Micro and Nanoscale Energy Transport Prof. Dr. Arvind Pattamatta Department of Mechanical Engineering Indian Institute of Technology, Madras

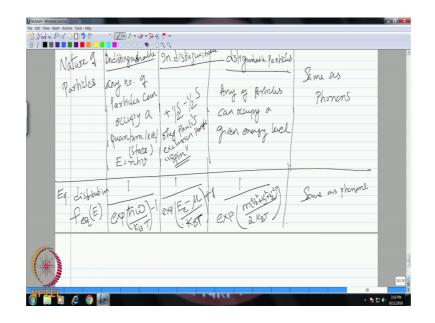
Lecture - 6 Microscopic Contributes to Internal Energy of Systems

(Refer Slide Time: 00:20)

			1 1	1
Enersy Prenentahion	Wave Velor K Frquency, is Modesand Polanjation	Wave vectors (p) Spin_	Momentum, P, Kinetic, Potential energies	Repenty D Polarization.
Particle Type	Bose-Eistein (Bosonis)	Fermi-Dirac (Fermions)	Naxwel-Boltmann dishibitin Castical dishibition	Jose-Einskin (Zoens).
		[

Very good afternoon, today we will continue our discussion related to the differentiation of the energy carriers in different media and their attributes that we are looking at. So, we will add on to the attribute where we stopped yesterday that was the type of particles, we classified for example phonons, which are responsible for heat conduction in semiconductors and die electrics. So, they are essentially described by the statistical distribution function called Bose Einstein distribution function and therefore, they are called bosons and what is the therefore, nature of this particle.

(Refer Slide Time: 01:17)



So, I mean when we are also talking about the corresponding you know particle type; we need to understand their nature, so let us also write down the classification based on the nature of particle. So, as I talked about now you should know that statistical thermo dynamics these different particles are classified for example, the bosons have a characteristics that they are indistinguishable and; that means, you cannot distinguish the character carriers themselves you know from each other, they all look alike and there is no limit to any number of particles fix or you cannot fix the number of particles which can occupy a quantum state and therefore, you can say that any number of particles can occupy by a given quantum state or energy state. Quantum state is nothing but an energy level or discrete energy level; we will see all those things in a short while or a quantum state.

So, this is maybe you can say something like integer multiples of h nu where n can be 1, 2, 3 and so on. So, these are discrete energy levels and at each energy level if there is no restriction on the number of bosons that can be that can occupy. Same thing follows also for the photons, which are also coming under the boson category; so they are also having the same as phonons and when we look at electrons for example, they are described by Fermi-Dirac distribution function and the nature of these particles is there also indistinguishable.

However you have a problem that for a given spin you have a plus half and minus half

spin quantum states, so only one electron can occupy a particular spin quantum state, you cannot have more than if you have a plus half spin that electron can occupy that quantum state and minus half spin can occupy the other one and so on. So, this has to obey therefore, Pauli's exclusion principle in terms of the occupation of the quantum states because of the spin electron posses this unique characteristic. So, therefore, only one electron can occupy a given quantum state plus half quantum state or minus half quantum state depending on the integer spin.

Now, the molecules coming to the molecules; now molecules are real atoms. So, you can actually distinguish between the molecules, molecular of a particular gas will be different from another gas and again. So, therefore, these are coming under the nature of distinguishable particles and again you know just like you have your bosons, you can have any number of molecules can occupy an energy level; however, these are governed by the distribution function called the Maxwell Boltzmann, which is not a quantum mechanical distribution function, but it is a classical distribution function; that means, the energy levels are not quantized or discrete like the case of Bose Einstein or Fermi-Dirac the Maxwell Boltzmann continuous energy levels, we will see all those things we will understand it gradually, but this is very important way of classifying the energy carriers.

