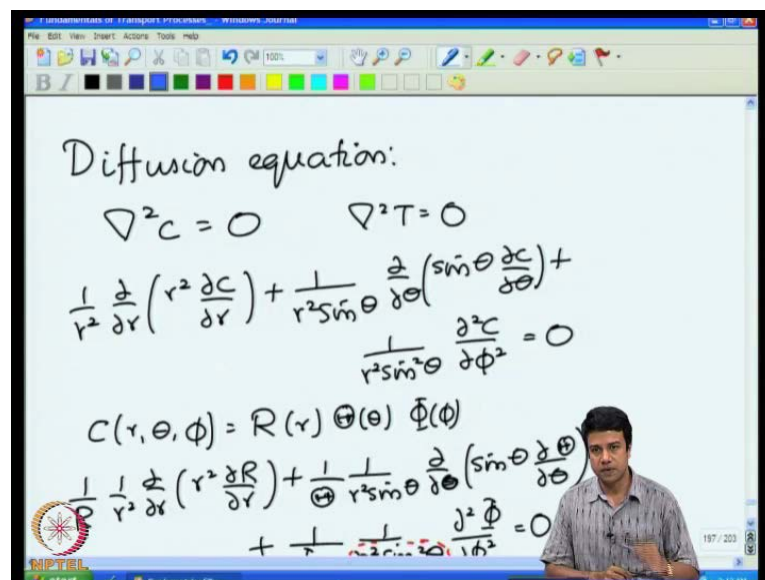


**Fundamentals of Transport Processes**  
**Prof. Kumaran**  
**Department of Chemical Engineering**  
**Indian Institute of Science, Bangalore**

**Lecture No. # 30**  
**Diffusion Equation Spherical Co-ordinates Separation of Variables**

So this is lecture number 30 where we were looking at transport processes in a spherical coordinate system in the limit of low ( $Pe$ ) number where diffusion effects were dominant when compared to convection effects.

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Diffusion equation:

$$\nabla^2 C = 0 \quad \nabla^2 T = 0$$

$$\frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial C}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial C}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2 C}{\partial \phi^2} = 0$$

$$C(r, \theta, \phi) = R(r) \Theta(\theta) \Phi(\phi)$$

$$\frac{1}{R} \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial R}{\partial r} \right) + \frac{1}{\Theta} \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial \Theta}{\partial \theta} \right) + \frac{1}{\Phi} \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2 \Phi}{\partial \phi^2} = 0$$

So we were basically solving the diffusion equation  $\nabla^2 C = 0$  or  $\nabla^2 T = 0$  in a spherical coordinate system. We had previously solved it in a Cartesian coordinate system for the particular case of the diffusion in a cubic solid. In that case we had homogeneous boundary conditions in one coordinate and inhomogeneous boundary conditions in the other coordinate and I showed you how to get solutions in the **the in the** form of basis functions sine and cosine functions in the coordinate which is homogeneous. The other solutions become exponentials. Those exponentials are determined from the orthogonality solutions from the boundary conditions along that direction.

We tried a similar procedure here for spherical coordinate system. In this particular case we did not make a specific reference to an underlying coordinate system. So, I had written down the concentration field as a combination as a product of three functions; one of which is only a function of  $r$ , the other is only a function of  $\theta$  and the third one which is only a function  $\phi$ . And I wrote down the equation for that  $1/r^2$   $d/dr$  of  $r^2$  partial of  $R$  with respect to  $r$  plus  $1/r^2 \sin \theta$   $d/d\theta$  of  $\sin \theta$  partial of  $R$  with respect to  $\theta$  plus  $1/r^2 \sin^2 \theta$   $d^2\phi/d\phi^2 = 0$ . Then I wrote down the equation for  $R$  and  $\theta$  separately,  $r^2 \sin^2 \theta$   $d^2\phi/d\phi^2 = -m^2$  and  $1/r^2$   $d/dr$  of  $r^2$  partial of  $R$  with respect to  $r$  plus  $1/r^2 \sin \theta$   $d/d\theta$  of  $\sin \theta$  partial of  $R$  with respect to  $\theta$  plus  $1/r^2 \sin^2 \theta$   $d^2\phi/d\phi^2 = 0$ .

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$$C(r, \theta, \phi) = R(r) \Theta(\theta) \Phi(\phi)$$

$$\frac{1}{R} \frac{1}{r^2} \frac{d}{dr} \left( r^2 \frac{dR}{dr} \right) + \frac{1}{\Theta \sin \theta} \frac{d}{d\theta} \left( \sin \theta \frac{d\Theta}{d\theta} \right) + \frac{1}{\Phi} \frac{d^2 \Phi}{d\phi^2} = 0$$

$$r^2 \sin^2 \theta \left[ \frac{1}{R} \frac{1}{r^2} \frac{d}{dr} \left( r^2 \frac{dR}{dr} \right) + \frac{1}{\Theta \sin \theta} \frac{d}{d\theta} \left( \sin \theta \frac{d\Theta}{d\theta} \right) \right] + \frac{d^2 \Phi}{d\phi^2} = 0$$

$$\frac{1}{\Phi} \frac{d^2 \Phi}{d\phi^2} = -m^2 \text{ If } C = +m^2, \Phi = A e^{m\phi} + B e^{-m\phi}$$

$$\text{If } C = -m^2, \Phi = A \sin(m\phi) + B \cos(m\phi)$$

$$\Phi(\phi + 2\pi) = \Phi(\phi)$$

We could with some manipulation reduce it to an equation in which one term dependent only upon  $r$  and  $\theta$  the other term dependent only upon  $\phi$  and for the term that depends only upon  $\phi$  since one term depends only upon  $r$  and  $\theta$  the other term depends only upon  $\phi$  both of these individually have to be constants. Otherwise, I could change  $\phi$  keep  $r$  and  $\theta$  a constant and only one term would change the quality will no longer be satisfied.

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$$\frac{1}{\Phi} \frac{d^2 \Phi}{d\phi^2} = -m^2$$
 If  $C = +m^2$ ,  $\Phi = A e^{m\phi} + B e^{-m\phi}$   
 If  $C = -m^2$ ,  $\Phi = A \sin(m\phi) + B \cos(m\phi)$   
 $\Phi(\phi + 2\pi) = \Phi(\phi)$   
 $m = \text{Integer}$

$$r^2 \sin\theta \left[ \frac{1}{R^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial R}{\partial r} \right) + \frac{1}{\theta^2} \frac{1}{r^2 \sin\theta} \frac{\partial}{\partial \theta} \left( \sin\theta \frac{\partial \Theta}{\partial \theta} \right) \right] - m^2 = 0$$

Therefore I separated it out into two parts; one depends only upon  $r$  and  $\theta$ , the other depends only upon  $\phi$  and for the  $\phi$  equation I told you that  $1$  over  $\phi$  times  $d^2 \phi$  by  $d\phi$  square has to be equal to minus  $m$  square where  $m$  is an integer. That follows from the requirement that when I increase the angle  $\phi$  by  $2\pi$ , I come back to the exact same location in space. Therefore, the properties, the concentration temperature at that point has to be exactly the same. That means that capital  $\phi$  at  $\phi$  plus  $2\pi$  has to be identical to capital  $\phi$  at the angle  $\phi$  itself and that fixes the value of the constant as minus  $m$  square where  $m$  has to be an integer.

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$$r^2 \sin\theta \left[ \frac{1}{R^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial R}{\partial r} \right) + \frac{1}{\theta^2} \frac{1}{r^2 \sin\theta} \frac{\partial}{\partial \theta} \left( \sin\theta \frac{\partial \Theta}{\partial \theta} \right) \right] - m^2 = 0$$

$$\left[ \frac{1}{R} \frac{\partial}{\partial r} \left( r^2 \frac{\partial R}{\partial r} \right) + \left[ \frac{1}{\sin\theta} \frac{\partial}{\partial \theta} \left( \sin\theta \frac{\partial \Theta}{\partial \theta} \right) - \frac{m^2}{\sin\theta} \right] \right] = 0$$

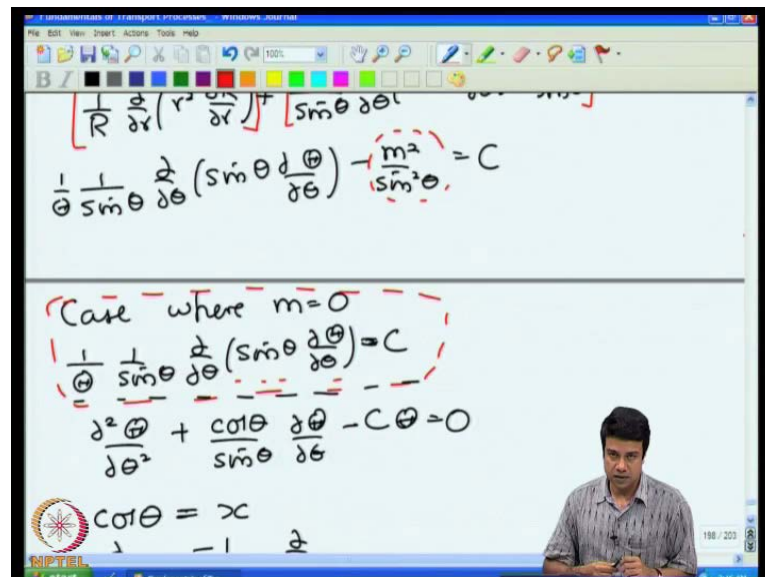
$$\frac{1}{\theta} \frac{1}{\sin\theta} \frac{\partial}{\partial \theta} \left( \sin\theta \frac{\partial \Theta}{\partial \theta} \right) - \frac{m^2}{\sin\theta} = C$$

Case where  $m=0$   

$$\frac{1}{\theta} \frac{1}{\sin\theta} \frac{\partial}{\partial \theta} \left( \sin\theta \frac{\partial \Theta}{\partial \theta} \right) = C$$

So that when you go around you come back to the same location and then we were left with the rest of the equation. Once again I separated that into one term which depended only upon  $r$  and the other term which depended only upon  $\theta$  and for the specific case where  $m$  is equal to 0.

