Semiconductor Optoelectronics
Prof. M.R. Shenoy
Department of Physics
Indian Institute of Technology-Delhi

Lecture-2
Energy Bands in Solids

Good morning and we start with lecture 2 energy bands in solids as I mentioned our objective will be to review the essential semiconductor physics. In the last class we discussed about the subject matter.

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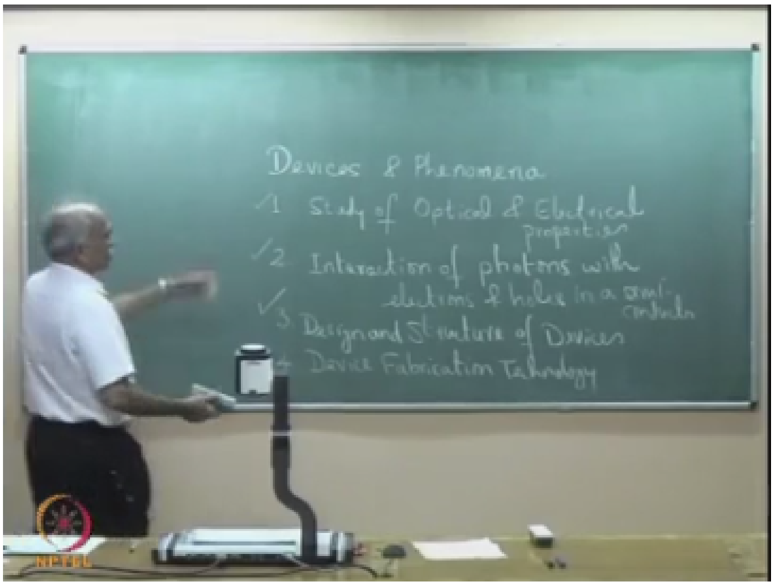

Devices & Phenomena

✓1 Study of Optical & Electrical properties

✓2 Interaction of photons with electrons & holes in a semi-conductor

✓3 Design and Structure of Devices

4 Device Fabrication Technology

The subject matter of semiconductor optoelectronics comprises of the deals with devices and phenomena and phenomena which involve interaction of optical processes with electronic processes. Therefore this will inter involve study of optical and electrical properties of semiconductor optoelectronic materials. Optical and electrical properties, it will involve interaction of a stud of interaction of photons with electrons and holes in semiconductor**.**

The technology will further involve design and structure of devices and of course fabrication technology, that is device fabrication technology. In this course we will consider these three aspects including design and structure of the devices, their performance, characteristics of devices, but not the device fabrication technology because there are other courses which cover device fabrication technology.

So these are the three aspects which we will cover in this course. So we start with the first one that is to study optical and electrical properties of semiconductor optical and electrical properties. So we start with the formation of energy bands all of you would have studied about this. So I am just recalling formation of energy bands in semiconductors.

So most of the semiconductors of practical importance are crystalline in nature most of them all the binary semiconductors that have written Silicon Germanium all are crystalline and most of them are also are characterized by the cubic lattice.

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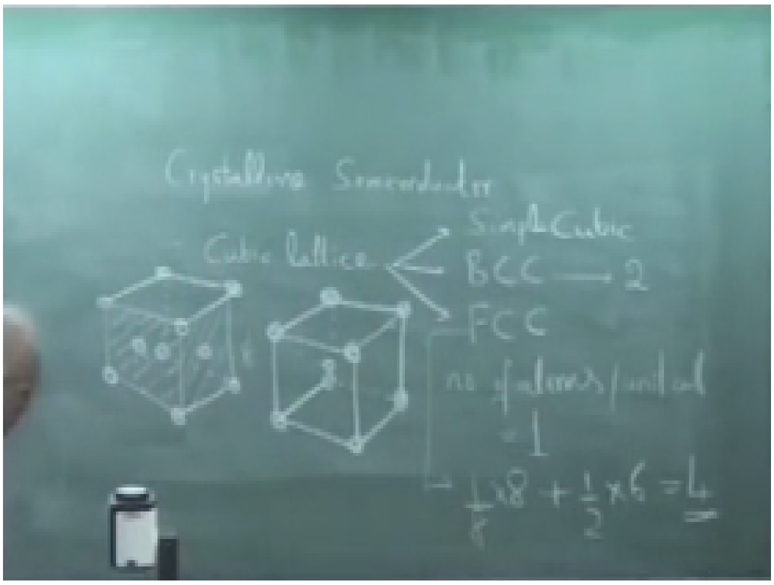

We may have different structures like diamond structures, zinc line structure, but most of them are characterized by a cubic lattice. In cubic lattice as you are aware that there are simple cubic, body centred cubic BCC and FCC face cantered cubic. So simple cubic if you draw a cube, the atoms are located at the corners of this cube. So naturally there are 8 atoms, 8 corners simple cubic.

But as you know the entire crystal structure each cubic cell here is shared for example there are further cubes on this side, further cubes on this side, so every atom here is shared with 8 other cells and therefore the contribution of this atom per sale is one eight and there are 8 atoms forming 1 cubic cell here and therefore number of atoms per number of atom per unit cell is equal to 1. If you take a body-centred cubic then there is one more atom at the centre here.