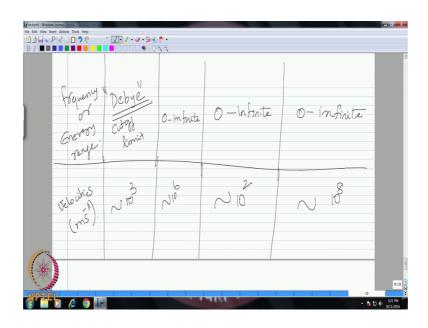
So, let us also write down in the corresponding distribution function now, we will derive this when we do this under statistical thermo dynamics. So, equilibrium distribution or occupancy function; so this is your f equilibrium as a function of the energy of the particle, so this is what we derive from the statistical thermodynamics. Describing the equilibrium what is the distribution of the particles at a given energy level under equilibrium conditions. So, if you look at the Bose Einstein distribution function you can write this as one over, exponential, e by k b t; where e is the energy.

Now in the case of phonons and photons, this energy is nothing but h nu is equal to h nu Planck's law. You can also write this h nu in terms of modified Planck's constant h cross, as h cross into omega the angular frequency, so we can multiply and divide by 2 pi, so 2 pi nu will be the angular frequency omega. So, h nu by the Boltzmann constant k b times t; the denominator entire thing minus 1. So, you have 1 by exponential h nu h cross omega by k b t; minus 1 is the equilibrium function given by Bose Einstein and the same thing holds for also the photons and when we look at the Fermi-Dirac distribution

function, structurally it looks little bit similar but you write this as the energy of the electron or the energy of that particular quantum state which the electron occupies minus this is called the Fermi energy; nu, sometimes people use this as e subscript f, which is the kind of a reference energy level, so divided by k b t.

Now, the major differentiator between the Bose Einstein & Fermi-Dirac instead of minus 1, there is a plus 1 here. So, otherwise structurally it looks very similar and then for the molecules which are given by the Maxwell Boltzmann distribution function, you can write this as 1 by exponential. Now the energy e for the case of molecule will be what primarily, kinetic energy, so you can write this as half m v square or m c square or m v square because c may confuses speed of light. So, v square is actually absolute velocity which includes speed and all the three directions because the molecule can actually collide with motion and all the three directions v x, v y, v z. So, therefore, you can actually write this as v x square plus v y square plus v z square divided by 2 and you have also the k b t, so this is your Maxwell Boltzmann distribution function.

(Refer Slide Time: 10:13)



All though they look very similar, we should understand that what is classical about the Maxwell Boltzmann distribution is that v x, v y, v z are speeds and they are continuous; minus infinity to plus infinity, whereas h bar omega, energy of quantum state they are all discrete. For example, although this says h bar omega they are n into h bar omega, so the discrete levels of energy 1, 2, 3, 4 depending on that. So, that is why the Maxwell

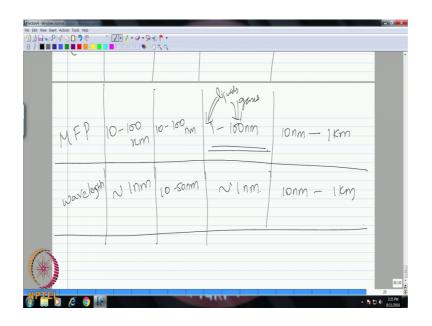
Boltzmann distribution is called a classical distribution function where are others are quantum mechanical distribution functions they exhibit this discrete nature.

So, what is the corresponding frequency or energy range, now when you talk about phonons what will be the maximum energy till phonons can posses is it 0 to infinity? No whereas for molecules, it can have 0 to infinite. Similarly for the electrons, it can occupy energy states all the way from 0 to infinite depending upon the temperature and depending upon the material, your photons can have energy levels from 0 to infinite, but your phonons being crystal.

So, there is a maximum frequency till which the phonon can be present and therefore the energy is limited by an upper cut off, so this is called as Debye cut off limit. So, this is Debye cutoff is basically dictated by the solid states, physics for which we describe the phonon dynamics. So, the material will dictate what can be the maximum possible frequency that a phonon can take this is called the Debye limit.