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$$\left[ \frac{1}{R} \frac{d}{dr} \left( r^2 \frac{dR}{dr} \right) \right] + \left[ \frac{1}{\sin \theta} \frac{d}{d\theta} \left( \sin \theta \frac{d\Theta}{d\theta} \right) - \frac{m^2}{\sin^2 \theta} \right] = C$$

Case where  $m=0$

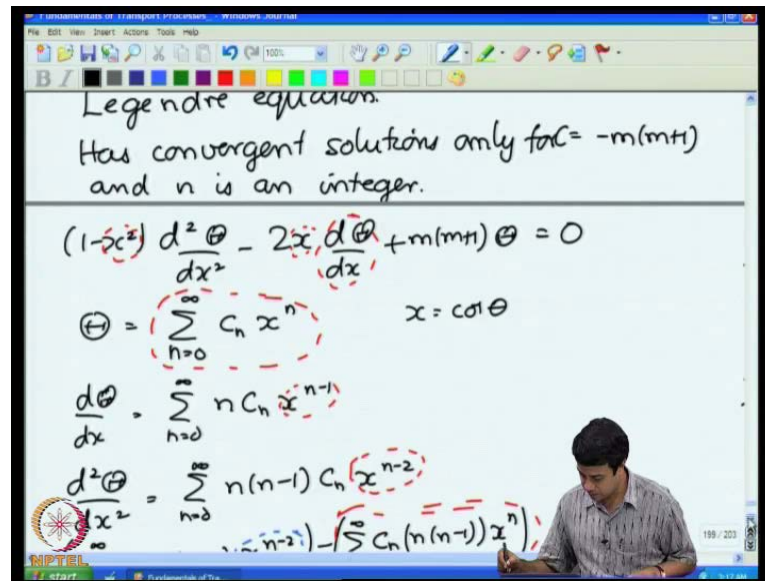
$$\frac{1}{\sin \theta} \frac{d}{d\theta} \left( \sin \theta \frac{d\Theta}{d\theta} \right) = C$$

$$\frac{d^2 \Theta}{d\theta^2} + \frac{\cot \theta}{\sin \theta} \frac{d\Theta}{d\theta} - C \Theta = 0$$

$$\cot \theta = \frac{\cos \theta}{\sin \theta}$$

There is no variation along the, that  $\phi$  direction. I showed you that if we postulate that this term which depends upon  $\theta$  that is one over sine  $\theta$   $d$  by  $d$   $\theta$  of sine  $\theta$  times partial of capital  $\theta$  with respect to  $\theta$  is equal to some constant. That constant has necessarily got to be equal to minus of  $n$  into  $n$  plus 1 where  $n$  is an integer and  $n$  has to be necessarily an integer.

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Legendre equation.  
Has convergent solutions only for  $C = -m(m+1)$   
and  $n$  is an integer.

$$(1-x^2) \frac{d^2 \Theta}{dx^2} - 2x \frac{d\Theta}{dx} + m(m+1) \Theta = 0$$

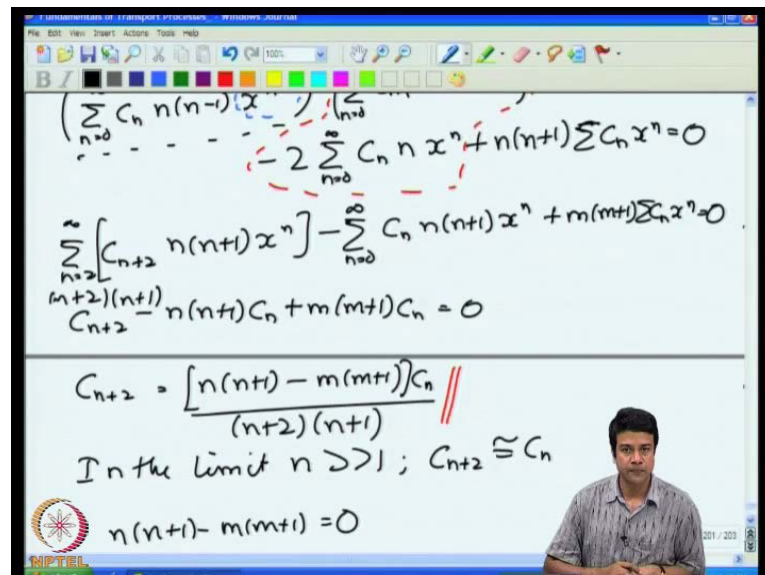
$$\Theta = \sum_{n=0}^{\infty} C_n x^n \quad x = \cos \theta$$

$$\frac{d\Theta}{dx} = \sum_{n=0}^{\infty} n C_n x^{n-1}$$

$$\frac{d^2 \Theta}{dx^2} = \sum_{n=0}^{\infty} n(n-1) C_n x^{n-2}$$

This has necessarily to be an integer in order for the  $C$  is solution that I get and expansion  $x$  power  $n$ . If that has to be finite at  $\theta$  is equal to 0 as well as  $\theta$  is equal to  $\pi$ ; then it is necessary that  $n$  is an integer. That is because the coefficient  $C_n$  I derived explicitly for you the coefficients  $C_n$  in this expansion.

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$$\left( \sum_{n=0}^{\infty} C_n n(n-1) x^{n-2} \right) - 2 \sum_{n=0}^{\infty} C_n n x^{n-1} + m(m+1) \sum_{n=0}^{\infty} C_n x^n = 0$$

$$\sum_{n=2}^{\infty} \left[ C_{n+2} n(n+1) x^n \right] - \sum_{n=0}^{\infty} C_n n(n+1) x^n + m(m+1) \sum_{n=0}^{\infty} C_n x^n = 0$$

$$C_{n+2} n(n+1) - n(n+1) C_n + m(m+1) C_n = 0$$

$$C_{n+2} = \frac{[n(n+1) - m(m+1)] C_n}{(n+2)(n+1)}$$

In the limit  $n \gg 1$ ;  $C_{n+2} \approx C_n$

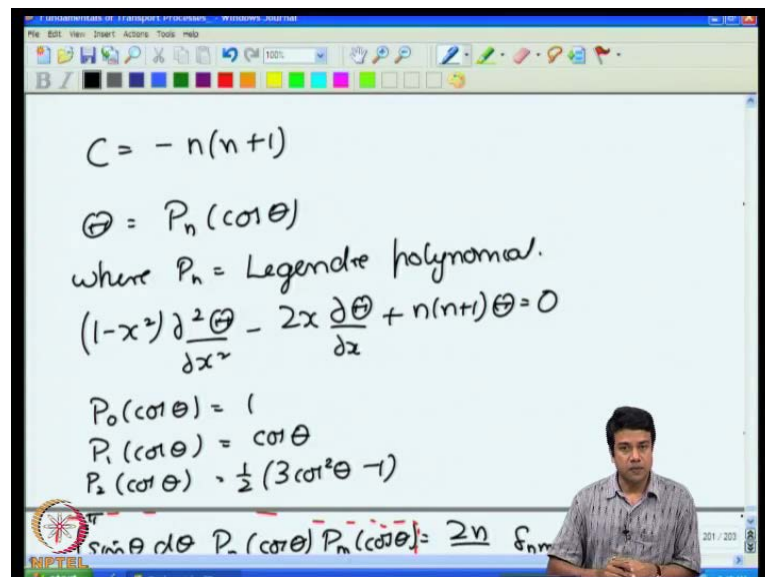
$$n(n+1) - m(m+1) = 0$$

There is one mistake here in the limit as  $n$  becomes large. The coefficients all approach the same value because  $n$  is becoming large  $m$  itself is finite. It is not changing very much. So, in the limit as  $n$  becomes large all these coefficients approach a constant

value. That means that that series has a form summation of some constant times  $x$  power  $n$ . If  $x$  is equal to plus or minus 1 then, the series does not converge because the higher terms are tending to constant values as any cases and a series in which each term tends to a constant value is not a convergent series.