And therefore number of atoms for BCC, number of atoms per unit cell si 2. If you take face centred cubic that means as you can see it comprises of 6 phase 2 up and down, 2 on the sides and 2 on the other side. So there are 6 faces, at the centre of each face if you wish you can draw another one another diagram. So these 8 atoms are in at the 8 corners plus on this face if I consider this phase 1 in the middle of this face.

The first phase here, second one here, each face there is one atom here and so on, so we have 6 atoms sitting on six faces. In addition to the 8 atoms in the corners, but each face is shared by 2 cells on 1 on this side and 1 on this side which means every cell the atom contribution for sale is half per face. So half*6 pieces, so we have 3 additional atoms which means for FCC we have 1 that is 1/8*8+1/2*6=4, number of atoms per cell is 4.

Three coming from the 6 faces and 1 coming from the corners. So number of atoms per unit cell is 6, is 4 now. Now why do I need this number will come to know in a minute my objective is to have an estimate of number of valence electrons. So to know the number of valence electrons I must know the number of atoms per unit cell and number of electrons per unit cell.

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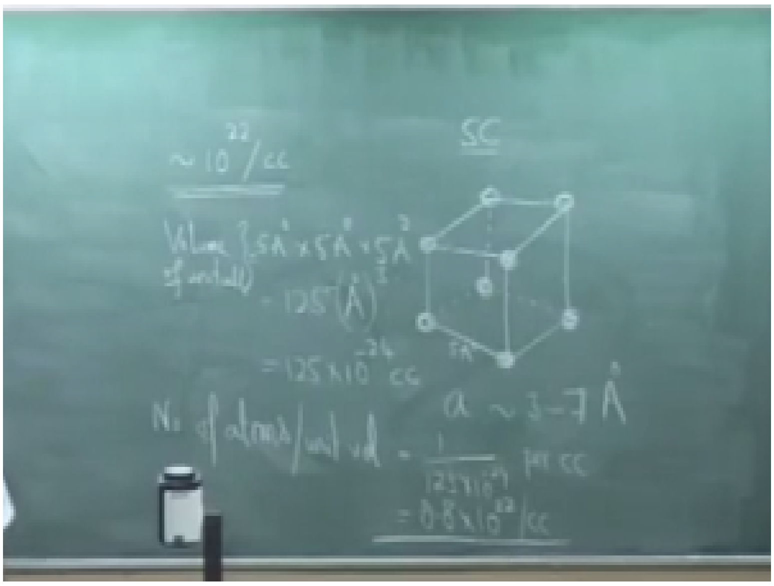

So I want to calculate how many number of atoms are present per unit volume of the material. So simple engineering estimates so you take the cubic cube again, so one atom if I take simple cubic SC simple cubic, then 1 atom per cell, I want to finally calculate the number of electrons or density of electrons which means number of electrons per unit volume, number of valence electrons per unit volume.

Because we would require the carrier concentration to determine the electrical properties and therefore I am starting with fundamentals in a semiconductor typically the inter atomic spacing that is inter atomic spacing A is anywhere in the range 3 to 7 angstrom **3** is the interatomic space, this one or this one approximately of that order. If you take gallium arsenide for example it is about 5.65 angstrom.

So 3-7 angstrom, so if I want to estimate what is the volume occupied by 1 unit cell let macro environment take this 5 angstrom ok, some intermediate value just an estimate 5 angstroms which means what is the volume of this, the volume is 5*5 angstroms, so the volume of unit cell which is equal to 1025 angstrom cube. So that is equal to 1 angstrom is 10 to the power of - 10 meters or 10 to the power of - 8 cm.

So this is 125*10 to the power of -24 cc or centimetre cube is the volume, volume occupied by 1 unit cell, what is our interest is to find out the number of atoms per unit volume. So what is the number of atoms per unit volume. Therefore number of atoms per unit volume=1/125*10 to the power of -24/cc. So this is nothing but 0.8*10 to the power of 22/cc, 0.8*10 to the power of 22/cc or the number of atoms per unit volume is of the order of 10 to the power of 22/cc.

Number of atoms per unit volume in a semiconductor is typically 10 to the power of 22/cc. If each atom contributes 1 valence electron then the number of valence electrons per unit volume is of the order of 10 to the power of 22, what is the number of valence electrons typically that we have, say it is a quick calculation to get an estimate. So I would like you to have this kind of practices to estimate very quickly starting from fundamentals.

So number of atoms, if you take silicon for example you know that the atomic number of silicon is 14, Germanium the most widely used semiconductors atomic number is 32, gallium 31, and arsenic 33, atomic number z. So if you write the electronic configuration this is 1S2, 2S2, 2P6, 3S2, 3P2, you see 14 valence shell by definition is the outermost shell which is either field or on field but the outermost shell where electrons are occupied.