And let us also look at the order of magnitude of the velocities; this is an meter second inverse. What is the order of magnitude of phonon velocity? This is speed of sound in a given lattice, usually this acoustic sound is of the order of 10 power 3 meters per second, may be few thousands; usually in crystals speed of sound is quite high. So, the order of thousand it could be even 10000 sometimes meters per second and now when it comes to electrons what do you think will be the speed of these electrons, free electrons of the order of 10 power 6 million meter per second and when you talk about molecules; gas molecules for example, it should be the order of few hundreds, 100s of meter per second. So, it is 10 to the power 2 and what about the speed of light; 10 power 08, so you know each of this energy carrier also limited by the corresponding speeds that they can take; the order of magnitude is quite different.

(Refer Slide Time: 14:42)



And we will also express the mean free path, which is a very important characteristic to understand sub continuum transport. So the mean free path of phonons typically ranging between, 10 to 100 nanometers. So if you are describing these lattice vibrations by representing them as particles, so the separation, the average distance between two of these phonons before they collide will be traveling around 10 to 100 nanometers distance. So, therefore, if you are having a device lens scale which is lesser than 100 nanometers then you are definitely falling in the sub continuum regime.

So, if you are talking about electrons they also possess a similar mean free path as a phonon, 10 to 100 nanometers; whereas the molecules can have even lesser mean free path especially we are talking about gases they can have very small values of mean free path close to even 1 nanometer, in liquids it can go to order of 100 nanometers. In fact, I think, so you have to be very careful with the order of mean free path that you are talking about sorry it should be the other way.

So, for the gases it should be of the order of 100 nanometers I am sorry and liquid it should be around 1 nanometer. So, the chances of therefore finding sub continuum with gases is very high, if you are having a 100 nanometer channel and full it with gas, you are already in the sub continuum level, whereas with liquid same dimensions of channel you will be still in the macro scale regime and when it comes to photon transport, so they also have similar starting value as the phonon and electron, but the ending value can be

very large depending on the kind of electromagnetic wave which spectrum part of the spectrum which you are in.

So, therefore, you have different length scale associated with each of this energy carriers, the other length scale that is required to understand the quantum mechanical aspects that is your wave length. So, the wave length of phonons is the order of 1 nanometer. So, now, if you are reducing your device dimension to the order of 1 nanometer, now you will start experiencing wave effects because yeah.

Student: (Refer Time: 17:50).

The photons mean path is you can approximate them to be similar to the wave lengths that you are electromagnetic waves are experiencing. If a wave length is of the order of kilometers you can, if you represent them with photons; that is the average separation between the photons before they interact something of that sort. So, similarly I mean in photons it is not very explicit like the way phonons because they are all in medium; the other three whereas electromagnetic waves they are operating in vacuum, so how do you explicitly, but here it is the scale of similar to the scale of wave length.

In fact, that is why now when I explicit put wave length, now I am going to say that for the case of photons again the wave length scale will be similar as the mean free path. So, you are just looking at the wave length and your mean free path is also of the same order. where as they are quite different for the other energy carriers if you are looking at electrons.

For example they can vary between 10 to 50 nanometers and again for molecules it can be the order of 1 nanometer. So, therefore, things are not so simple I mean when you say Knudsen of 10, it depend on first the kind of media that you are talking about and again you have to be careful whether this approaches the wave length. So, then the quantum wave effects will also start appearing you have to be dealing those aspects as well.

So, over all this is a very elaborate classification of the energy carriers. So, I think by now you should fairly understand how these energy carriers appear in order to us; I mean out of these phonons and photons are virtual particles. Since we are talking about micro microscopic picture, we talked about approximating the lattice vibration with phonon gas and so on, similarly electron gas and we talked about the characteristics.