The only way the series will converge is if  $C n$  plus 2 turns out to be equal to 0 for some particular value of  $n$ . Once  $C n$  plus 2 is equal to 0, then all higher terms in the series all odd or even terms in the series all become 0 and you end up with a finite series in that case.

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$$C = -n(n+1)$$

$$\Theta = P_n(\cos \theta)$$

where  $P_n = \text{Legendre polynomial.}$

$$(1-x^2) \frac{d^2 \Theta}{dx^2} - 2x \frac{d\Theta}{dx} + n(n+1)\Theta = 0$$

$$P_0(\cos \theta) = 1$$

$$P_1(\cos \theta) = \cos \theta$$

$$P_2(\cos \theta) = \frac{1}{2} (3 \cos^2 \theta - 1)$$

$$\int_{-1}^1 P_n(\cos \theta) P_m(\cos \theta) \sin \theta d\theta = 2\pi \delta_{nm}$$

So, the requirement that the series has to converge that it has to a finite value at  $\cos \theta$  is equal to 1 or  $\cos \theta$  is equal to minus 1 or at  $\theta$  is equal to 0 and  $\phi$  itself implies that one has to have  $n$  being an integer in this expansion.

So,  $n$  can take only discrete values and those discrete values **for those discrete values** 0 1 2 3 etcetera I showed you that the solutions are in the form of Legendre polynomials. I have written down the first few polynomials in this series here 1  $\cos \theta$  half of 3  $\cos^2 \theta$  minus 1 and so on.

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$$P_0(\cos \theta) = 1$$

$$P_1(\cos \theta) = \cos \theta$$

$$P_2(\cos \theta) = \frac{1}{2} (3 \cos^2 \theta - 1)$$

$$\int_0^\pi \sin \theta \, d\theta \, P_n(\cos \theta) P_m(\cos \theta) = \frac{2n}{2n+1} \delta_{nm}$$

$$(1-x^2) \frac{d^2 \Theta}{dx^2} - 2x \frac{d\Theta}{dx} - \frac{m^2}{1-x^2} = -n(n+1)$$

$$\Theta = P_n^m(\cos \theta)$$

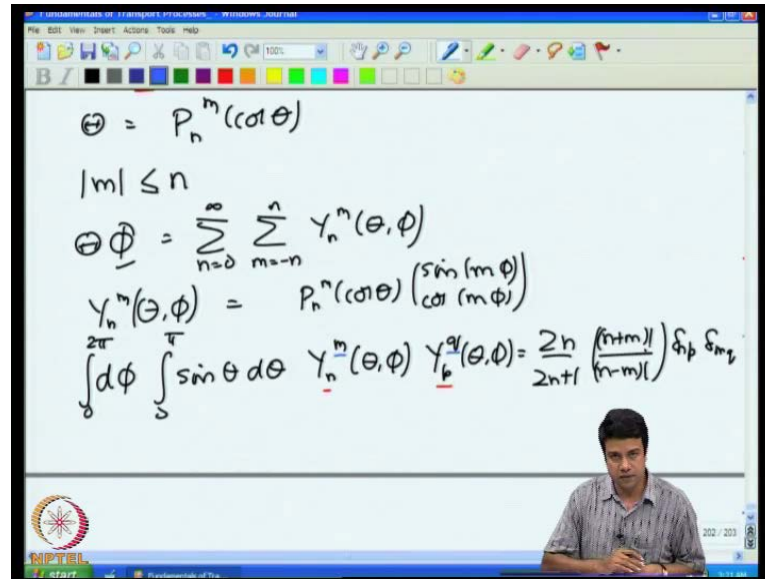
$$|m| \leq n$$

And these Legendre polynomial actually satisfy an orthogonality relation that the product of two polynomials integrated over 0 to pi multiplied by sine theta is non zero only when n is equal to m. So, products of these Legendre polynomials are non zero only when the the the two polynomials are identical and they are 0 when the polynomials are different.

The same thing actually carries over even when I have a non zero value of m. Even in this case where I have a non zero value of m, the same principle carries over. Only thing is that there is an additional requirement. n has to be an integer can go from minus infinity to plus infinity. n has to be an integer. I showed you it has to go from 0 to infinity because the series is only over positive values of n when m is non zero then m can vary only between minus n and plus n.

So for example, for n is equal to 2; m varies from minus 2 minus 1 0 plus 1 plus 2. So, there are 5 solutions. n is equal to 1 there are 3 in general for any value of n the number of solutions is 2 n plus 1.

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$$\Theta = P_n^m(\cos \theta)$$

$$|m| \leq n$$

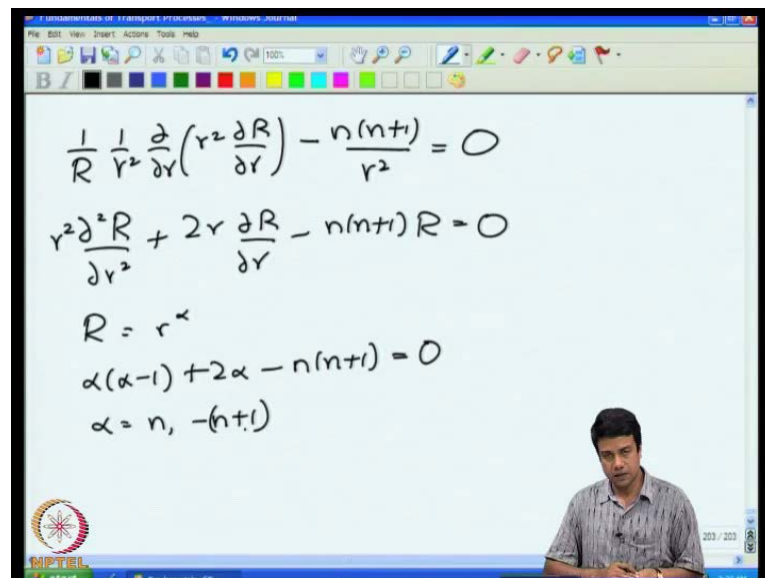
$$\Theta \Phi = \sum_{n=0}^{\infty} \sum_{m=-n}^n Y_n^m(\theta, \phi)$$

$$Y_n^m(\theta, \phi) = P_n^m(\cos \theta) \begin{pmatrix} \sin(m\phi) \\ \cos(m\phi) \end{pmatrix}$$

$$\int_0^{2\pi} d\phi \int_0^{\pi} \sin \theta d\theta \underline{Y_n^m}(\theta, \phi) \underline{Y_l^q}(\theta, \phi) = \frac{2n}{2n+1} \frac{(n+m)!}{(n-m)!} \delta_p \delta_m$$

I told you that the Legendre polynomials along with sine and cosine of theta can be put together to give you spherical harmonics,  $P_n^m$  of  $\cos \theta$  times  $\cos$  and  $\sin$  on  $m \phi$  gives you a spherical harmonic expansion which also satisfies the orthogonality relation.

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$$\frac{1}{R} \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\partial R}{\partial r} \right) - \frac{n(n+1)}{r^2} = 0$$

$$r^2 \frac{\partial^2 R}{\partial r^2} + 2r \frac{\partial R}{\partial r} - n(n+1)R = 0$$

$$R = r^\alpha$$

$$\alpha(\alpha-1) + 2\alpha - n(n+1) = 0$$

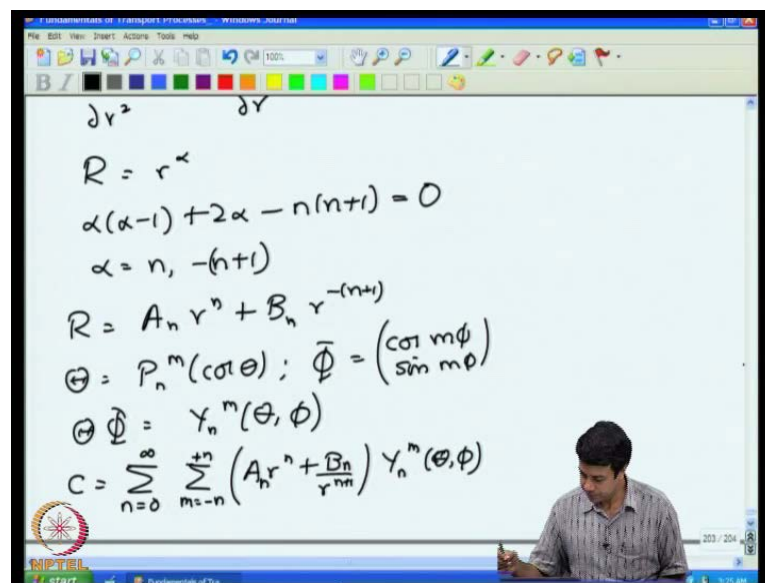
$$\alpha = n, -(n+1)$$

And now finally, we are left with solving the equation for the  $r$  coordinate. The equation that we are left with is  $\frac{1}{R} \frac{1}{r^2} \frac{d}{dr} \left( r^2 \frac{\partial R}{\partial r} \right) - \frac{n(n+1)}{r^2} = 0$  where  $n$  was the discrete solution. The discrete Eigen value for the Legendre polynomials that I had earlier.