So 3S2, 3P2, so there are 4 electrons in the valence shell, so 4 electrons, that is why it is in group 4 right germanium 32 1S2, 2SS2, 2P6, 3S2, 3P6, 3D10, 4S2, 4P, you see the fourth shell is the outermost shell and again you have 4 valence electrons. If you see gallium here it is 31, it has the same structure, same electronic configuration, but 4S2 and 4P1. So this has 3 valence electrons, this has 4, this has 3 valence electrons.

And as you know that gallium is group 3 element, arsenic on the other hand will have the same configuration of this here we have 4S2, 4P3, so 5 valence electrons, arsenic is in group 5, Silicon, Germanium, gallium arsenide yesterday as mentioned is a 3,5 compound very important semiconductor in of optoelectronics. Therefore 1 atom has in this case 5 valence electrons we have 3, here 4, and so on.

In other words therefore the number of valence electrons per unit volume is this number multiplied by number of valence electrons per atom which means in general n the number of electrons in the valence shell is per unit volume is of the order of 10 to the power 22 to 10 to the power of 23/cc ok. Let me come to the second issue.

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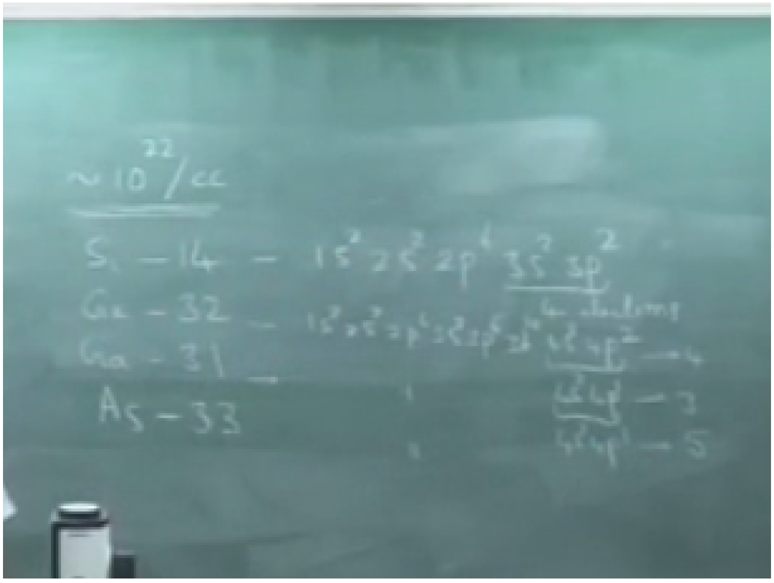

So I have in this discussion I have made use of the fact that most of the useful semiconductors are crystalline of course there are what first semiconductor but most of the useful semiconductors in optoelectronics are crystalline in nature. Let me use another fact that our topic as you can see is energy band in solids.

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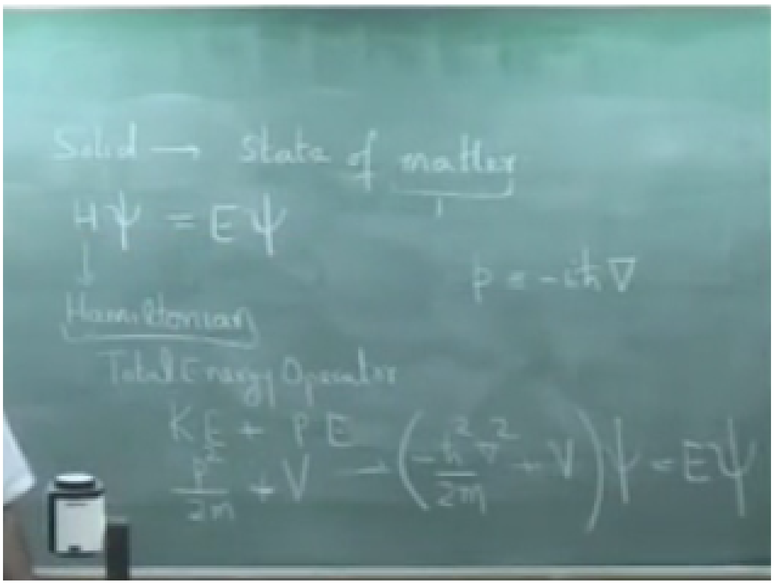

Solid → State of matter

$H\psi = E\psi$

Hamiltonian

Total Energy Operator

$p = -i\hbar\nabla$

KE + PE

$\frac{p^2}{2m} + V \rightarrow \left(\frac{-\hbar^2\nabla^2}{2m} + V\right)\psi = E\psi$

So solid is a state of matter is basically collections of atoms and atoms comprise of a central positively charged nucleus and negatively charged electrons. The motion of constituent of an atom are described by the quantum mechanics, the laws of quantum mechanics in particular the motion of constituent are described by the Schrodinger equation.