(Refer Slide Time: 20:25)

	Moder & Cassial Mechanics of Quantum Mechanics	
	$\frac{G_{negy}}{T_{Ruslation}} = \frac{m}{2} \frac{2}{2\pi} \frac{2}{2m} \frac{1}{2m} $	
	Robotional $E_{70k} = \frac{IW^2}{2}$ $E_{70k} = \frac{RB}{2}$ $E_{70k} = RB \frac{1}{2}$ $E_{70k} = RB \frac{1}{2}$ $E_{70k} = RB \frac{1}{2}$	
	Vibrohind Evibrohin $= \frac{1}{2}mc_1^2 kx^2$ $\left[\frac{E_{\text{tribular}}}{v_1 + 2} + \frac{1}{2}kx^2 - \frac{1}{2}\frac{E_{\text{tribular}}}{v_2 + \frac{1}{2}\frac{1}$	
*		

So, the next question will be talking about how much energy or momentum can each of these energy carriers poses, that will be the next question right. So, each of this particles micro scale level will be governed by the corresponding momentum or energy they process. So, what is it? How is it classified? So, let us also give some kind of classification of that. So, when we say energy again we have to be little bit more explicit about micro scale that we can talk about either a classical energy like kinetic energy, when you are looking at the particle nature or if you are talking about wave nature that is very very small dimensions or the wave length becomes significant order as the characteristic dimension, then the wave effects will now bring in quantum mechanical things into picture.

So, therefore if you are talking about particle nature, you are having the classical mechanics, to study the energy possessed by the particular energy carrier. If you are talking about the wave aspects then you have quantum mechanics to understand the energy, posses by these carriers. So, therefore, we will classify this into the energy in the quantum mechanics regime and the classical regime.

Now, again we have different modes of energy, now when you look at particles for example, what are all the different kinds of energy this particle can posses. So, for example, atoms single atoms, monatomic structure. So, what can one it can have transits very good translational energy. So, for a single atomic substance, one atomic gas for

examples can there be rotational energy? Cannot be, for diatomic molecule then then rotational energy can also.

So, you can talk about rotational energy and then what about also you have for example, the picture of phonon which is nothing, but 2 atoms connected by a spring you have vibrational energy same thing with inter atomic potential between molecules and so on. So you also have vibrational energy. So, these are the 3 major microscopic energies which added together, will decide what is the average total energy process by the particle that will contribute to on the macro scale internal energy. Internal energy on the macro scale is nothing, but the sum of all this three microscopic energies.

Now, these can be there both from the classical mechanical perspective as well as quantum mechanical perspective, depending on what scales you are looking at. Now when you are talking about for example, the translation energy from classical mechanical perspective what is the translation energy? half m v square, you have a particle with velocity v and therefore, the corresponding momentum m v, the energy is half mv square. So, if you write this into terms of momentum. So, let us say momentum p is equal to m times v. So how can we write this in terms of p.

Student: p square.

P square by 2 m right, now what we will do here is quickly switch on suddenly from the particle to the wave nature. So, there is a relationship between the momentum and the wave vector, if you look at the wave nature. So that is given by modified planks constant time K, where k is nothing but wave vector related to wave length lambda, 2 pi by lambda. So, therefore, if you substitute his into the relation h cross times k you are p will be nothing, but p by h by lambda.

So, this wave length lambda which is h by p is called the Deborah of the wave length. So, this says that the wave length is related to the momentum of this particular wave. So, you can easily switch between toggle between the particle picture, wave picture, whenever p square by 2m is from the particle picture, in the equivalent wave picture if you are substituting for p as h cross times k, modified plans constant times k. So, this will be h cross square k square by 2 m.

Now, the k is you know wave vectors; it is a vector in space and therefore, when you say

k square, is the square of the magnitude of the wave vector. So, therefore, we can write it this as K x square, plus K y square, plus K z square, but here this is classical mechanics so this is continuous waves.

