Semiconductor Device Modelling and Simulation
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Lecture – 55
Solving Schrodinger Equation

Hello, welcome to lecture number 55. In last class we discussed about the basic postulates of quantum mechanics, so, there were four rules, basically that were discussed and then we concluded that Schrodinger equation can be solved to find out the state function psi. Now, in today's lecture we will discuss how to solve this Schrodinger Equation. So, we begin our discussion in last class regarding the solving solution to Schrodinger equation and where there we use the method of variable separable.

Now, we will consider some scenario like quantum bell or so, some potential structure, where we will solve this ordinary equation. We will solve both analytically as well as numerically.

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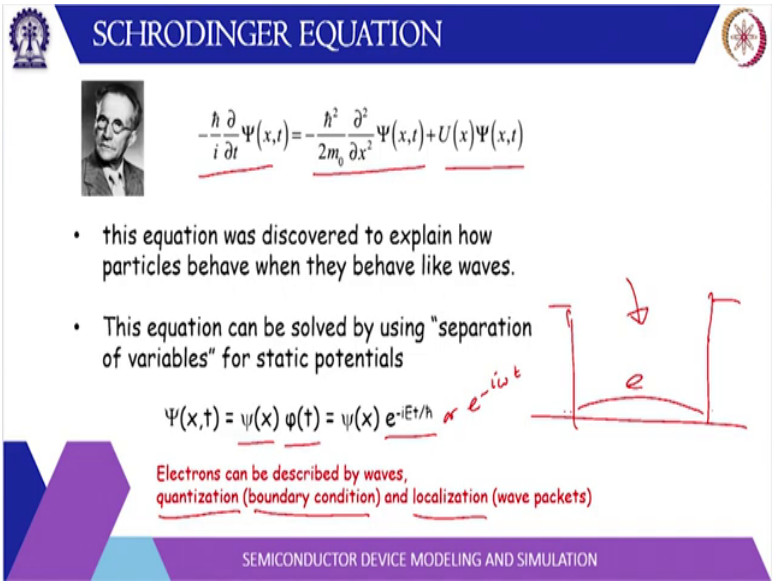

So, let us recall the Schrodinger equation this is a time dependent form so, d psi by dt – h by iota h bar by iota, is equal to position dependent derivative d 2 psi by dx square multiplied by – h bar square by 2m + U psi Now, we can recall the solution to this equation using variable separable. So, psi is a function of x unless another function phi which is function of t, can return as e to the power – iota E t by h bar or it can be written as e to the power – iota omega t.

Because this energy is H bar omega. Now, this is a general solution and we did not explore any boundary condition. It is a boundary condition that give rise to the quantization. So, if electron is freely moving in the space, it can assume any energy. But when you constrain it then only energies of the electron which can satisfy this boundary condition will be allowed. So, this is a quantization this is a boundary condition that give rise to the quantization and the localization.

Because by applying the boundary condition, let us say there is some potential here. So, there is high potential here and then some electron is confined here. So that means this electron is localized here that is probability of finding electron will be the high here. And because of this boundary condition, only certain energies of electron will be allowed. That is called quantization.

That means this electron cannot assume arbitrary energy, energies has to be some discrete numbers.

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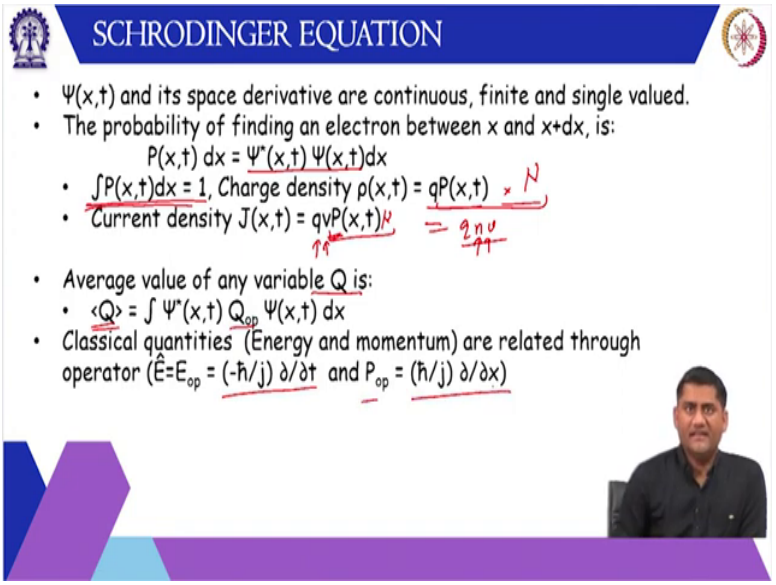

