now this equation is actually a little misleading because, what you are supposed to write is in this equation you are supposed to write x as a function of y. So, I should actually write this as p of x of y. So, wherever I have x in the expression for p of x, I replace it by y. Divided by d y by d x and again d y by d x should be this should be expressed as a function of y. So, let us go ahead and do this. So, what you have is y equal to x square d y by d x is equal to 2 x, but this is express as a function of x. So, if you want to express is that of express this as a function of y you will get 2 root square root of y because x is nothing, but square root of y and so what you will get, now I can write p of y. So, what I have is 1 over square root of pi and 1 have e to the minus x square is nothing, but e to the minus y and then I have to divide this by this derivative. So, it should be into 1 over 2 square root of y.

So, what we had initially was p of x is equal to 1 over square root of pi e to the minus x square and when we set x square equal to y, within the probability distribution for y not only does this change, but also there is an there is an additional factor. So, this problem is a very general problem that shows how you go from distribution of one variable to distribution of another variable. So, it can be used, it is a general method that can be used to transform from one variable to another.

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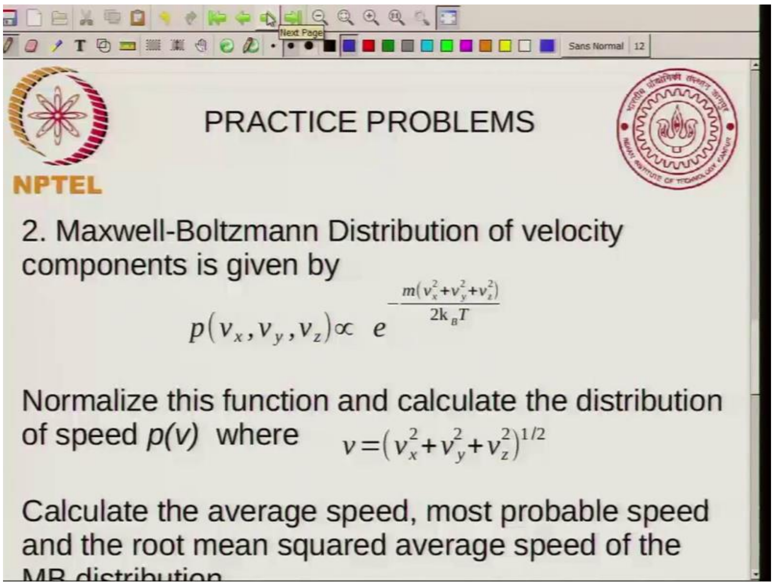

So, the next problem that I want to do is a more specific problem and this is related to the Maxwell Boltzmann distribution of velocity components and will also use some of what we learned from the previous problem here. So, p of v x, v y, v z is proportional to e to the minus m v x square plus v y square plus v z square divided by 2 k B T. So, what you are asked to do is to normalize this function and calculate the distribution of speed. So, this is a distribution of 3 components. So, it is a multi dimensional distribution, it has 3 components and you convert it to a distribution of a single quantity V, which is given by square root of v x square plus v y square plus v z square and then you calculate the average speed, most probable speed and the root mean square average speed of this Maxwell Boltzmann distribution.

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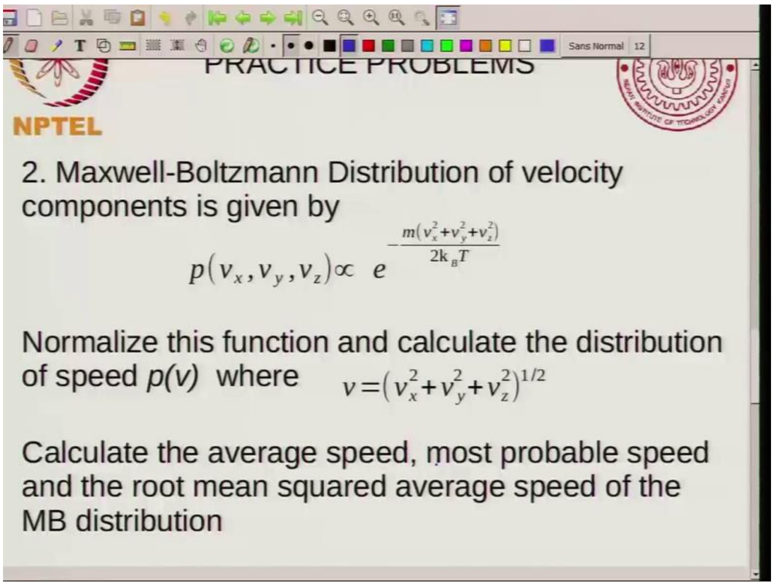