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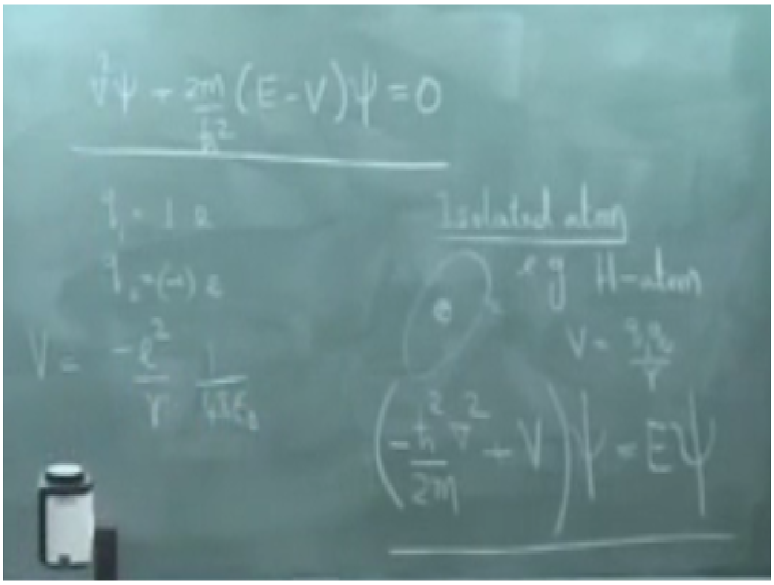

$\nabla^2\psi + \frac{2m}{\hbar^2}(E-V)\psi = 0$

$q_1 = 1\,e$

$q_2 = (-)\,e$

$V = \frac{-e^2}{r}\frac{1}{4\pi\epsilon_0}$

Isolated atom

e.g. H-atom

$V = \frac{q_1 q_2}{r}$

$\left(\frac{-\hbar^2\nabla^2}{2m} + V\right)\psi = E\psi$

The spelling actually either you have to put two dots or Schrodinger equation, I do not know how many of you are familiar with this, but basically Schrodinger equation si defined by H shy=E shy where H is called the Hamiltonian which means it is basically total energy operator which means it is an operator corresponding to the kinetic energy and potential energy which means it corresponds to p square by 2 m+V.

Where P is the momentum, M is the mass and V is the potential energy. If you replace this moment I'm here by the corresponding momentum operator part of the basic quantum mechanics momentum operator which is -IH cross dell and substitute here then you will get the Schrodinger equation. So this gives you H cross square by 2m with minus sign*dell square+V.

So this is H, multiply this by shy the wave function which is equal to E shy where E is the energy Eigen values, shy are the Eigen function and E are the energy Eigen values, there could be more than one Eigen energy values and therefore E representative. So this is nothing but the Schrodinger equation which you can rewrite you can rewrite in the form delivery square shy+2Mi H cross square*E-V shy=0.

For every given potential variation V you can find out an energy Eigen value which gives the energy of the particle under consideration. And shy being the wave function H is Planck's constant, H cross is H/2phy, H is Planck's constant and M is mass of the electron. If you are finding energy of Eigen values of electrons then M is the mass of, if you can an isolated atom.

For example hydrogen atom I am very quickly recalling all the basics that you have already studied. If you take the hydrogen atom it has a central positively charged protons here and electrons surrounding it as a cloud. So the potential energy V is given by Q1Q2/r which means in the case of hydrogen Q1 is this, Q1=1E, the quantum of electric charge and Q2 is -1*E charge of an electron therefore Q1Q2/r is -E square/r. V=-V square/r, in CGS system you have an additional factor which is 4,5 0.

If you substitute this V here you can find out the energy Eigen values for hydrogen atom.

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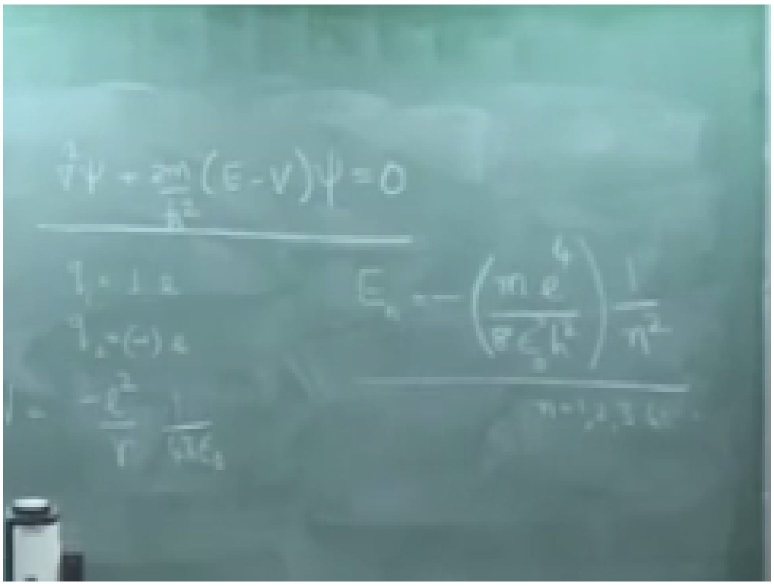

$$\nabla^2\psi + \frac{2m}{\hbar^2}(E-V)\psi = 0$$

$q_1 = 1e$

$q_2 = (-)e$

$$V = \frac{-e^2}{r}\frac{1}{4\pi\epsilon_0}$$

$$E_n = -\left(\frac{me^4}{8\epsilon_0^2 h^2}\right)\frac{1}{n^2}$$

$n = 1, 2, 3, \ldots$

So this gives you the solution for hydrogen atom gives you energy Eigen values which are En=-m E to the power 4/8 actually 0 square, H square*1/n square. These are the energy Eigen values where n=1, 2, 3, 4, etc. correspond to the principle quantum number 2 or energy levels of a hydrogen atom. Since n is discrete it immediately means that En is discrete, so for hydrogen atom if you put values for this.