So, this is the final solution. I can expand this out to give partial square R by partial r square plus 2 minus n into n plus 1 R is equal to 0. Just by expanding this out this equation as you can see is equi-dimensional in small r. Therefore, the solutions have to be of the form R is equal to r power alpha where the value of the index alpha the exponent alpha is determined by inserting into this equation and then solving.

If I insert into this equation and solve, I will get alpha into alpha minus 1 plus 2 alpha minus n into n plus 1 is equal to 0 or alpha is equal to n and minus n plus 1.

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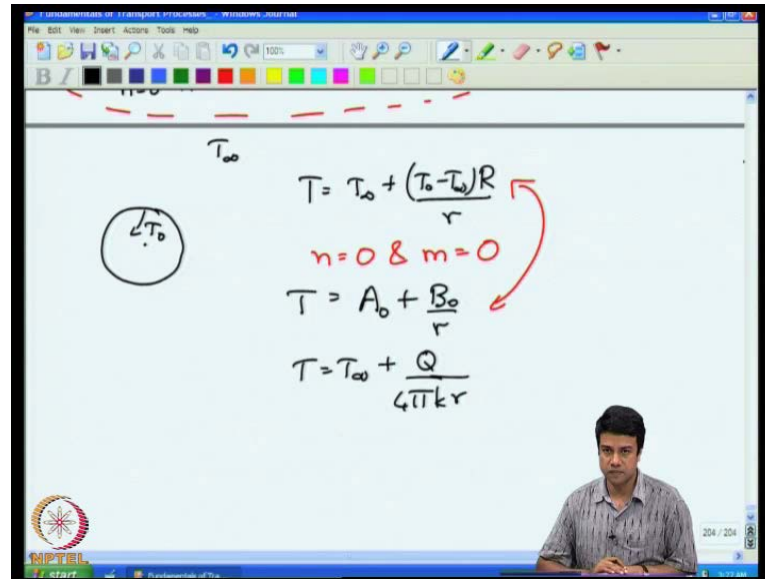


$$\begin{aligned} \nabla^2 R &= 0 \\ R &= r^\alpha \\ \alpha(\alpha-1) + 2\alpha - n(n+1) &= 0 \\ \alpha &= n, -(n+1) \\ R &= A_n r^n + B_n r^{-(n+1)} \\ \Theta = P_n^m(\cos \theta); \quad \Phi = \begin{pmatrix} \cos m\phi \\ \sin m\phi \end{pmatrix} \\ \Theta \Phi &= Y_n^m(\theta, \phi) \\ C &= \sum_{n=0}^{\infty} \sum_{m=-n}^{+n} \left( A_n r^n + \frac{B_n}{r^{n+1}} \right) Y_n^m(\theta, \phi) \end{aligned}$$

Therefore, the solutions for R are of the form R is equal to A n r power n plus B n r power minus n plus 1 for a specific value of n. And for that specific value of n the solution for theta is of the form P n m of cos theta and phi is of the form cos m phi and sine m phi or alternatively I can write theta times phi of the form Y n m of theta phi where Y n m is the spherical harmonic. So, putting all these together the final solution for C will have n is equal to 0 to infinity, m is equal to minus n to plus n. I told you that m has to go only from minus n to plus n for the series to be convergent times A r power n plus B by r power n plus 1 Y n m of theta phi.

So, this is the final solution for the concentration field where A n and B n are in general constants which have to be determined from boundary conditions. A n and B n are constants which have to be determined from boundary conditions. We have already seen this expansion for the special case where n is equal to 0.

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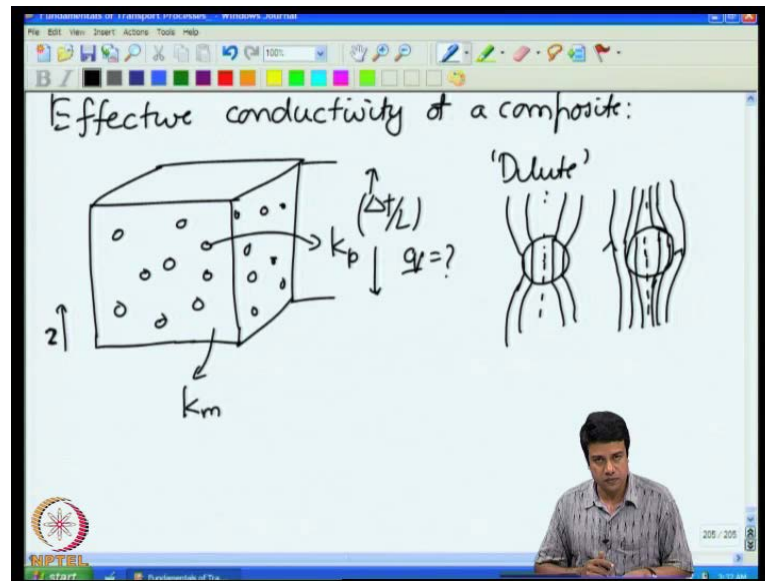


If you recall we solved the heat transfer problem for conduction from a sphere where the surface was at temperature  $T_0$  and the temperature was  $T_\infty$  far away and we got the solution as  $T_\infty + T_0 - T_\infty \frac{R}{r}$  sorry by  $r$ .

This thing corresponds to Legendre polynomial, the spherical harmonic solutions  $n$  is equal to 0 and  $m$  is equal to 0. Of course, if  $n$  is equal to 0 then  $m$  of course, has to be equal to 0 because  $m$  can vary only between minus  $n$  and plus  $n$ . Therefore, this corresponds to this particular solution. For  $n$  is equal to 0 and  $m$  is equal to 0, the solution is of the form  $T$  is equal to  $A_0 + \frac{B_0}{r}$  because  $T_0$  of  $\cos \theta$  is equal to 1 and  $\cos$  and  $\sin$  of  $m \phi$  1 and 0 respectively. So, it just reduces to this particular form and you can see that these two solutions are identical with  $A_0$  is equal to  $T_\infty$  and  $B_0$  is equal to  $T_0 - T_\infty$  times capital  $R$ .

So, the heat conduction from a heated sphere that we did corresponds to the spherical harmonic expansion with  $n$  is equal to 0 where  $m$  is by default is equal to 0 and in that case if you recall we had got the temperature  $T_\infty + \frac{Q}{4\pi k r}$ . So, at this particular case if we take the limit as the radius of this sphere goes to 0 this corresponds to the point source and the total amount of heat coming out of this point source is equal to  $Q$ . So, this is what is called a source term it is called a source. So,  $n$  is equal to 0 and  $m$  is equal to 0 corresponds to a source of heat or a source of mass.

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Now, let us consider a slightly more complicated example that is the effective conductivity of a composite. So, I have some composite material which has spherical inclusions in it and the matrix has conductivity  $K_m$ , the particles have conductivity  $K_p$ . And I want to find out what is the effective conductivity of the medium as a whole. What does one mean by effective conductivity? That is if I apply a temperature difference  $\Delta t$  across the material what is going to be the heat flux? The heat flux is equal to what? So, if I can get a relation between the heat flux and the temperature gradient then I know what is the effective conductivity.

If the particles were not present the effective conductivity would just be the conductivity of the matrix itself. However, because the particles are present there is going to be either an increase or a decrease in the conductivity of the material depending upon whether the particles are more or less conducting than the matrix.

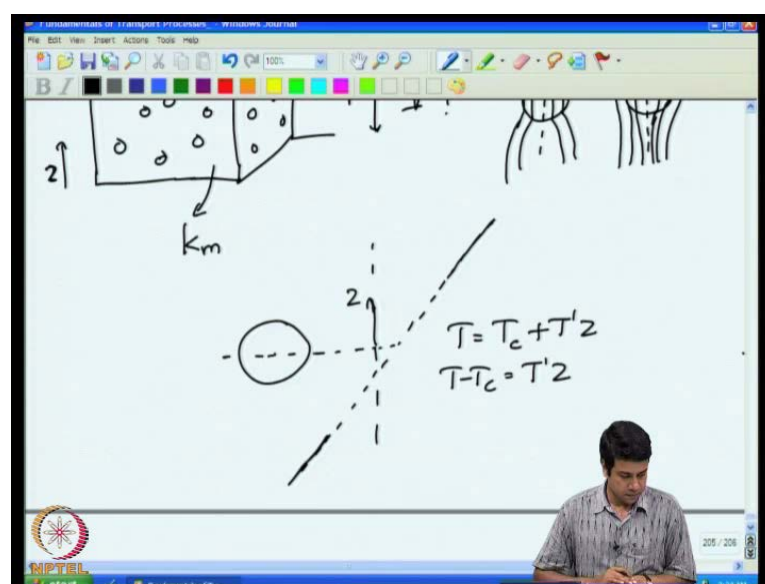
So, now we will solve this equation for the particular case where the **the the** composite is what is called dilute and let me try to explain what that means. If I have a spherical particle and there is a temperature difference across this particle then of course, the heat flux through this particle or the **the** flux lines through this particle will depend upon whether the particle is more or less conducting than the matrix. If the **if the** particle is more conducting than the matrix then the flux line will curve towards the particle.