So, again you can do this it is a very standard exercise when you do kinetic theory of gases. So, just to show, how you will go ahead and do this, so first let us look at the normalization.

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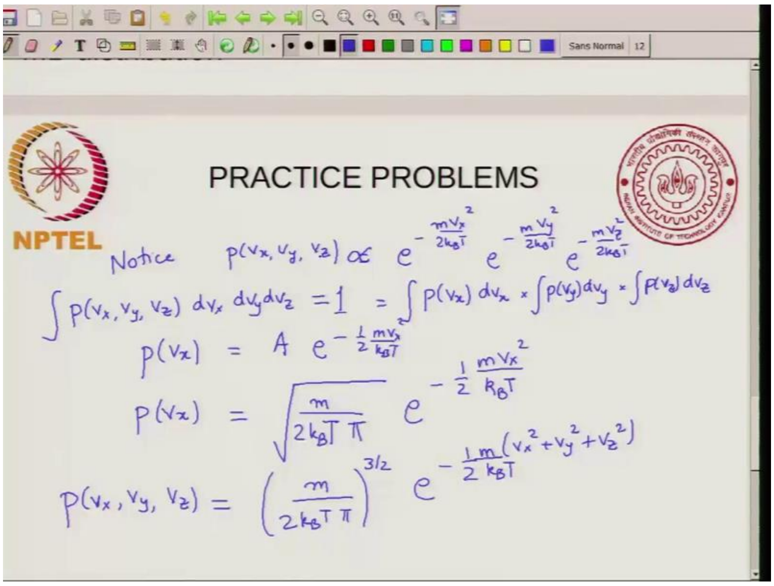

So, notice that, p of v x, v y, v z is equal to e to the minus m v x square by 2 k B T into e to the minus m v y square by 2 k B T into e to the minus m v z square by 2 k B T. So, what we realized is that this distribution factors into 3 distributions, one that depends only on v x other that depends only on v y and the third that depends only on v z. So, what can you do with this? Now, your condition is that integral p of v x, v y, v z. Know this is I should write this is proportional to d v x, d v y, d v z is this should be equal to 1. Now, what I can do is, I can write this because I see that my this factors into 3 factors I can write this as integral p of v x, d v x, into integral p of v y, d v y into integral of p of v z, d v z and what I am going to do is going to insist that each of these is equal to 1. I am going to normalize each of these distributions separately. So, you know the normalization constant for if you just take 1 v x then you have this, this is equal to A e to the minus half m v x square by k B T.

So, what you can say immediately is that, you know the value of this normalization constant to because this is just a Gaussian function. So, the normalization constant I can write as square root of this quantity A, which is which is the m, m divided by 2 k B T square root of a divided by pi. So, that is the normalization constant for this and what you can see is that the same normalization constant will appear will apply for p y and p z and so what I can do with this whole exercise? I will just complete the writing of this quantity. So, this is my normalized p v x, again we use the idea we took this a just from a usual Gaussian function. So, if instead of if you add e to the minus a x square then the normalization constant the square root of a by pi.

So, here instead of A, you have m by 2 k B T. So, that is what is replaced A by that. So, now, we have the normalization constant for v x, we can do similarly for v y and v z. So, I can write p of v x v y v z is equal to m by 2 k B T pi raise to 3 by 2 because, because, I will get half factor from each of them and I will have e to the minus half m v x square plus v y square plus v z square divided by k B T. So, this is the normalized Maxwell Boltzmann distribution of velocities.