These are all constant, mass of electron, charge of electron, permittivity of free space, H is Planck's constant. So this will come out to be -13.6*1/n square Ev. If you put n=1 that is the ground state then you know that ground state of hydrogen atom is -13.6 EV is energy of hydrogen atom. You may be wondering why I am discussing this. So the point is if you take an isolated atom it is characterized by discrete energy levels.

So this is n=1, n=2, iniquity we actually the separation today increased because and square is in the dinner it's a n square it goes as health square and finally it goes 20 which pen and becomes very large this was 200 is the free state walking stick so as you go here they come closer and closer and closer and finally that is the vacuum stick the vacuum state here we are -13.6 EV states of the atom do you have nucleus which is surrounded by various orbits.

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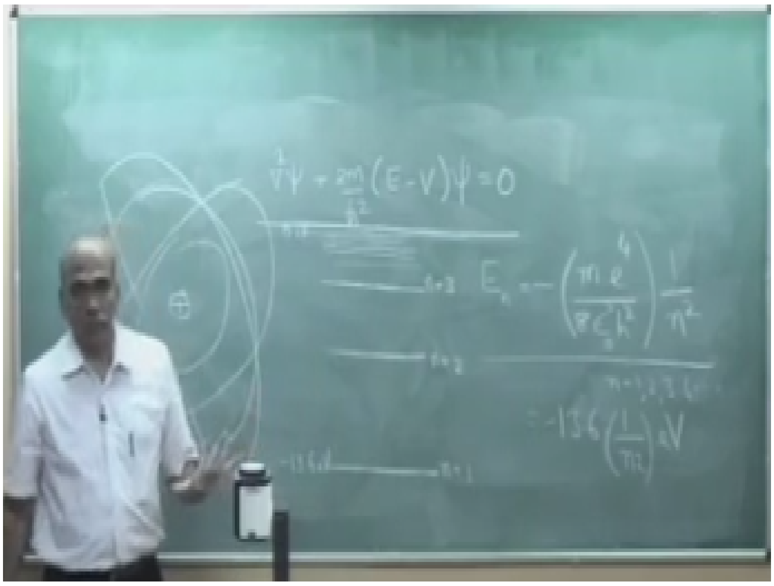

I am just showing randomly some orbits and energy corresponding to various shells and energy corresponding to various levels or what is given here. So the ground state of hydrogen atom is -13.6. What we are interested is from this discussion is to see that an isolated atom is characterized by discrete energy levels, this is the point. So I have taken just an example which already you have studied is the hydrogen atom.

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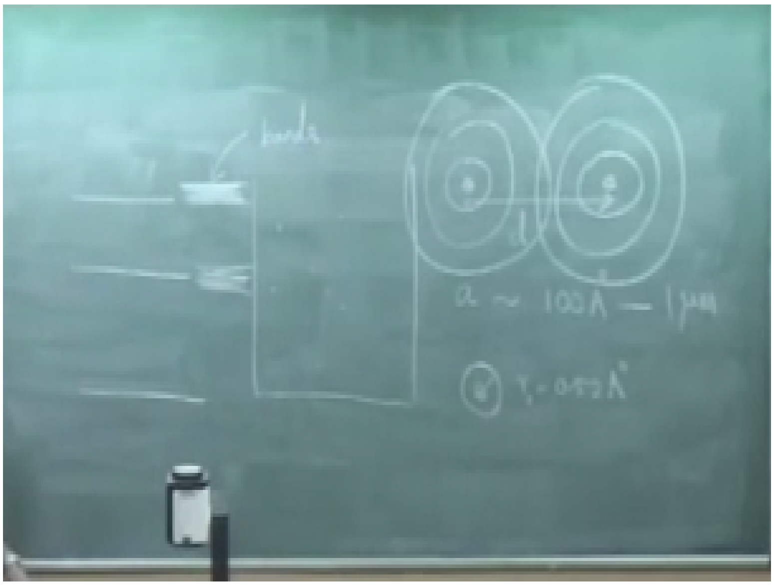

Let me recall the argument again matter is a collection of atom and solid is densely packed collection of atoms. If you to take a gas at low pressure the interatomic separation you know that if you take a container, a gas at low pressure then the gas molecules are continuously in a state of motion. The average interatomic spacing depends on the pressure of the gas, lower the pressure, largest is the interatomic spacing.

So typically the interatomic spacing A, if I want to call the interatomic spacing A is anywhere from the of the order of 10 or 100 angstrom to 1 micron, typically the interatomic spacing that is between atoms in a gas, what is the size of an atom, the of an atom there is no fixed size of an atom, but the size can be estimated if you know that the ground state of hydrogen atom here has a radius here which is called the bohr radius is 0.52 angstrom which means the size is typically about 1 angstrom.