So, if the particle more conducting than the matrix the flux lines will curve towards the particle where as if it is less than the conducting than the matrix, the flux lines will curve away from the particle. In either case, it is going to be a disturbance to the temperature field in the matrix because of the presence of this particle. Either the disturbance is towards the particle if it is more conducting or the disturbance is away from the particle if it is less conducting.

If I had another particle nearby, then the disturbance to the temperature field due to the first particle is going affect the temperature field around the second particle. That makes it a much more complicated problem. For the present case I will assume that the particles are sufficiently far separated by sufficient distance that the temperature field around one particle is not affected by the temperature disturbance due to a second particle. That is what I mean by the dilute limit for this particular case. Therefore, the assumption here is at temperature field around one particle is not affected by the temperature field around another particle. So, in this dilute limit we want to find out what is the effective thermal conductivity of the entire system.

So, I apply a temperature delta  $t$  over a distance  $L$  and I want to find out what is the flux in the vertical direction? Let me call this vertical direction as the  $z$  axis. So, I want to find out what is the flux  $q_z$ . Now, since the distance between the particles is relatively large, there is a large distance between neighboring particles.

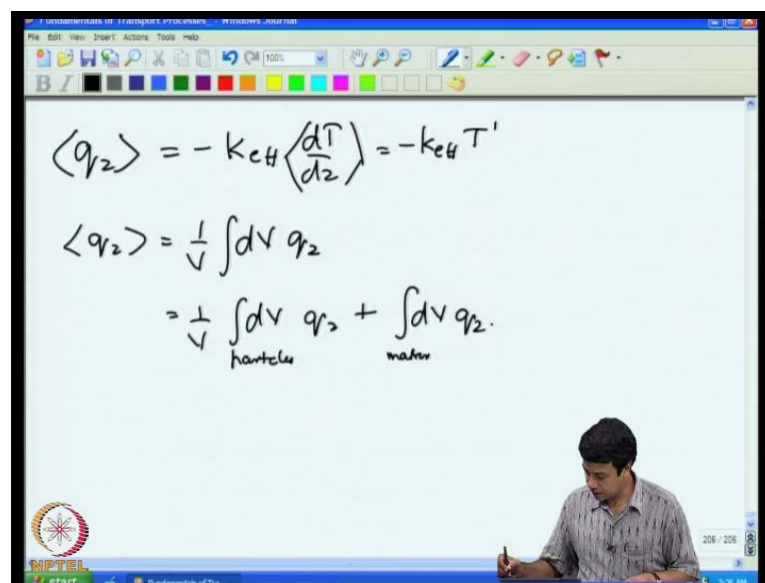
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So, if I look at a second, a single particle it looks like particle that has been placed in a temperature gradient which is nearly linear far from the particle. Of course, when I come close to the particle there is going to be disturbance due to the temperature field because this particle is either more or less conductive. However as a function of this, of the distance  $z$  if I go sufficiently far away **if I go sufficiently far away** I should recover back this temperature gradient even though close to the particle there is a disturbance due to the presence of this particle and that temperature gradient far away is going to be of the form  $T$  is equal to  $T_e$  at the center of this particle. The **the** value of the temperature the center of this particle plus a correction  $T' \text{ times } Z$ .

Without loss of generality, since I am interested only the heat flux; the heat flux depends only upon the derivatives of the temperature it does not depend upon the constant temperature that is there. So, without loss of generality this I can take it as  $T'$  **(( ))** times  $Z$ .

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$$\langle q_z \rangle = -k_{eff} \left\langle \frac{dT}{dz} \right\rangle = -k_{eff} T'$$

$$\langle q_z \rangle = \frac{1}{V} \int dV q_z$$

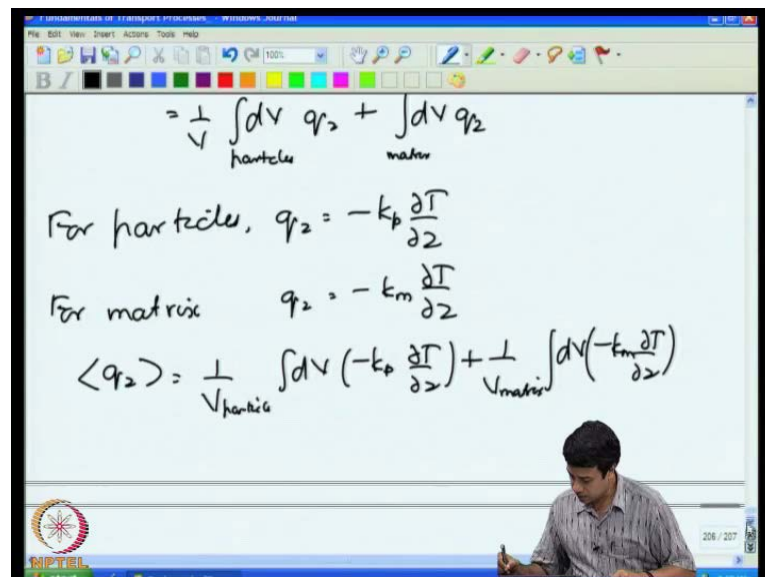
$$= \frac{1}{V} \int_{particle} dV q_z + \int_{matrix} dV q_z.$$

Now how I am going to determine the thermal conductivity of the entire system? So, for the entire system particles plus matrix, I have to get an equation of the form minus  $k$  effective times  $dT$  by  $dz$ , the average which is basically equal to  $k$  effective times the difference in temperature divided by the length, is equal to  $k$  effective times the difference in temperature between the top and bottom surfaces divided by the length.

So, this is going to be minus  $k$  effective times  $T$  prime. Now, I can define this heat flux as a volume average or an ensemble average. If the ergodic hypothesis holds both should be equal this is a non equilibrium system. Therefore, it is better to use averages which does not depend upon the ergodic hypothesis. For the present I will use  $q_z$  is equal to a volume average  $1$  over  $V$  integral over the entire volume, particles plus matrix of the local value of  $q_z$ .

So, this is the average over the entire volume. Now, this I can separate it out into two parts; one over the particles  $q_z$  plus integral over the matrix.

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$$= \frac{1}{V} \int_{\text{particle}} dV q_z + \int_{\text{matrix}} dV q_z$$

For particle,  $q_z = -k_p \frac{\partial T}{\partial z}$

For matrix  $q_z = -k_m \frac{\partial T}{\partial z}$

$$\langle q_z \rangle = \frac{1}{V_{\text{particle}}} \int dV \left( -k_p \frac{\partial T}{\partial z} \right) + \frac{1}{V_{\text{matrix}}} \int dV \left( -k_m \frac{\partial T}{\partial z} \right)$$

For the particles; for  $q_z$  is equal to minus  $K$  particles  $dT$  by  $dz$  and for the matrix minus  $k_m dT$  by  $dz$ . Therefore, I can write this as average of  $q$  is equal to  $1$  over  $v$  particles summing to over the particles and over the matrix.

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$$\begin{aligned}
 &= \frac{1}{V} \int_{\text{total volume}} dV \left( -k_m \frac{dT}{dz} \right) + \frac{1}{V_{\text{particle}}} \int dV \left( -(k_p - k_m) \frac{dT}{dz} \right) \\
 &= -k_m \left\langle \frac{dT}{dz} \right\rangle + \frac{1}{V_{\text{particle}}} \int dV \left( -(k_p - k_m) \frac{dT}{dz} \right) \\
 &= -k_m T' + \frac{N}{V_{\text{particle}}} \int dV \left( -(k_p - k_m) \frac{dT}{dz} \right)
 \end{aligned}$$

Rather than do it this way it is more convenient to write this as 1 over the total volume **the total volume** where I have used the matrix conductivity for the **for the** total volume plus a contribution which is basically the disturbance over the particles. So, I have written this as an integral over the matrix plus particles of  $k_m dT$  by  $dz$  plus over the particles alone of minus of  $k_p$  minus  $k_m dT$  by  $dz$ .

So, there are two contributions; one due to the particles and the other is due to the total volume. The particle contribution only contains the difference in the fluxes in the **in in in** thermal conductivity between the particles in the matrix. You can see straight away from this that when particle conductivity is equal to the matrix conductivity there is no disturbance.