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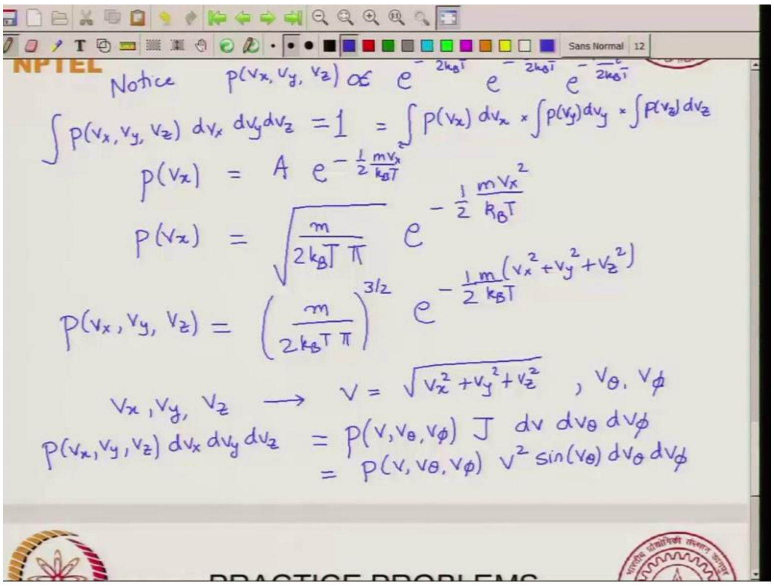

Now the next thing that we wanted to do if you go back to the problem is you wanted to calculate the distribution of the speeds p of v. So, to do this, we will just look at this distribution and then what you want to do here you have v x, v y, v z and what you want to calculate is the distribution of the speed v v. So, here we have 3 variables and here you have only 1 variable. So, actually what you need to do is to can you look at the expression for v v is equal to square root of v x square plus v y square plus v z square and you immediately realize that this is nothing, but the length of this velocity vector. So, you are going from x y z to a length and that should remind you that what you are doing is actually a transformation of coordinates from x y z to spherical polar coordinates. So, you are going from this to there should be 2 other components 1 is a theta component and a phi component. Again these are not the important in this description because you can work it out by normalization ok.

So, when you do this transformation, then is the easy way to see what this transformation should be is to insist that you should have p of v x, v y, v z, d v x, d v y, d v z this should be equal to p of v v theta and v phi. So, these are the 2 angular components I am just calling them v theta and v phi times Jacobean for this transformation times, d v d v theta d v phi. So, the way d v x, d v y, d v z that transforms us j times this and this j for spherical polar coordinates is actually equal to v square sin v theta d v theta d v phi and what we notice is that this distribution this p depends only on v x v y it depends only on the sum of square. So, it depends only on v its independent of v theta and v phi. So, this independent allows us to write the following expression.

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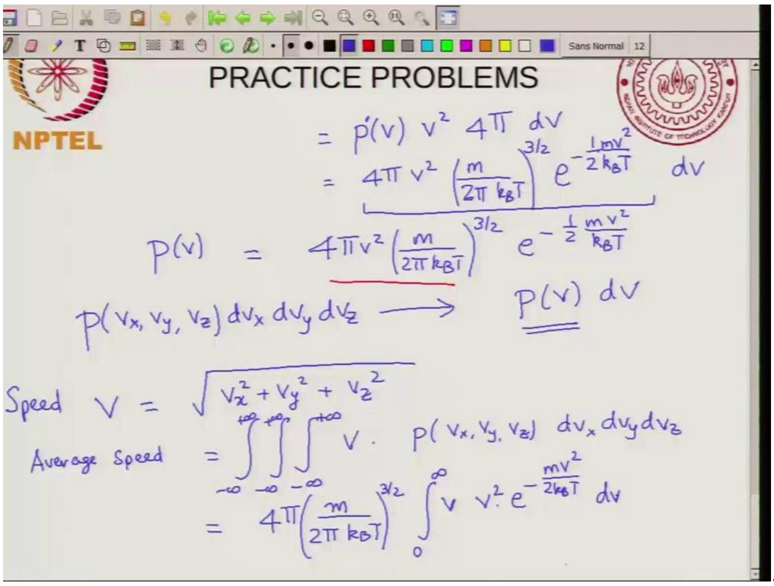

So, you can write this as p of it depends it is independent of theta and phi. So, I will write it as p of v times, v square and this sin theta v theta d theta d phi and then you have a d v. So, this whole factor I can just replace by 4 pi and then I have a d v. So, these are very standard things that you do when you work with a curvilinear coordinates or spherical polar coordinates. So, you have a 4 pi e square d v.