Then these are the relationship that we can recall that probability density is psi star psi dx over region x. Then for real situation, we can basically normalize this probability density function that psi star psi dx = 1. So that means if there are N number of electrons in the system then star density can be written as Q times probability multiplied by this N. So, this N times P is the number of electrons basically, per unit area volume.

Then current density we know the expression for the current density q times n times v that is the expression. So, if we write in terms of probability density function then we can again use the q here and v here and this electron is written by P times N. So, N is a total number of electrons times their probability in that particular region or that particular time. This is, we are using it because we are normalizing with respect to 1.

If you do not normalize, you can just directly write P. Then it will not give the probability because it will give the number of electrons so, to satisfy the meaning of the name that it is a probability density we have to normalize it to the 1. Then for any variable Q we can use its operator that is Q of to calculate the average value of that particular physical quantity. For example, for energy the operator is –h bar by j times d by dt or for operator for momentum is h by J d by dx. So, this we have discussed in last class also.

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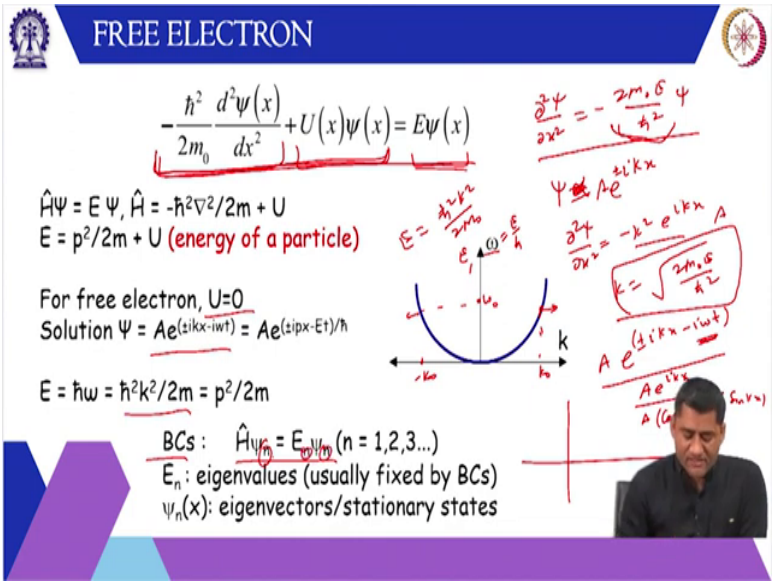

Now, let us consider a free electron, so, free electron means it is freely moving in the space. There are no constraints, no boundary conditions. So, let us only consider the position dependent Schrodinger equation. Because we are using the variable separable method and this will be already derived, so, we can directly use this part of the equation. Now, here you see that some operator, this is basically kind of operator h.

So, we say h psi is equal to E times psi. So, E are the energy or there are Eigen values of this particular equation. This these equations are called Eigen equation. This left side of this equation you can say there are two terms here one is a double derivative that is basically

telling about the kinetic energy. And then U times psi that is telling of the potential energy. So, there is a total energy of the particle is equal to E.

Now, if you consider this free electron in a space where potential is 0, so, we can conveniently set u equal to 0. Then we have this double derivative is equal to d 2 psi by dx square is equal to – 2m naught E by h bar square times psi. So, this is simple equation and we can say the solution of this equation is psi is equal to this term. Here can be represented by some let us say some constant.