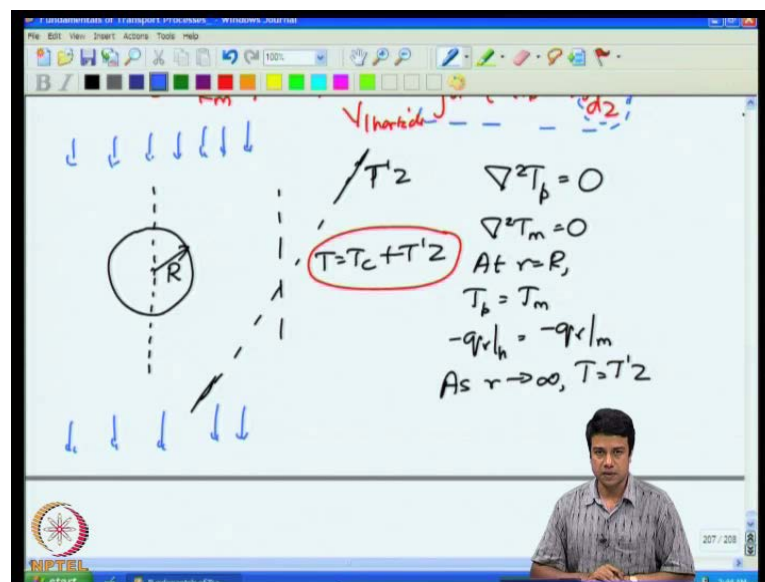
So, this I can write this integral over the entire volume is equal to minus  $k_m$  into the average of  $dT$  by  $dz$  plus 1 over the particles integral  $dV$  of minus of  $k_p$  minus  $k_m dT$  by  $dz$ . So, this second term here gives me the correction to the heat flux due to the presence of this particle. This first term here is just the average contribution of the matrix. This is just equal to minus  $k_m$  times  $T'$ . The heat flux due to the imposed temperature gradient and this second term here gives me the additional contribution due to the presence of the particles.

This is an integral over all the particles. However, at the beginning I had made the assumption that the system is dilute so that the presence of one particle does not affect

the temperature field around the second particle. In addition, this depends only upon the temperature gradient locally near the particle.

So as far as this is concerned, I can write this as number of particles divided by the volume of one particle integral  $dV$  of minus of  $k_p$  minus  $k_m$   $dT$  by  $dz$ . So, this is equal to the total number of particles divided by the volume of one particle. This is basically the number of particles per unit volume times  $dT$  by  $dz$  and this is the contribution that I have to calculate by actually calculating the temperature field near one particle. I need to calculate the temperature near one particle and from that I need to calculate what is this contribution.

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So let us calculate the temperature field near one particle. I have a particle and I have a temperature field which far away goes as  $T$  prime times  $z$ . It is a linear temperature field far away from the particle. Of course, there is some disturbance. So, the temperature if I take will be equal to  $T_c$  plus  $T$  prime times  $z$ . This is the temperature field that is at a large distance from the particle. Near the particle itself, there is going to be a disturbance due to this temperature field because the thermal conductivity of the particle is not equal to a thermal conductivity of the matrix.

So, let us evaluate this temperature field. So, we have to solve the equations for the particle phase I have to solve  $\nabla^2 T_{\text{particle}} = 0$ . For the matrix I need to solve  $\nabla^2 T_{\text{matrix}} = 0$  and I have conditions at the surface. So, if I

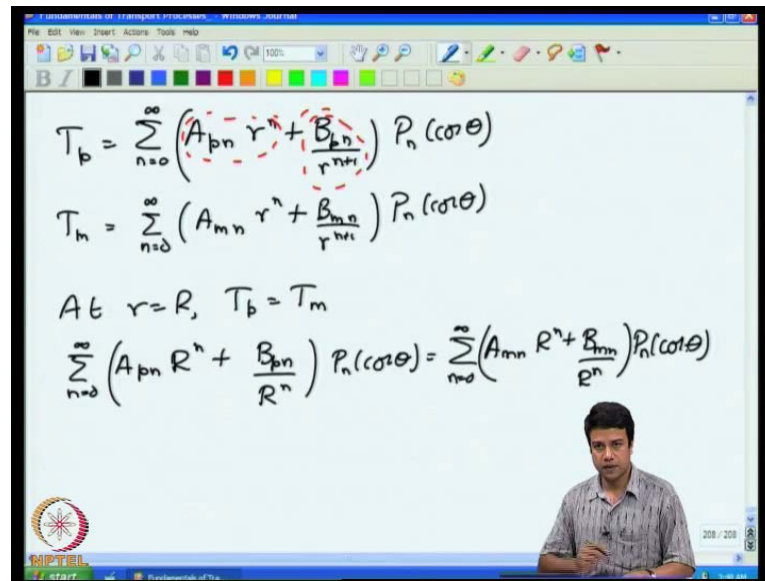
choose the particle radius as  $R$  then, at  $r$  is equal to  $R$   $T$  particle is equal to  $T$  matrix. So, I require that the temperatures in the particle and the matrix phase are both equal. Also, the heat fluxes normal to the surface have to be equal minus  $q_r$  in the particle is equal to minus  $q_r$  in the matrix. So, the heat fluxes in the two phases have to equal and in the limit as  $r$  goes to infinity goes to infinity, I should require that the temperature has to have this form. The temperature has to be the prime times  $z$ . As I said as far as the temperature field is concerned I can determinate only to within a constant because the contribution to the thermal conductivity depends only upon the **the** derivative of the temperature.

So, without loss of generality I can assume that the temperature at the center of the particle as far as this calculation is concerned the temperature at the center of the particle is equal to 0. So, first things first I have a **a** temperature field that is linear. So, far away my flux lines are all straight lines because the temperature field is linear. Near the surface there is going to be a disturbance to this depending upon whether the particle is more or less conducting than the matrix. I will have a disturbance to this temperature field and that is the disturbance that I would now like to calculate.

So  $\nabla^2 T$  particle is equal to 0 and  $\nabla^2 T$  matrix is equal to 0. That means that I can use this spherical harmonic expansions for both the particle and the matrix in a coordinate system with center at the origin of the sphere.

So, I choose a coordinate system with the center at the origin of the sphere and within that coordinate system I can then write down my equations, my spherical harmonic expansions which satisfy  $\nabla^2 T$   $\nabla^2 T$  particle is equal to 0 and  $\nabla^2 T$  matrix is equal to 0. First of all note that this is an axis symmetric problem. There is no variation in the  $\phi$  direction as I go around the axis because the temperature field is only in the  $z$  direction the temperature gradient is only in the  $z$  direction. So, for this particle there is no variation in the  $\phi$  direction as I go around  $z$  axis. That means that my solutions for in the  $\phi$  direction will basically be constants  $m$  is equal to 0. Remember that when I had solved for the  $\phi$  direction I got  $e$  power plus or minus  $i m \phi$  or  $\cos$  and  $\sin$  of  $m \phi$ .

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$$T_p = \sum_{n=0}^{\infty} \left( A_{pn} r^n + \frac{B_{pn}}{r^{n+1}} \right) P_n(\cos \theta)$$

$$T_m = \sum_{n=0}^{\infty} \left( A_{mn} r^n + \frac{B_{mn}}{r^{n+1}} \right) P_n(\cos \theta)$$

At  $r=R$ ,  $T_p = T_m$

$$\sum_{n=0}^{\infty} \left( A_{pn} R^n + \frac{B_{pn}}{R^n} \right) P_n(\cos \theta) = \sum_{n=0}^{\infty} \left( A_{mn} R^n + \frac{B_{mn}}{R^n} \right) P_n(\cos \theta)$$

These are constants only if  $m$  is equal to 0 therefore, I can restrict attention to solutions for  $m$  is equal to 0 alone. For the particle I will have solutions for  $m$  is equal to 0  $n$  goes from 0 to infinity of  $A_{pn} R^n + B_{pn} / R^{n+1} P_n$  of  $\cos \theta$  and  $T_{matrix}$  is equal to summation  $R^n + B_{mn} / R^{n+1} P_n$  of  $\cos \theta$ . At the coefficients  $A$  and  $B$  for the particle and the matrix have to be determined from the boundary conditions. As  $r$  goes to infinity; so first things first let us look at the particle. The particle consist of two terms one is a growing harmonic, one is a growing term which increases as  $r$  increase and the other is a term which decreases as  $r$  increases. Similarly, the matrix also contains a term that increases as  $r$  increases and another term which decreases as  $r$  increases. At the surface at  $r$  is equal to capital  $R$  I require that  $T_p$  is equal to  $T_m$  which means that summation  $n$  is equal to 0 to infinity of  $A_{pn} R^n + B_{pn} / R^{n+1} P_n$  of  $\cos \theta$  is equal to summation infinity of  $A_{mn}$ .

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$$A_{pn} R^n + \frac{B_{pn}}{R^n} = A_{mn} R^n + \frac{B_{mn}}{R^n}$$

$$q_r = -k_p \left. \frac{\partial T}{\partial r} \right|_{r=R} = -k_m \left. \frac{\partial T}{\partial r} \right|_{r=R}$$

$$k_p \left[ A_{pn} (n R^{n-1}) - \frac{B_{pn} (n+1)}{R^{n+2}} \right] = k_m \left[ A_{mn} n R^{n-1} - \frac{B_{mn} (n+1)}{R^{n+2}} \right]$$

Since the Legendre polynomial are all orthogonal to each other **since the Legendre polynomials are all orthogonal to each other** I can multiply this entire equation by  $P_n$  of  $\cos \theta$  and integrate and I will just get that the coefficients are both equal that is  $A_{pn} R^n + B_{pn} / R^n$  is equal to  $A_{mn} R^n + B_{mn} / R^n$ . So, this is one set of conditions from the temperature being equal at the bounding surface. In addition, the flux is also equal the flux  $q_r$  is equal to minus  $k_p$  partial  $T$  by partial  $r$  at  $r$  is equal to  $R$  is equal to minus  $k_m$  partial  $T$  by partial  $r$  for the matrix at  $r$  is equal to capital  $R$ .