So, now I can write this as 4 pi v square now p of v is just p of v you can get by looking at the expression for. So, we notice that this whole thing in this this whole expression is just equal to v square. So, that allows us to write this as. So, you keep the normalization factor as it is. So, you have m divided by 2 pi k B T this thing raise to 3 by 2 and you have e to the minus half m v square by k B T. So, this is the Maxwell Boltzmann distribution of speeds, d v and what you can say from this is that p of v this is equal to, I should call this p prime of v here because, what you are doing is you are expressing the original distribution in terms of v x, v y, v z in terms of in terms of v.

So, finally, what you will get is you will just identify this whole thing as p of v. So, you will say this is 4 pi v square m by 2 pi k B T raise to 3 by 2 e to the minus half m v square by k B T. So, once you have this then, you can say that what we did is we had a P of v x, v y, v z and you had d v x, d v y, d v z and you went to p of v d v. So, this is what gives you the Maxwell Boltzmann distribution of speed. So, then this p of v is given by this quantity. Notice that what you have is you do not have just a Gaussian. In this case we have a Gaussian multiplied by a v square in front. So, this is the very standard Maxwell Boltzmann distribution of speeds that you have seen in your kinetic theory of gases.

Now, the next thing is to calculate the average speed, most probable speed and the root mean square average speed of this Maxwell Boltzmann distribution. So, the average speed v is equal to square root of v x square plus v y square plus v z square. So, this is speed an average speed is equal to integral v times P of v x, v y, v z, d v x, d v y, d v z and this is a triple integral actually because you are integrating over v x, v y and v z. So, I will just write this as a triple integral and each of v x v y v z go from minus infinity to plus infinity. So, if you want to calculate the average speed then, what you do is again, again, you do the transformation to spherical polar coordinates and you can use p of v and what you will get is I can write this as 4 pi and then I take the m by 2 pi k B T raise to 3 by 2. So, I am just copying this expression from here.

So, I am just taking this this expression and bringing this here. I, I took all this outside the integral and then I have a single integral from 0 to infinity. So, v the speed can only be positive. So, v goes from 0 to infinity. Now, I have a v’s v into v’s v square e to the minus m v square by 2 k B T d v. So, that is essentially the expression that you get and now you have to evaluate this integral now this integral goes only from 0 to infinity and you have v cube e to the minus m v square by 2 k B T and you have to evaluate this integral ok.

So, this is how you will calculate the average speed. So, the average speed is given by this expression and we can go ahead and do the calculation.

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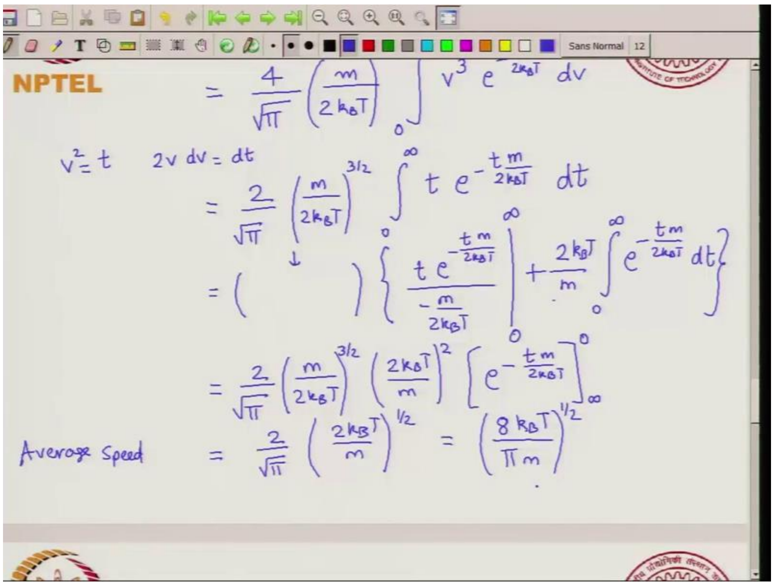