You can say that the size of an atom is approximately 1 angstrom, of course higher orbits will be that is higher electrons will have a larger spatial extent, but the size is typically 1 angstrom. When the interatomic spacing if you now considered 2 atoms 1 atom sitting here and 1 atom sitting here, the interatomic spacing here the separation between these. When this separation D is large then the electrons here do not see any effect due to the electric field.

The electrostatic field here the field here does not experience the field due to the other atom because it is quite far there is hardly any interaction. But if they start coming closer then the field here gets perturbated because of the field here or the electrons here starts seeing the second atom or they get influenced by this. The influence leads to splitting of the energy level, the energy levels which were originally discrete.

If you start bringing 2 atoms together then the energy levels split into 2, the outer walls are the more affected one, because the inner electron shells are inside here they are not seeing the influence of the other atom, the outer electron I am just showing circular orbits like this as you can see the outer orbits or outer electron start seeing each other or the interaction is stronger there for the perturbation felt by the outer electron is more.

And therefore you start seeing splitting of the outermost electron energy level. This is considering 2 2 atoms, if you have a large number of atoms the levels here split into multiple levels. First point when 2 atoms are well separated there is very little interaction between them and therefore the entire collection of atoms are characterized entire collection is characterized by discrete energy level.

Because each atom has this energy level, therefore the entire collection is characterized by this discrete atomic energy levels, but if you start bring them closer and closer then the energy levels get perturbed or splitting of energy levels take place, allowed levels become more than one corresponding to 1 you now have several energy level and therefore if the number increases this goes over to a back.

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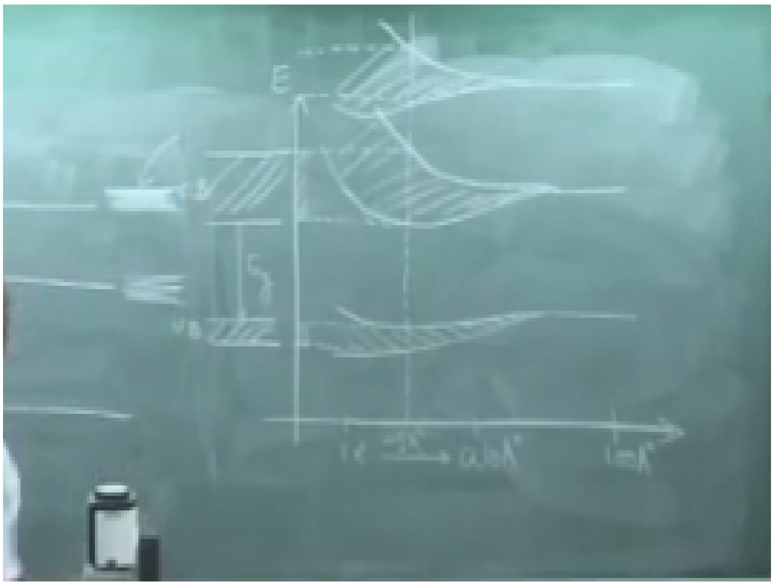

So they go over as you decrease the interatomic spacing the energy levels this is illustrated by a nice diagram which you generally seen in books. So this is the interatomic spacing A interatomic spacing versus the energy. So when the interatomic spacing is very large. So let me put some number ok I will put the number ok 1 angstrom, 10 angstroms, this action sees energy E.

So when the interatomic spacing is sufficiently large you have energy levels which are discrete. They are not equally spaced I am just qualitatively illustrating as you reduce the interatomic spacing the levels start splitting, you could have seen this diagram in many books, so what you have is a range of allowed energy level, a quality to explanation I am offering there are so semiconductors have an interatomic spacing approximately 5 angstrom.

So if you go here let us say 5 angstrom, what are these, these are the allowed energies, we see these levels correspond to allowed energy value has the interatomic spacing reduced the allowed energy values become more that is the result the range of energy values corresponding to each level, a range of energy balance and as you reduced it further it started splitting further.

Hence in for some values they may also start overlapping with each other, typically for semiconductors where interatomic spacing is about of 5 angstrom, you can see therefore in this energy access if I draw the range of energy values which are allowed please see this is the range of energy values allowed here. This is the range of energy values allowed here and this is the range of energy allowed.

So what do I have, I have a range of energy values range of allowed electron energy values inside semiconductor and this is nothing but the bands. So what you have are the band diagram that you see this basically this and the separation here where there are no allowed states correspond to the forbidden gap. I have written EG but please remember the highest band which is completely filed is called the valance band.

The highest band which is completely filled is the band and the next band is called the conduction band and the energy separation of the forbidden gap between the valence band and the conduction band is the band gap. There may be many more bands but no electrons there and therefore we are not concerned with them.