Therefore the equality of the flux requires that  $k_p$  into  $A_{pn} R^{n-1} - B_{pn} (n+1) / R^{n+2}$  is equal to  $k_m$  into  $A_{mn} n R^{n-1} - B_{mn} (n+1) / R^{n+2}$ . Just doing the same thing these will of course, have the Legendre polynomials sitting beside them and I should be equating the summation of these two. But, since the Legendre polynomials are all orthogonal, I can without loss of generality set the coefficients equal to 0. This is for all values of  $n$ .

However, these are the flux conditions. Four constants; I have one condition for the temperature the other condition for the flux. I also have conditions to satisfy at the center of the particle as well as in the limit as  $r$  goes to infinity; far away from the surface of the particle.

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$$k_p \left[ A_{pn} (n R^{n-1}) - \frac{B_{pn} (n+1)}{R^{n+2}} \right] = k_m \left[ A_{mn} n R^{n-1} - \frac{B_{mn} (n+1)}{R^{n+2}} \right]$$

At  $r=0$ ,  $\frac{\partial T_p}{\partial r} = 0 \Rightarrow B_{pn} = 0$  for all  $n$

As  $r \rightarrow \infty$ ,  $T = T' z = T' r \cos \theta = T' r P_1(\cos \theta)$

$$\sum_{n=0}^{\infty} \left( A_{mn} r^n + \frac{B_{mn}}{r^{n+1}} \right) P_n(\cos \theta) = T' r \cos \theta = T' r P_1(\cos \theta)$$

$$\Rightarrow A_{m1} = T' \text{ \& } A_{mn} = 0 \text{ for } n \neq 1$$

At the center  $r$  is equal to 0; I require that the derivative partial  $p$  by partial  $r$  is equal to 0. This you will recall is a symmetry condition at the center of the particle itself if this is not 0 then you get different slopes as you approach the center from different directions the only way that the **the the the** slope will be identically equal to 0 regardless of the direction that you approach it from is if partial  $T$   $p$  by partial  $r$  is equal to 0.

So the condition at the center of the particle implies that all of these terms are identically equal to 0 at the center of the particle because they are 1 over  $r$  power  $n$  plus 1. These terms diverge as  $r$  goes to infinity. Therefore, you have terms that go only as 1 over  $r$  power  $n$  plus 1. Since these go to infinity the coefficients  $B_{pn}$  has to be equal to 0. Therefore, this implies that  $B_{pn}$  is equal to 0 for all  $n$  **this implies that  $B_{pn}$  is equal to 0 for all  $n$ .**

Therefore these terms basically cancel out in these conditions. Within the particle you have you can have only growing harmonics because the decaying harmonics go to infinity at the center of the particle. How about the matrix? As  $r$  goes to infinity, I require that  $T$  is equal to  $T' z$ .  $z$  is equal to  $r \cos \theta$   $T' r \cos \theta$  which is equal to  $T' r P_1$  of  $\cos \theta$ . If you recall, when we did the Legendre polynomial expansion we had said that  $P_0$  of  $\cos \theta$  is equal to 1,  $P_1$  is equal to  $\cos \theta$ ,  $P_2$  is equal to  $\frac{3}{2} \cos^2 \theta - \frac{1}{2}$  and so on. And these are all orthogonal to each other.

Therefore this contribution in the limit as  $T$  prime as  $r$  goes to infinity the solution has to converge to  $T$  prime times  $T$  times  $\cos \theta$ . What that means in the equation for the matrix is that you can see this term here  $A_{m,n} R^n P_n(\cos \theta)$ . So, this has to be equal to  $T$  prime times  $\cos \theta$  in the limit  $T$  prime times  $r \cos \theta$  in the limit as  $r$  goes to infinity. So, I require that summation  $A_{m,n} R^n P_n(\cos \theta) + B_{m,n} r^{n+1} P_n(\cos \theta)$  is equal to 0 to infinity is equal to  $T$  prime  $r \cos \theta$ . Of course, as  $r$  goes to infinity these terms all decrease to 0. But, if you look at the growing harmonics in the limit as  $r$  goes to infinity for  $n$  is equal to 1 it increases proportional to  $r$ , for  $n$  is equal to 2 it increases proportional to  $r$  square, for  $n$  is equal to 3 it increases proportional to  $r$  cubed and so on. So, these terms do not decrease to 0. This equality will be satisfied, this is equal to, now I can use orthogonality relations. I can multiply both sides by  $P_m(\cos \theta)$  and integrate  $\sin \theta d\theta$ .

If I integrate both sides; the right hand side is non 0 only when  $m$  is equal to 1. If I integrate if I multiply by  $P_m(\cos \theta)$  where  $m$  is some other coefficient the right hand is 0 only when  $m$  is equal to 1. So, this I will get  $T$  prime  $r \delta_{m,1}$ . So, what this implies is that on the left hand side, I have the coefficients. The right hand side is 0 unless  $m$  is equal to 1 which means that  $A_{m,1}$  is equal to  $T$  prime and  $A_{m,n}$  is equal to 0 for  $n$  not equal to 1. So, the coefficient  $A_{m,1}$  is equal to 0, coefficients  $A_{m,2}$   $A_{m,3}$  etcetera all other coefficients are identically equal to 0.

So, that is what you get by the orthogonality relations in the limit as  $r$  goes to infinity. So, from the orthogonality relations, so from the symmetry boundary conditions at  $r$  is equal to 0  $B_{p,n}$  was equal to 0. Orthogonality relations as  $r$  goes to infinity  $A_{m,1}$  is equal to is non 0, is equal to  $T$  prime all other coefficients are equal to 0. So, let us put this for the conditions that I had for the temperature and the flux.

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$$A_{p1} R = A_{m1} R + \frac{B_{m1}}{R^2}$$

$$k_p A_{p1} = k_m A_{m1} - \frac{2 B_{m1}}{R^3}$$

For  $n > 1$

$$A_{pn} R^n = \frac{B_{mn}}{R^{n+1}}$$

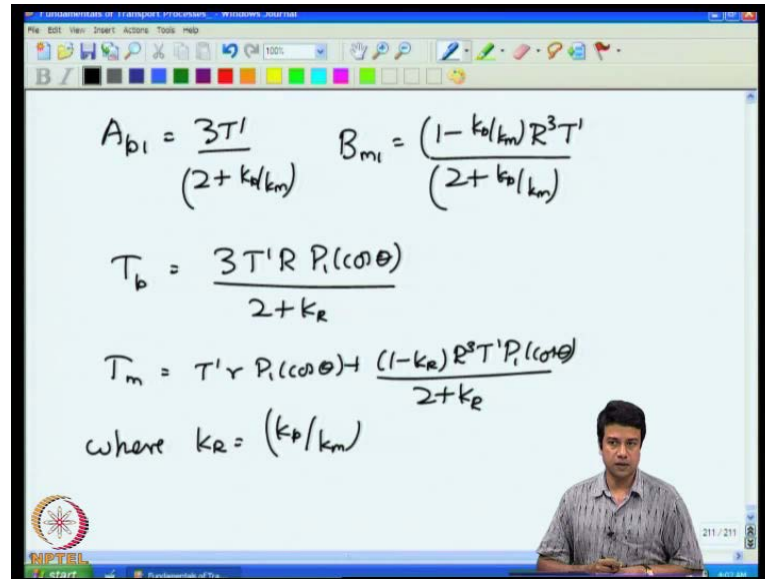
$$k_p A_{pn} n(R^{n-1}) = -\frac{k_m B_{mn}(n+1)}{R^{n+2}}$$

$$A_{pn} = 0 \text{ \& } B_{mn} = 0$$

So, I have  $A_{pn} R^n$  is equal to  $A_{m1} R$  plus  $B_{mn} R^{n+1}$ . This coefficient one is this is non 0 only for if so let us just write out the coefficients separately for  $n$  is equal to 1 and for all other coefficients. So, for  $n$  is equal to 1  $A_{pn} R^n$  is equal to  $A_{m1}$   $A_{p1} R$  is equal to  $A_{m1} R$  plus  $B_{m1}$  by  $R$  square and  $k_p A_{p1}$  is equal to  $k_m A_{m1}$  minus  $2 B_{m1}$  by  $R$  q. So, these are the coefficients for  $n$  is equal to 1. For all other values of  $n$   $A_{mn}$  is equal to 0. So, I will have the **the** temperature condition is  $A_{pn} \times r$  is equal to  $B_{mn}$  by  $R$  power  $n$  plus 1 and  $n r$  **yeah** and  $k_p A_{pn} \times R^{n-1}$  is equal to minus  $k_m B_{mn}$  by  $R$  power  $n$  plus 2 into  $n$  plus 1.