I will just write this in a slightly different form. So, I will take the factor of pi outside. So, I will have a pi raise to 3 by 2. So, I will just write it as 4 divided by a square root of pi. So, and then and then, what all write is m by 2 k B T this raise to 3 by 2 and what I have is integral v cube e to the minus m by 2 k B T v square d v from 0 to infinity. Now, this is actually a standard integral you can do this using gamma functions, but I will just show you how to do it explicitly. So, I will just show how to do this integral explicitly. So, what will do is we will put v square equal to t then 2 v d v equal to d t and so what I can write this. So, I will get 2 by root pi and I have m by 2 k B T raise to 3 by 2 and what I have is integral 0 to infinity.

Now, I have t e to the minus t into the factor of m divided by 2 k B T i and is have d t. So, this is; what the expression looks like and now you can do this integral integrate by parts? So, when you integrate this by parts you will get 2 terms, the first term will be t times the value of this integral and then the value of this integral is just exponential divided by a constant and basically you have t times e to the minus. So, I will just write this factor as it is I want to write it out again, but what I will have is a 2 terms. The first term will be t e to the minus t m by 2 k B T divided by minus m by 2 k B T and this has to be evaluated from, from 0 at the boundaries 0 and infinity and the other term will look like integral will look like. So, minus, minus at will become plus, plus 2 k B T by m and I have integral e to the minus t m by 2 k B T d t from 0 to infinity. So, these are the 2 terms you have and instantly you realize that this term when t equal to infinity e to the minus infinity goes to 0 much faster than t the t goes to infinity.

So, this product goes to 0 at infinity it goes to 0 at 20 equal to 0 this term goes to 0. So, this term is equal to 0. The second term we will just have this times this integral. So, the factor of 2 k B T by m times this e to the minus t m by 2 k B T you can easily do this integral and what that will do this will give you an additional factor of 2 k B T by m. So, what this will give is, is. So, I will just write it alright now. So, 2 by root pi and I have m by 2 k B T raise to 3 by 2 and I have 2 k B T by m square whole square and then what I have is.

So, the second square came from doing this integral and I have e to the minus t m by 2 k B T, but there is a minus sin. So, the limits are actually infinity to 0 when t equal to 0 this is equal to 1 when t equal to infinity this is equal to 0. So, this is just 1. So, finally, what I can right this as. So, I have 2. So, I can write this as 2 by root pi into 2 k B T by m raise to half. So, if I want to take this to inside I have the square this. So, 2 square a 4 4 into 2 I can write this as 8 k B T divided by pi m raise to half. So, this is a expression for the average speed. So, this is a standard expression that you have seen in lot of the books and we saw how you can get this from the Maxwell Boltzmann distribution.

Now, what about the other, other speeds that you were asked to calculate you are asked to calculate the most probable speed and the root mean square speed. So, the root mean square average p it is actually again fairly easy to calculate.

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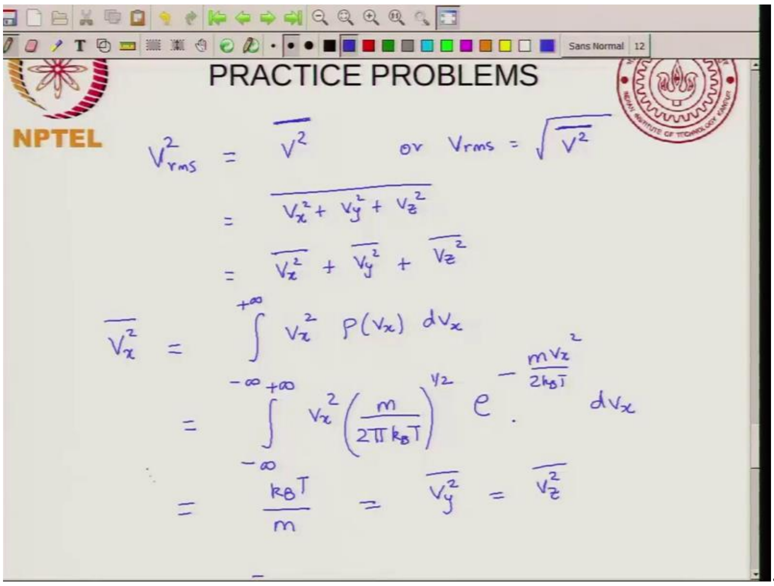