Let us say k or you can say this is basically see if you consider the size of the form e to the power iota kx. So, double derivative d 2 psi by dx square will be – iota k times iota k. So that will be – k square e to the power iota kx. So, if there is some coefficient a we can just put a here. Then we can use high quality sign now. This is basically k square so, from here you can find out that k is equal to 2m naught E by h bar k square.

So, this is A times e to the power iota kx. So, whether U is + iota kx or – iota kx you will get the same expression basically because minus, minus will become plus. So**,** iota square k square. So, this is the solution and the other part which is time dependent, is e to the power – iota omega T. So, overall solution will be A times e to the power +– iota kx – iota omega t. So, this is the solution if you look at the physical meaning of this equation, it simply means a plane wave.

You see iota kx – omega T. So, if you use plus sign that means it is moving in the positive x direction and if you use other sign, it means it is moving in minus x direction. There is a simply a meaning of this, so, this direction, basically, we say phase velocity, so, it is how the phase is changing. You can basically plot this at different time, so, you can think like this. Let us say this is A times e to the power let us consider plus sign so, iota kx.

So, A times e to the power iota kx there is to be some kind of so, you can write A times cosine kx + iota times sin kx. Then, basically, you can observe the evolution of this wave with time you change the time, so, this will slightly change the phase. So, this phase will basically decrease basically. So, you can see a plane wave which is moving in x direction. Now, another thing you can see we found the k is equal to root 2m E by h bar square.

So that gives you a relationship that E is equal to h bar square k square by 2m naught where m naught is the mass of this particle. So, energy is proportional to k square, so, this is E by h bar E is equal to H bar omega. So, omega determines E by h bar. So, you can use this axis as E or omega and this can be written as k. So, both are proposal to actually k square. So, this omega k or Ek diagram will have this parabolic nature.

Now, here in this case, there is no constraint on the value of k or all on the value of energy. That means all the energy on this curve are allowed but if you select certain omega or k if you select omega then corresponding k is fixed. Let us say this is omega naught so, corresponding you can have either plus k naught or – k naught. So, + k naught means it is moving in x direction – k naught, is moving in – x direction.

So, space velocity is in + x direction is phase velocity is in – x direction, so that is the meaning. So, corresponding to one energy there are two waves one moving in x direction, other moving in – x direction. So, this is for one dimension case. You can use the same logic to extend this idea to 2D do 3D cases. So now, when we put the boundary conditions here is a plane wave unconstrained.

So, when we apply the boundary condition then this discrete nature will come into the picture. So, to summarize, this slide a free electron as Ek relationship which is parabolic in nature and this is written by x psi is x psi is equal to E psi, where E is the energy. Now, for unconstrained electron there is no quantization. So, you do not have to use this N here, all the values of energy it can assume and psi are basically the Eigen vectors or stationary states of the electron.

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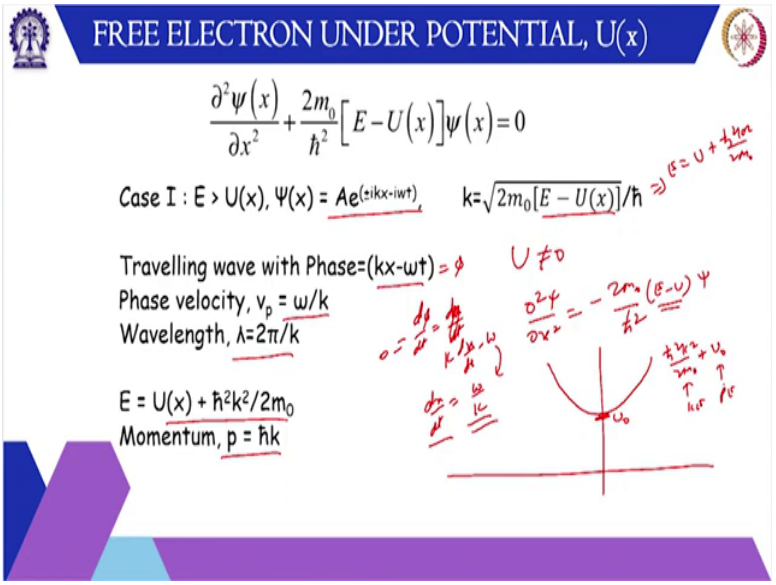

Let us introduce a background potential U. So now, in this case U is not 0 so, U is not 0. So, again, this is simple case. You can write d 2 psi by dx square is equal to – 2m naught y h bar square. We can replace E by E – U times psi. So, everything will be same except now E is replaced by E – U, U is the background potential. So, it is E – U and rest is same E to E times e to the power + – iota kx – omega t.