So, for  $n$  greater than one you can see that in these two equations for  $A_{pn}$  and  $B_{mn}$  there is no inhomogeneous term in the equation for  $A_{pn}$  and  $B_{mn}$  **There is no inhomogeneous term in the equation** which means that the only solution is that for each value of  $n$   $A_{pn}$  is equal to 0 and  $B_{mn}$  is equal to 0. So, you do not have any contributions to the expansion for  $n$  greater than 1. You have contribution only for  $n$  is equal to 1 that is because the forcing in the limit as  $r$  going to infinity was only for  $n$  is equal to 1 there was no forcing for  $n$  greater than 1. For  $n$  is equal to 1 you have this inhomogeneous term  $t A_{m1}$  is equal to  $T$  prime and because of that you have this in homogeneous term and for the combination of these two equations you can get solutions for all of the constants within the equation you can solve the simultaneous equations quite easily.

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$$A_{p1} = \frac{3T'}{(2 + k_p/k_m)} \quad B_{m1} = \frac{(1 - k_p/k_m)R^3 T'}{(2 + k_p/k_m)}$$

$$T_p = \frac{3T' R P_1(\cos\theta)}{2 + k_R}$$

$$T_m = T' r P_1(\cos\theta) + \frac{(1 - k_R)R^3 T' P_1(\cos\theta)}{2 + k_R}$$

where  $k_R = (k_p/k_m)$

And I will just give you the final solutions that you get  $A_{p1}$  will be equal to  $3 T'$  prime by 2 plus  $k_p$  by  $k_m$  and  $A_m$  sorry  $B_{m1}$  is equal to 1 minus  $k_p$  by  $k_m$  into  $R$  cubed  $R$  prime by 2 plus  $k_p$  by  $k_m$ .

So, these are the final solutions for the temperature fields. So, there is in the particle and that is in the matrix. That means that the temperature field in the particle is equal to  $3 T'$  prime  $R P_1$  of  $\cos \theta$  by 2 plus  $k_R$  and  $T_m$  the matrix equal to  $T'$  prime  $r P_1$  of  $\cos \theta$  plus 1 minus  $k_R R$  cubed  $T'$  prime  $P_1$  of  $\cos \theta$  by 2 plus  $k_R$  where  $k_R$  is equal to the ratio of the conductivities of the particle and the matrix.

So these are the solutions that we get for the temperature fields in the particle and the matrix. Using these now we can determine what is the effective thermal conductivity of the composite.

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where  $k_R = (k_p/k_m)$

$$\langle q_z \rangle = -k_m T' + \frac{N}{V} \int dV (-k_p - k_m) \frac{\partial T}{\partial z}$$

$$= \left[ -k_m T' + \frac{N}{V} \int dV [-(k_p - k_m)] \left( \frac{3T'R}{2+k_R} \right) \right]$$

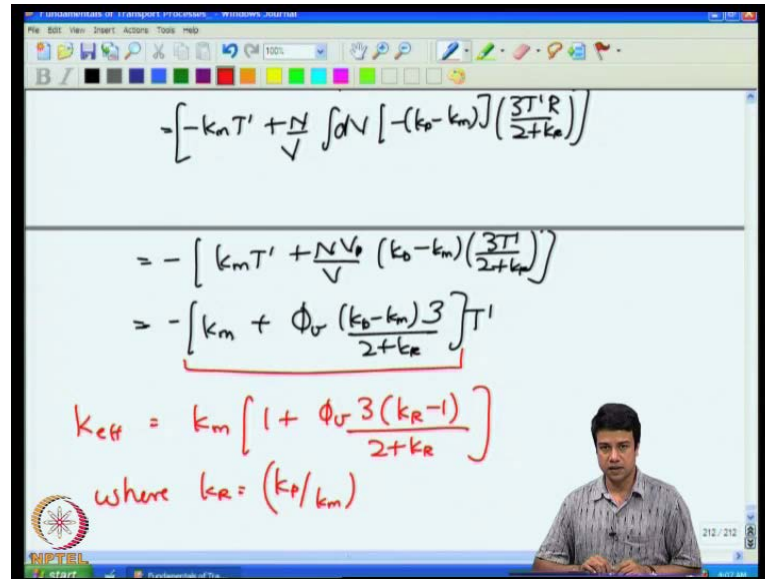
$$= - \left[ k_m T' + \frac{N V_p}{V} (k_p - k_m) \left( \frac{3T'}{2+k_R} \right) \right]$$

$$= - \left[ k_m + \phi_v \frac{(k_p - k_m) 3}{2+k_R} \right] T'$$

If you recall we had said that  $q_z$  is equal to minus  $k_m T'$  plus integral over plus 1 over the volume of one particle, integral over the particle volume of minus of  $k_p$  minus  $k_m$  times  $dT$  by  $dz$ . For the particle this can be written as  $R$  into  $P$  1 of  $\cos \theta$  is just  $z$  itself  $P$  1 of  $\cos \theta$  is  $\cos \theta$  itself. Therefore,  $R$  into  $P$  1 of  $\cos \theta$  is just  $z$  itself. So, we just take the gradient of this with respect to  $z$  I will finally, get what is the temperature field. If I take the derivative of this with respect to  $z$  this becomes minus  $k_m T'$  plus  $N$  by  $V$  integral over the volume of minus of  $k_p$  minus  $k_m$  into  $3 T' R$  by  $2$  plus  $k_R$ .

This derivative is independent of the particle volume position. This derivative is just a constant. So, I can just take it out of the differentiation sign this will give you minus of  $k_m T'$  plus  $n$  into that volume of one particle divided by the total volume. This was total volume. Volume of one particle divided by the total volume into  $k_p$  minus  $k_m$  into  $3 T' R$  by  $2$  plus  $k_R$ . The number of particles times the volume of one particle divided by the total volume is just the volume fraction is equal to minus of  $k_m$  plus the volume fraction  $\phi_v$  into  $k_p$  minus  $k_m$  into  $3$  by  $2$  plus  $k_R$  into  $T'$ .

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$$\begin{aligned}
 & - \left[ -k_m T' + \frac{N}{V} \int dV [-(k_p - k_m) \left( \frac{3T' R}{2 + k_p} \right)] \right] \\
 & = - \left[ k_m T' + \frac{N V_p}{V} (k_p - k_m) \left( \frac{3T' R}{2 + k_p} \right) \right] \\
 & = - \left[ k_m + \underbrace{\Phi_v \frac{(k_p - k_m) 3}{2 + k_p}} \right] T' \\
 & k_{eff} = k_m \left[ 1 + \frac{\Phi_v 3(k_p - 1)}{2 + k_p} \right] \\
 & \text{where } k_p = (k_p / k_m)
 \end{aligned}$$

So this finally, gives me the conductivity of a composite material. This entire coefficient here is the effective conductivity.  $k_{\text{effective}}$  is equal to  $k_m$  to 1 plus the volume fraction into three into  $k_R$  minus 1 by 2 plus  $k_R$ .

You can easily see  $k_R$  is equal to  $k_{\text{particle}}$  by  $k_{\text{matrix}}$ . So, the correction to the conductivity of the composite material is proportional to the volume fraction in the very dilute limit because as the volume fraction goes to the 0; you have to recover the conductivity of the matrix itself. Conductivity increases as the particle has a higher conductivity because  $k_R$  minus 1 is positive. The effective conductivity decreases if the particle has a lower thermal conductivity than the matrix because  $k_R$  minus 1 is negative.

So in this limit for non interacting particles that is when the particles are sufficiently far, that the temperature field around one particle does not affect the temperature field around another particle; we were able to solve for a single particle in temperature field which is a linear function of  $z$  axis far away. From that we were able to calculate the conductivity. Turned out to be quite simple. The original expansion that we had was for  $n$  is equal to 0 to infinity here an infinite number of terms. However we found that in this particular case only the term with  $n$  is equal to 1 was non 0 all other terms were identically equal to 0.

We look at a little in a little more detail, look at the symmetries a little more detail in the next lecture. Why we said that we were able to get a solution quite easily? Previously when we did the **the** solution in **in in** Cartesian coordinate system for a cube; the solution was an infinite sum of coefficients times the times the sine and cosine functions and in that case you are getting all coefficients to be non zero. In this particular case, we got only one coefficient to be non zero. The coefficient proportionate to  $P_1^0$  of  $\cos \theta$  that is because of symmetries and we will see that a little later in the next lecture and we look at another interpretation of this particular spherical harmonic expansion. It is not just some function of  $\theta$  and  $\phi$ ; it has other physical interpretation in the form of sources, dipoles and multi pole expansions. So, look at that in a little more detail in the next lecture. So, we will continue this discussion of spherical harmonics expansions in the next lecture and we will give a more detailed interpretation of this in **in in** another physical sense, in terms of sources, dipoles and so on. So, we will continue in the next lecture.

**Thank you.**