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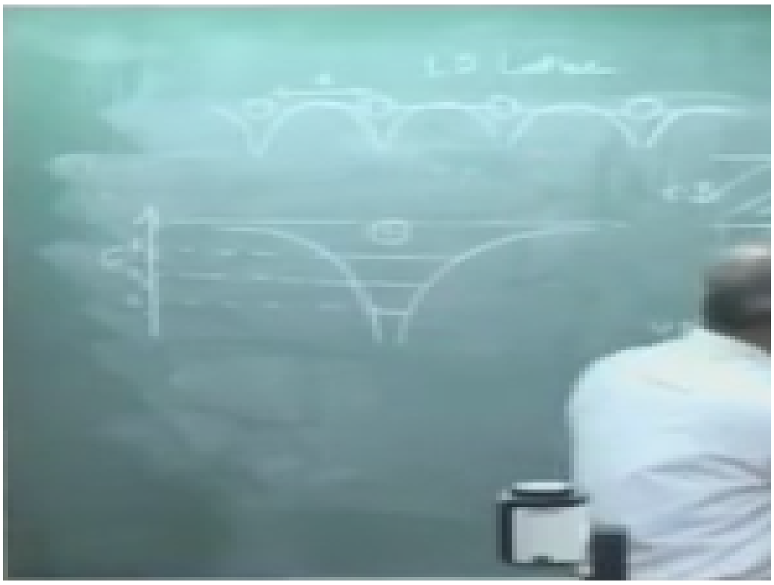

So a semiconductor is characterized by energy bands. I have given a qualitative explanation here, let us make it little bit more quantitative, little bit more rigorous and see whether this is really true or not. Those of you have study solid state physics, you have studied the kronig penney model. If you consider a 1 D lattice, so what I am showing these are the atoms which are separated an interatomic spacing of A.

Consider a 1 deluxe if you consider an isolated atom single atom what will be the potential energy variation V=-Q1Q2/r. So if you plot the potential energy variation where r is the distance from the nucleus then the potential energy variation looks like this, it is 1/r variation, r=0 here, at the nucleus r=0, so this is the potential energy variation, this is 1/r variation and minus, that r=0 it tends to infinity.

That is why you see I am sure all of you have seen this potential energy variation. This is for 1 atom. If you have a series of 1 D lattice of periodically placed items then we will have a corresponding potential energy variation**.** If you solve this problem like in hydrogen atom you will get, so this is the potential energy here V, and you will get different discrete energy levels, permitted values of energy level.

So this is P1, P2, P3 are permitted values of energy levels. These are the discrete energy levels of the isolated atom. But now what I am showing is a 1D lattice separated by A. when you have an isolated atom like a hydrogen atom with one electron it is exactly solvable you have analytical solutions, but if you have many atoms with many electrons then it becomes a multibody problem.

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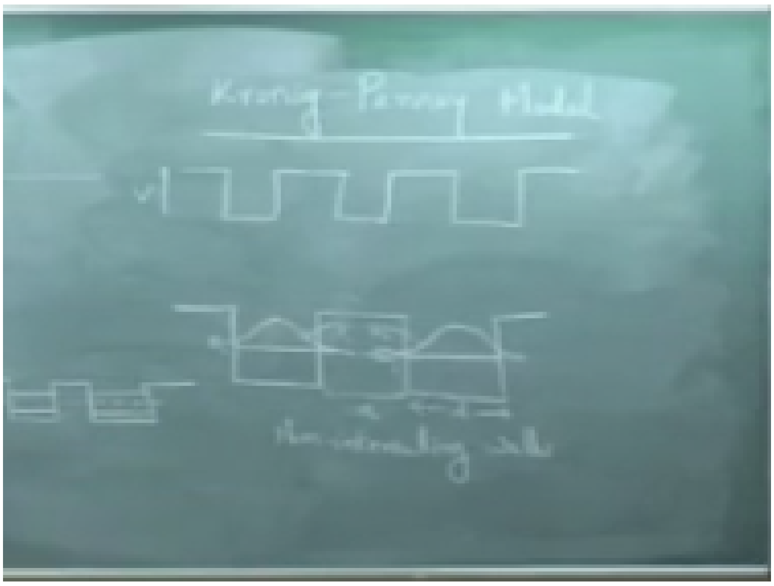

And you cannot have analytical solutions for many such problems. But you can solve them numerically or you make certain approximations. So you may be familiar with kronig penney model and just recalling what you have studied, those of you have not studied do not worry basically we are interested in the concept and the result. Finally we are interested in the concepts because this is not part of this course.

So we will not going to the analysis of this, but in kronig penney model what he did was he approximated this potential variation by a potential well a rectangular potential well, a periodic potential well and then you have this periodic potential well, the potential energy variation here, this is the and this is the separation between them. If you consider a single potential well this is a particle in a potential box problem we study even in first year undergraduate engineering.

If you take a potential well here this supports analytical solution, this supports different discrete Solutions even the ground state, the second statement and it may support depending on the height and the width it may support many solutions. For simplicity let me take a potential well which supports only one solution. So there is one solution here E1, one allowed solution which is the fundamental mode, fundamental solution or fundamental state which is the ground state.

And if you see the wave function it typically looks like this, it has a oscillatory behaviour inside the well and evanescent behaviour outside the well hmm hmm. This is the ground state of particle in a potential well a single well. If I bring a second well close to this reasonably close to it, so that they start interacting if the separation here, this is the separation let me call this as D the separation.