So, travelling wave so, this is the phase iota kx, kx – omega t. So, phase velocity can be found from the phase. So, this lets say this is a phase you can write d phi by dt will be dk by dt k times dx y dt – omega. So, this is a derivative phi. Now, if you want to find the constant phase, so then this d phi by dt has to be 0. So, if you equate this to 0 then it gives you the dx by dt is equal to omega by k. So, this is basically the phase velocity omega by k.

So, this is basically point how the particular phase point is moving and there is another concept of group velocity that we will discuss only. Now, this wavelength is of course, 2 pi by k and now energy U naught if you use this equation, it tells you that energy is now U + h bar square k square by 2m naught. So, this is the expression for energy and momentum is h bar k. So if we plot it, what you will get?

Now this curve will is slightly shifted, so, this minima will not be 0 but it will be U 0. Then so energy is h bar square k square by 2m + U 0. So, this is a potential energy, this is the kinetic energy, so, this is kE, this is a potential energy. So, this electron in background with background potential U.

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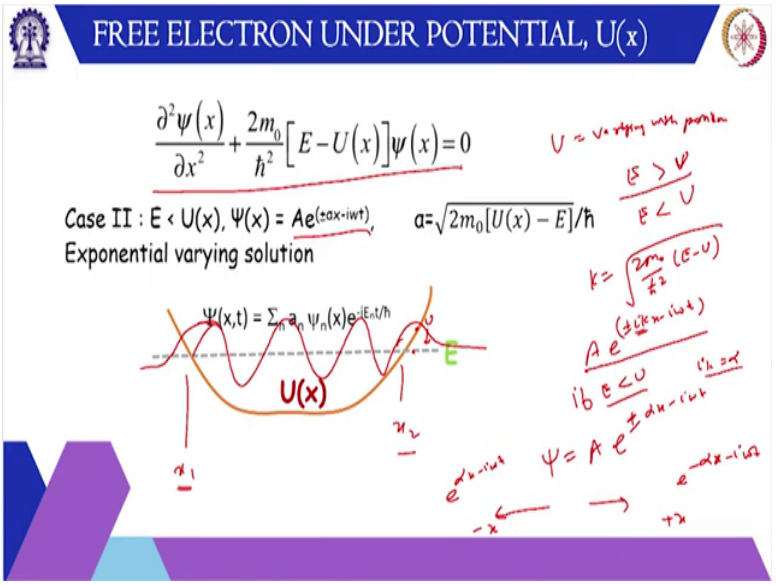

Now, we can vary the background potential. So now, this background potential U is not constant. So, U is varying with position, so, you can discuss two scenarios. Even in the previous case, there can be two scenarios that the energy of electron which is E is more than U or energy of electron is less than U. So, when energy is more than U then we can say it is a traveling wave because what you will get here?

The solution is let us say that k is equal to 2m naught by h bar square times E – U square root. And the solution was a times e to the power + – iota kx – iota omega t. So, this k is happen to be real when E is more than U this is real. So, iota kx – iota 2 omega t is a plane wave which is not decaying. For the second case, if E is less than U then this k becomes imaginary.

So, iota k will become real, so, you will have solutions e to the power +– iota k can let us write it as alpha. Because now this is real so, +– alpha x – iota omega t. Now, for a positive triangle with traveling wave when x goes to infinity, we cannot use + sign because this psi goes to infinity this is not possible basically. So, we can have minus sign for positive x axis, so, it will be e to the power – alpha x – iota omega t.

And for negative axis we can have e to the power alpha x – iota omega t. So, this will basically kind of decay. So now, if you consider a situation where there is this potential is U and which is less than E in certain region let us say x 1 to x 2 and outside this energy is less than the potential energy. So, potential is more here and less in this region. So that means between x 1 and x 2 you will have the solution e to the power +– iota kx – iota omega t.