So, therefore, the wave vector k in the x direction K x, K y and k z is all continuous. So added together they will contribute to the translational energy. Now in the quantum mechanics how do we find this translational energy, so, this is done by solving the Schrodinger wave equation and the typical system that you will consider as called the Particle in a box. This is one of the simplest systems to which Schrödinger equation solved easily, analytical solutions possible.

So, you have what is called as a quantum well, where you have a single particle like this and within the well have a certain potential and outside the well this particle cannot escape because the potential will be infinite outside. So, it cannot escape from that well. Within the well the particle has a certain potential energy u, but it cannot come out of that well. So, it always confined to that well. So, this is called a Particle in a box or quantum well. Quantum well is 1d, if you make it 2 dimensional it becomes a box. Let us confinement in both directions left right top bottom also.

So, in this case when we solve this Schrodinger's wave equation, which we will do next week, you will end up getting expression for the energy .So, how we calculate, how do we find energy in quantum mechanical state? So, this energy turns out to be the Eigen value of Schrodinger's equation. When we Schrodinger's equation is a partially differential equation, we have to solve that by method of separation of variables, we separate that into an o d which is a function of space and another which is function of time and the equation o d is function of space will have a certain Eigen value, and that Eigen value will give you the energy and if you calculate that, it turns out to be very similar to what we have for the classical particle. Except the fact that, the k now becomes discrete energy states, for example, if you are talking about K x you can write this as some l pie by d, where l is an integer it can go from1,2 3,0, 1,2, 3,4,and so on infinite number of energy states. Similarly in the y direction it will be another integer, m pi by d and in the z direction it could be n pi by d.

So, now this is very where the quantum mechanical energies are different from the classical energy. Classical energy is a continuous, where as quantum mechanics what it is

doing the particle, when you put it in a box it is confined and now this confinement because of the wave nature we are talking about the box, which is of the order of nanometers 1 nanometer, 2 nanometer So the wave nature is going to break this continuous wave into discrete energy levels. So, this is called Quantum confinement. This d is basically the width of this particular well.

Student: Sir what is procedure significance (Refer Time: 31:21) where we represent in terms of wave vector.

Generally mean in physics, especially quantum mechanics all this waves posses certain momentum of energy and they are all functions of the wave vector. This is how I have given, this is the fundamental expression which relates some momentum, similarly energy also can be related, we have related also now energy with respect to the wave vector, and momentum is also related to the wave vector.

So, you want to understand what is physically a wave vector; So, for that we will take few more classes, down the line I will explain the wave vector space, just like you have a physical coordinates space x y and z that is the space where you can talk about velocities, momentum space, v x, v y, v z analog us to that is your wave vector space k x, k y, k z because this wave vectors are nothing, but related to a momentum particle momentum. So therefore, you can transform your momentum space into a wave vector space. The particles also posses' velocity is in each direction they can be plotted on that map v x, v y, vz map and they have a certain vector which is pointing in the direction of v vector, the same way is the k vector.

So, in quantum mechanics what we find is, basically this energy levels are no more continuous, but they get discretize because of the quantum confinement. You are confining this waves to a certain dimensional because of that they split of, that is no single value of energy, but there are multiple levels that they discrete levels also. So, this is where the quantum effects, what people say quantum effects start appearing. So, the all the wave vectors now become discrete integer, multiples of pi by d. But however, the gross expression here looks structurally similar to the classical mechanical expression.

Now, if you talk about rotational energy, in the classical mechanical perspective how do you calculate rotational energy, you replace your mass with moment of inertia and your linear velocity with your.

Student: Angular.

Angular velocity as simple as that; now in quantum mechanics we will solve Schrodingers equation, for the simplest rotational atom that is a hydrogen atom. The 2 atoms and they are rotating. So, for that we solve the Schrodingers equation to describe the energy content in the rotational due to rotation and we see once again they are quantized and that energy is again discrete energy, which is given as h into capital B into l into l plus one. So, where this l is the integer, 0, 1, so on infinite levels.