If this or let me call this as A, the cell is of width D and separation A, if A is sufficiently large much greater than D then the 2 wells are non interacting wells. So this will have one solution here, this also has the same solution if it is identical size and identical height then this also has a solution corresponding to the same energy value for non interacting well**.**

Two potential wells which are non interactive or you can imagine as it as two atoms which are well separated not interact. So this is the potential well which is approximating this potential actual potential where is like this, but it is approximated by the box equal and box because this has analytical solutions easily you can solve this. If you when A is much larger than D there is no interaction between them.

But if A starts reducing, so each one of these is characterized by the Eigen state here the fundamental solution of the ground state when you start reducing this that the evanescent tail of this field here, this site interact with the evanescent tail of the shy here. If I want to call this is shy1 and shy2. We are actually same states but the tails start interactive, they start overlapping which means there is an interaction between the wells.

This is original when A was much larger than D they were non interacting wells, when A started reducing this started interacting, when they start interacting if you solve this double well problem then you will get 2 solutions corresponding to this interacting double wells, now you get 2 solution, that is one here. This was the original level let us say this was the original level E1.

Now the new values are one about that and 1 below. So there are 2 allowed energy values, you have two solutions earlier there was only one solution, now you have two solutions. I do not wish to go into the details because they are not symmetric solutions, antisymmetric solutions and so on. However what is important is if there was only one energy level initially when you have 2 interacting wells there are two solutions.

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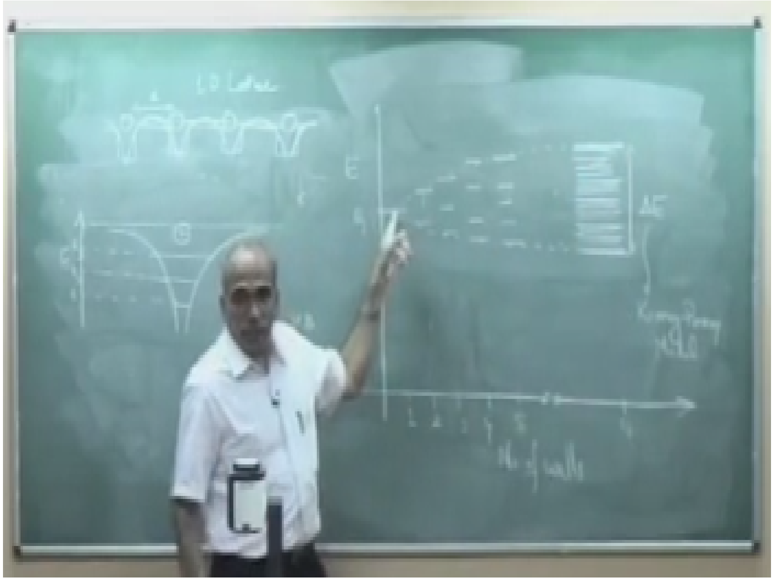

If there are 3 interacting wells there will be 3 solutions and if there are end interacting wells there will be n solutions, n allowed states and therefore if I plot so what I am going to plot, let me erase this if I plot the number of wells here this is number of wells versus energy allowed energy E, this is some state I am discussing about E1. So this was my E1 original E1 when I had only one value of energy I had this. This is E1.

When I have number of wells 2 then I have 2 allowed values 1 slightly below and another slightly above. So 2 allowed energy states, if I have 3 wells please see the relevance I have considered a 1D lattice where atoms are sitting along a line. They are like interacting atoms. So equivalently each atom is characterized by a potential well. So I have a series of interacting potential wells.

And I am now writing depending on the number of wells how many energy states are permitted. So the allowed energy state for this 3 is here, 1 above, 1 below, when I go to 4 then it is here 1, 2, 3, 4. This is exactly numerical is horrible, this is not so solve this Schrodinger equation for the 4 interacting wells you will get the 4 solution. These are solutions which are actually you can calculate the solutions.

As the number of cells increase, so you go to 5 it becomes 1, 2, 3, 4, 5 and so on. So the number of cells increase and when the number of cells become very large some end then you see that this saturates to very large number of allowed states, the number of allowed states here, we see that the discontinued here in the access because the number is very large there I have shown discontinuity.

Let me show this again 5 and this is number of this is some large number N, there are large number of cells. So this varies something like if I draw it leads to saturation and this separation here delta E is the width of the energy band, the corresponding width of the energy band that you get, now there is a range of allowed energy values because you have n interacting atom.

There is the range of allowed energy values, this delta E comes out to be the same that you get from kronig penney model. This calculation was not from kronig penney model, this calculation is from quantum mechanics. So the quantum mechanical calculation gives this separation as the same which you get from the kronig penney model.

So what is the point in this discussion is that when you have a closely packed arrangement of atoms periodically arranged atoms in a lattice. They are characterized by discrete energy bands. This is corresponding to 1 energy level, similarly for the next energy level if I had the next level E2 there are also I would have got is splitting into bands corresponding to E2.