So that that means traveling wave can exist in this region but outside this region this k becomes imaginary because energy is less than U. So, this is U this is E so, this is energy is less than potential energy. So, it will be decaying function basically, so, you can think of it like this, so, you can have some kind of traveling wave here. Then here it will basically decay. So, this kind of wave will exist. Now, what will happen?

Because of this boundary condition, it cannot be a simple sinusoidal wave it has to respect the boundary condition basically. So, the solution will can be evaluated by solving this Schrodinger equation. So, for arbitrary potential profile we may not be able to get the analytical solution. So, we may have to go through the numerical solution but there are some regular profile where we can get the analytical expressions.

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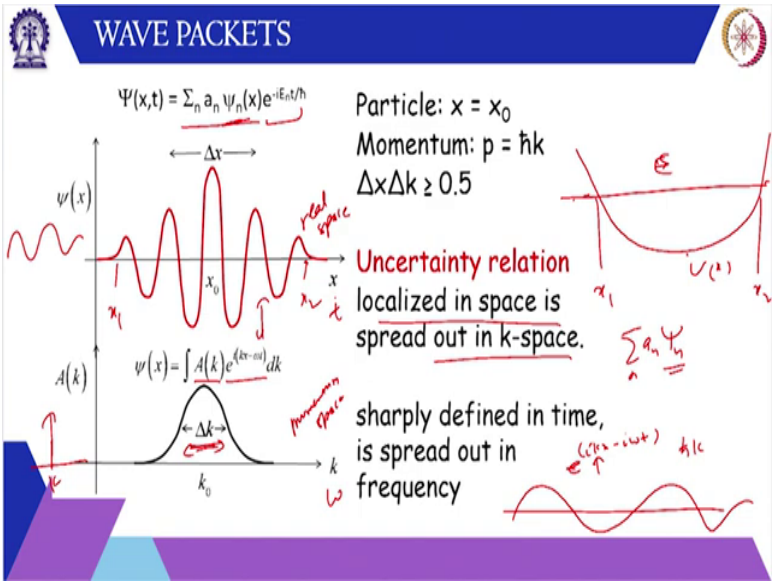

Now, if you consider a potential profile like this and this, let us say the energy of the electron. So, here, if you see this is U this is function of position? This is energy, so, this E is more than U. So, there is a high probability of finding electron here and there is a of course here it is decaying. So, there is a less probability of finding electron in this region. That say this is x 1 this is x 2.

So, between x 1, x 2 there is a high probability of finding electron beyond x 1 or beyond x 2 this is a less probability of finding electron. So now, actual waveform may look something like this. So, let us say this is your x 1 this is let us say, x 2. So, in between you will find the

so that means this electron is now localized. So now, this waveform is not a single psi n but it is a combination of psi n.

So, you can write some a n coefficient times psi n and that is added over some n basically. So, you have this one then multiplied by e to the power – iota omega t or iota e by h times t. So that means this waveform or this electron is localized in this region. Now, we can recall the Heisenberg uncertainty principle that if it is localized in position then it is momentum cannot be determined with accurately.

So that means it will have some spread in k. So, you can see here this psi n basically. So that means they have different each psi n will have different k. So that means there will be range of momentum and if you compare this thing with e to the power iota kx – iota omega t, here is a plane wave unlimited and this momentum is fixed is h bar k. So, it is momentum is basically.

For a plane wave it is some kind of this thing as some k value it is fixed. Then this is basically moving like this. When it is constant in x direction then this momentum basically spreads. You can see some spread here, so, this psi x. If you write in momentum space, you can write some coefficient times e to the power iota kx – omega t dk. So, there is some kind of Fourier relationship between real space and the momentum space.

So, this we call real space and this we call momentum space. So, this basically satisfies the uncertainty relationship that it is localized in position real space it is spreads out in k space. And similar relationship exists between time and frequency. So, if you look in terms let us say this is the same. If it is versus time then this versus omega the similar relationship you can explore in time and frequency space. So that part we will not explore.

We are only exploring the position space but you can solve this equation with respect to time and frequency and get the similar relationship.