So this b here should be function of the moment of inertia I and then this become quantized and this quantization is nothing, but discrete levels, splitting of the energy into discrete levels and that is given by this integer 1 0 1 to infinity. This way this will also show under Quantum mechanics. Now when we go to vibrational energy, I will first if you look at the vibrational energy in the classical perspective, the simplest way to look at it is the spring mass system.

Student: Spring.

(Refer Slide Time: 35:39)

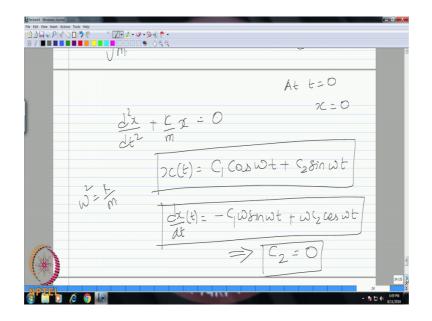
	Z₽ Z • Ø • 9 % ₱ • □ □ □ ● 0 ९ ٩		
	E K-18prild Constant	dt	
	1 2=0	$ \begin{array}{c} $	
*			22,

The atom can be assumed to be a mass and then the forces of attraction between the atoms can be assumed to be having a spring constant like nature, we are not considering damping now, will have only a spring constant and a mass, so therefore if you write down the equation of motion for this spring mass system.

So, let us say initially this is at some level x is equal to 0 and then you from this level you disturb it you pull it and let it go. So, the displacement is basically x is a function of time, depends on the amount of mass that you have and also this spring constant. So, you want to track the displacement as a function of time the velocity as a function of time. So, therefore, we solve the equation for this particular system.

So, you have mass into acceleration is equal to minus k x, this is where k is spring constant. So, if you solve this condition that at t is equal to 0. So, you have the fact that your velocity is 0, you start from resting state and then and you let it go.

(Refer Slide Time: 37:37)



So, therefore, d x by d t is equal to 0. So, how many conditions you need? You need 2 conditions, one is d x by d t and what about x, also at t equal to 0, x is equal to 0. So, what is the solution to this particular expression we can write this as, d square x by d t square plus k by m. I can represent this k by m I can use omega to describe square root of k by m. So, we will hold on to this we have k by m into x is equal to 0.

So, the solution to this will be basically as a function of sine and cosine right. So, therefore, we have x of t will be C1 cops square root of k by m. Now will replace it with omega plus C2 sin omega t and therefore, the velocity d x by d t differentiated will be C1 omega sin, omega t plus omega C2 into cos omega t. So now you please apply the initial conditions x equal to 0 and d x by d t is equal to 0 find out the constants C1 and C2.

So, the condition d x by d t is 0 should give you what? C2 should be 0. Therefore the other condition that x equal to 0, at t equal to 0. If you apply that, C1 cannot be 0 otherwise the solution becomes striver so $\cos \cos \cos t$ should be 0.

e4 - Windows Journal		
it View Insert Actions Tools Help		
	L • @ • 9 • 1 * •	
	=7 6	= () (
		0
	Coswt=0	
	0003 60 0 = 0	
	,	
	$U = dx = -C_{\mu} \omega sin$ $z = -C_{\mu} \omega sin$	24.
	U = = = (wan	WC
	ct	
	$r - C_1 COSU$	NE I
	C	
5	never = KE. + PE	
E E	nergy = Kt. + Pt	
	1er84	
		2 2 2
		Culenut
	= mu + ice	quoma
	2. 6 6	12 2 2 1
	$=\frac{1}{2}mv^{2}+\frac{1}{2}kx^{2}=\frac{1}{2}$	+ - CW LESNE
all a state		- 2'
***		22
sile 🔁	Enerry =) 1	νw
- Aller		
TEL		25
		 ► 12 ● 349 PM 8/11/201

(Refer Slide Time: 40:00)

So, this will give you the corresponding value of omega, so that should be expressed just a moment. We do not have to worry about that now. I think for calculating the energy, all we need is only the d x by d t only the velocity is required. So therefore C2 is equal to 0. So, therefore our velocity of motion d x by d t is given by minus C1 omega, sin omega t. and therefore, your x is C1 cos omega t.