So, the v root mean square. So, this is defined as, as the. So, I can say the v square root mean square is the average of v square. So, you take the average of v square then you will get v root mean squares the square of that or you can write v root mean square is the (Refer Time :23:40) have been using the slightly different notation for average. So, I will just stick to that and use our notation. So, it is the average of v square or you can write v root mean square as the square root of average of v square. So, essentially what you need to do is to, you need to calculate the average of v square. So, this is nothing, but the average of v x square plus v y square plus v z square. This I can write as average of v x square plus average of v y square plus average of v z square and now, now, if you look at the Maxwell Boltzmann distribution the 3 directions are identical, so the 3, if you look at the Maxwell Boltzmann distribution of velocities.

So, there is nothing that that distinguishes x y and z. In fact, whatever you get for v x square you will get the same for average of v y square and you will get the same for average of v z square. So, I can go ahead and I can calculate v x square average. So, I can calculate this. So, now, this is only a function of x. So, I can write this as integral from minus infinity to plus infinity v x square times p of v x d v x and this, this you, you can show this again the using the using the integrals that we have seen. So, you write this as minus infinity to plus infinity.

Now I have v x square now p of v x what we said that hat was equal to m by 2 pi k B T raise to half the half because, you are looking only at v x and e to the minus m v x square by 2 k B T d v x. So, this is the average of v x square and you can show that this is equal to when you, when you do this integral you will get this equal to k B T by n.

So, all the other factors will go off and what will be left which is k B T by m and you can similarly show that this is equal to v y square average and this is equal to v z square average. So, this part it takes a little bit of work to show, but it is not very difficult.

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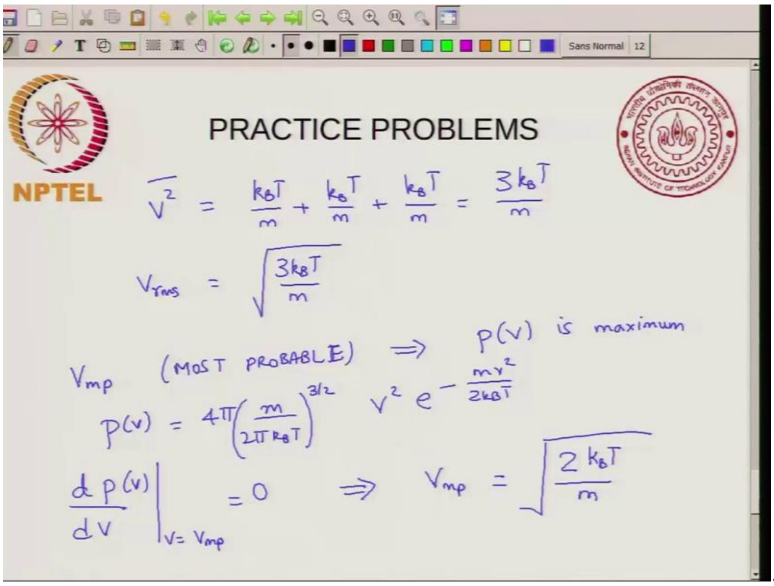

So, then you can write v square average is nothing, but k B T by m plus k B T by m plus k B T by m equal to 3 k B T by m or v r m s is equal to square root of 3 k B T by m. So, this tells you what v r m s is. Now, what about v most probable? So, v most probable, so this implies p of v is maximum, where is p of v maximum. So, p of v we wrote as 4 pi into m by 2 pi k B T raised to 3 by 2 and you had v square e to the minus m v square by 2 k B T and so this is maximum means the derivative of this with respect to v should be 0. So, d p of v by d v at v equal to v most probable equal to 0 and so you have to take the derivative of this quantity and this if you work out you will get v most probable equal to 2 k B T by m on the root of that. You have to work this out and you will get this result.

So, with this I conclude this practice problem and in the next class we will go to the second module.

Thank you.