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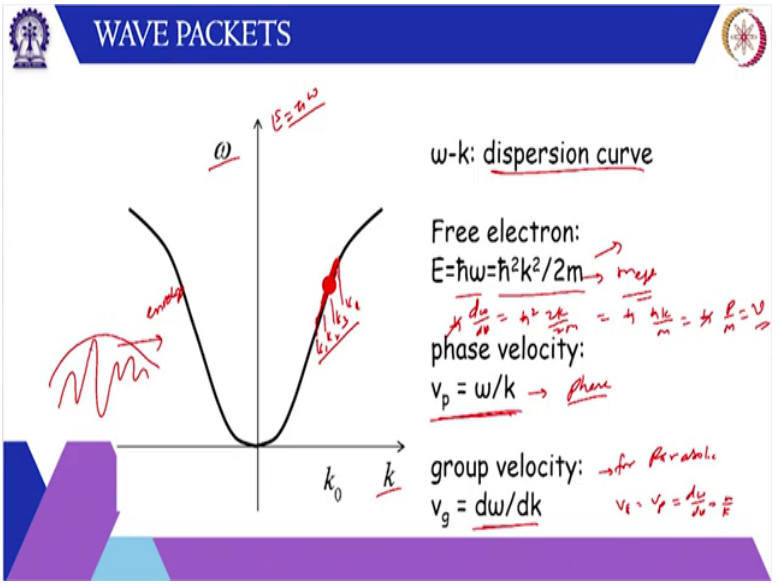

Now in real life situations or for example, in semiconductor band structures. We have this relationship omega versus k or Ek diagram because e is equal to h bar omega only different by a constant. So, this relationship is called a dispersion curve omega k or Ek diagram is called the dispersion curve. So, for free electron energy is h bar omega and is equal to h bar square k square by 2m.

But that is not satisfied here may be near this bands you have this relationship. And this mass is actually replaced by some effective mass. So that is because to take care of the **(()) (20:58)** effect and for parabolic you can write phase velocities omega by k and group velocity is d omega by dk. So for parabolic band structure this V g is equal to V P, d omega by dk is equal to omega by k.

You can differentiate here see if you differentiate h bar times T omega by dk is equal to h bar square 2k by 2m. So that is h bar into h bar k by m, so that is h bar times h bar k by omega. So, 1 h bar will cancel out and then h bar k is P by m. So, this d omega by d k this P by m is velocity basically. So, d omega by dk is velocity, so, you basically the phase velocity group velocity are same in case of parabolic dispersion curve.

And but in real crystals there is some and division from this relationship. So, the group velocity and phase velocity are different. Now, to highlight more about it phase velocity is basically the ratio of omega by k. So, this is basically that the if you consider phase and if you take the derivative d phi by dt is equal to 0. Then you will get this relationship that how a position with a constant phase is moving. So that is the phase velocity.

Group velocity is more related to this slope here. So, if you consider all these values, let us call it k 1, k 2, k 3, k 4 and then this will give you some kind of this relationship. And then how this envelope is moving basically, so that is the group velocity, so, group velocity is the movement of this envelope. Of these always these values in that region, k 1, k 2, k 3, k 4 and phase velocities is individual related to individual phase movement. So, individual phase point how it is moving that is omega by k.

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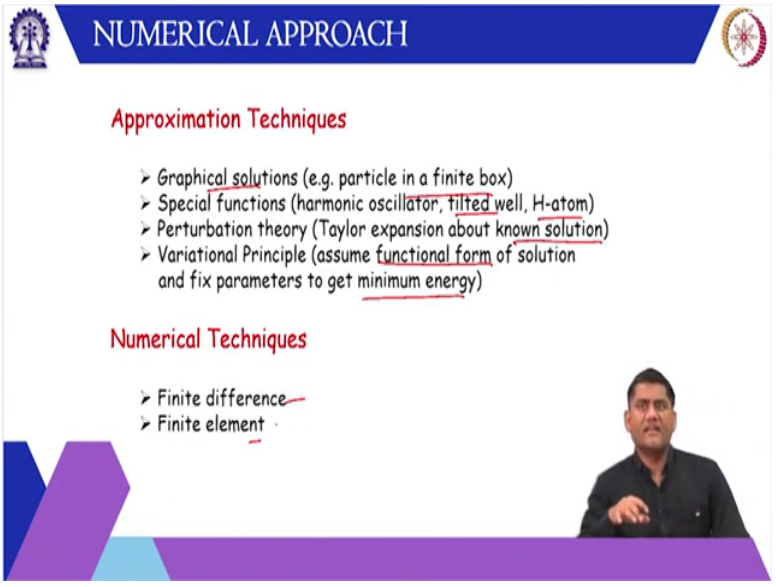