So, therefore, the total energy in this case will be summation of your kinetic energy plus your potential energy. To a kinetic energy is the component of half m v square and potential energy is due to spring constant half k x square. So therefore, the total vibrational energy that we are talking about here consists of, both the kinetic and potential energy is together.

So, if you substitute for v into this expression and x into this. So, you have therefore, C1 square, omega square, sin square, omega t plus half into k can be now again written in terms of omega and m, as k square should be omega times n. So, you have omega times m and again m you can write in terms of again we can express k by m and therefore, m can be written as k by omega square. So they should be C1 square, omega square into cos square, omega t. essentially they come up to half C1 square omega square. So, this is

your total energy.

So, this is therefore for your vibrational energy, that we wanted to ill up to that consist of the summation of your kinetic and potential energy that is your half m v square plus half k x square, for the case of assumption of equivalent spring mass system which is a linear system, this turns out to be half of m C1 square, omega square. Just I will give you a couple of minutes to work it and check again or some of you are doing it slowly. I will go back to this point make sure that work out all the steps.

I think missed m here.

Student: (Refer Time: 45:04).

Yeah you are write that is what I was also thing here it should be m here, m C1 square, omega square because energy cannot be independent of mass right here I have written correctly good.

Similarly, in the quantum mechanical vibrational energy, we also considered similar problems spring mass problem, but we solved Schrodinger's equation for that, So, in that case we again have a quantized vibrational energy level and the energy for the vibration is given as h nu times n plus half, where your nu is nothing but 1 by 2 pi square root of k by m and your n can take the value 0, 1, 2, so on. So, this is some integer multiples of h nu, but instead of integer multiple we have n plus half coming into this picture and n is these are discrete levels.

When we solve the Schrodinger's equation, then you will understand why this is coming this way, but I mean there since e is the Eigen value, so you have this Eigen value of the Schrodinger's equation, this is coming as function of h nu, where nu is 1 by 2 pi square root of k by m. So, here also if you take the Eigen value you find the Eigen value from this expression. So, you should be able to come to a similar expression. So, have cos may be you can just try it this yourself here, we are doing the classical energy computations. So, putting the other initial condition tells you that your cos omega t is equal to 0, that means, omega t should be.

Student: (Refer Time: 46:43).

Is it n pie by 2 how about 2 n plus1.

Student: 2 n plus 1.

2n plus 1.

Student: pi by 2.

Pi by2. So, in this case you are saying that omega is equal to omega t is basically 2 n plus 1 pi by 2. So, this are the Eigen values, for n is equal to 0, 1, 2, 3, and so on. Similarly for the Schrodinger's equation, the Eigen vales are giving the vibrational energy levels, h nu into n plus half. So, this is what we will do in the next few classes, we will go into quantum mechanics solve the Schrodinger's equation and we will see how the Eigen values are obtained and how do we actually derive this particular expressions.

So, what I would like to do is now stop here. So, we have I think had lot of classes for introduction, I think spend couple of weeks only on the introduction part, but it gives very good foundation now you are able to understand different kinds of energy carriers, different media and their characteristics and also you should able to appreciate that energy when we talk about as a micro microscopic basis and also in micro scale there can be energy associated with the particle based picture, as well as Quantum mechanical picture. So, the next week we will go into the quantum mechanics, to derive these energy expressions from Schrodinger's equations.

So, I will do a little bit basic at the same time I will also go a little bit fast. So, you can also do reading parallel on these topics, I will try to make it. So, that people who do not have any understanding of quantum mechanics can pick up. So, it will be mostly conceptual I will also try to parallel derive the expressions.

Thank you.