Now, we will discuss how to numerically solve the Schrodinger equation. So, there are several approximation techniques for example there are graphical solutions for particle in a finite box. Then there are some special function that are used to discuss harmonic oscillator tilted well, or hydrogen atom. Then they are perturbation theory. So, using the Taylor series, expansion are about non solutions.

So, to get the solutions in the vicinity of known solutions then they have variational principles where some functional form is assumed for the solution. Then these parameters are fixed to get the minimum energy. So, through energy minimization we get those wave functions a numerical technique. We can use finite difference of the finite element method here.

So, in this lecture we will discuss how the finite difference method a simple method which is very useful to solve the Schrodinger equation.

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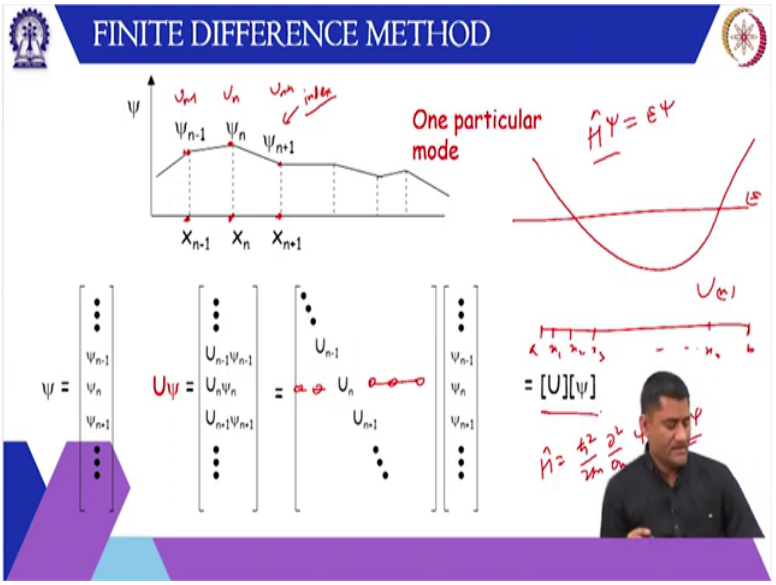

So, for example, we can consider any potential profile. Let us say this is the potential profile U as a function of position. So, we will solve for only one dimension. Let us say this is the energy. So, if you recall that the Schrodinger equation time independent Schrodinger equation is h psi is equal to e psi where size of wave function. So, h is basically d 2 psi by dx square + U times psi.

So, there are two terms here basically one is the derivative term double derivative and other is a u psi. So, what we can do? Let us consider this let us say this is your x axis so, from a to b these are the point x 1, x 2, x 3 and so on. Let us say, x n so, what we do? Let us say this is the how we discretize. So, this is x n, x n + 1 x n – 1. And this is the whole x axis which is discretized then on each axis we can basically do the Taylor series expansion of the differential equation.

And we can assume that this is a psi here. So, at x n the value is psi n, x n + 1 psi n + 1. So, this n, n + 1 are the index or they are tailing all the position basically. So, this indexed tailing all the position. So, at each point we can have. What is the value of potential? U n, U n + 1 U n – 1. So, if you see this h is h cap is h bar square by 2m del 2 by del x square times psi + U psi.

So, U psi is basically product of potential at that particular position multiplied by the value of wave function at that particular position. So, this will be U 1 psi 1, U 2 psi 2 and so on U n psi n U n + 1 psi n. So, we will get one vector basically for one dimensional case and if you

write it as a product then what you can write? You can write this as a some diagonal matrix multiplied by unit by a column vector.

So, if you multiply first row, you get U 1 psi 1. Second row you will get U 2 psi 2 and so on. For of this row, you will get u n psi n because others are 0 basically here. So, this zeros are not shown here so, this is U psi.

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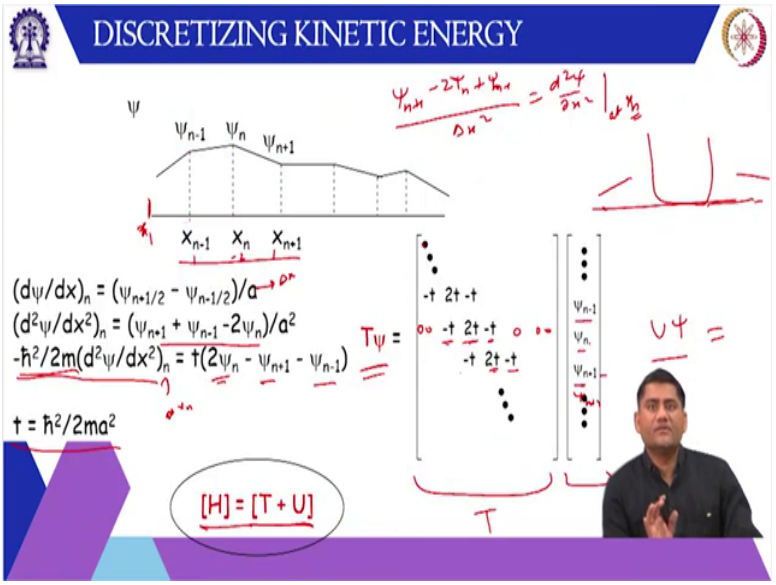

Then other term is the double derivative d 2 psi by dx square. So, this you can recall we discuss over the finite difference expression. So, this is the central difference for the double derivative. So, this is written as psi of n + 1 – 2 psi n + psi of n – 1 divided by delta x square. This is d 2 psi by dx square so, this is what, in this form, we can write. So, this is a derivative at n at x n so, you can say at x n, this is a derivative at x n.

So, at nth position, this double derivative is basically 2 times the psi at x n and then 1 times at n + 1 and n. So, these are the two neighbouring points basically. So, the coefficient is –2 here coefficient is 1 here 1 here n divided by this delta x square times h bar square by 2m. So, here delta x is written as a. So, this a is actually the delta x. Now, this we are assuming uniform grade expressing if it is non-uniform then you have to accordingly discretize.

Now, if you multiply this vector h bar square by 2m times d 2 psi by dx square at x n. So, the derivatives at x n. So, this a square and h bar square 2m can be combined and we will call it let us say T. So, this h bar square by 2ma square is called T, so, the coefficient is 2T for psi n

and – T and – T for psi n + 1 and psi n – 1. So, again, this can written as T psi again this is a matrix multiplied by psi vector.

So, if you consider, let us say any nth term here so, this will be this others will be 0 here. So, nth psi n is multiplied by 2T. So, psi n – 1 is multiplied by – T and psi n + 1 is multiplied by – T and so on. If you go to next term then psi n + 1 is multiplied by 2T. So, psi n by – T and psi n + 2 by – T. So that is how you can basically write another point you might like to know what happens at the end? So, at the end basically let us say this is a last point.

Let us say this is x 1. So, this is a last point so, here what you will write? So, this boundary condition thing we have already discussed. There can be drizzling boundary condition. Then you already know the value of psi. So, for example, in a situation you can assume that far away from this as the psi is 0, so, you can put Rich lead boundary condition or you can put other boundary condition where the derivative of psi is some value.

So that is called Newman boundary condition. So, here we will use a digital boundary condition because sufficiently away from this, let us say psi is 0. So now, we have two expressions this is T psi the other one is U psi. So, T psi + U psi = e psi. So now, what we do? We have, this H = T + U. So, T is this matrix, U is this matrix. So, when you add T + U then you have to just get the Eigen solution of this matrix.

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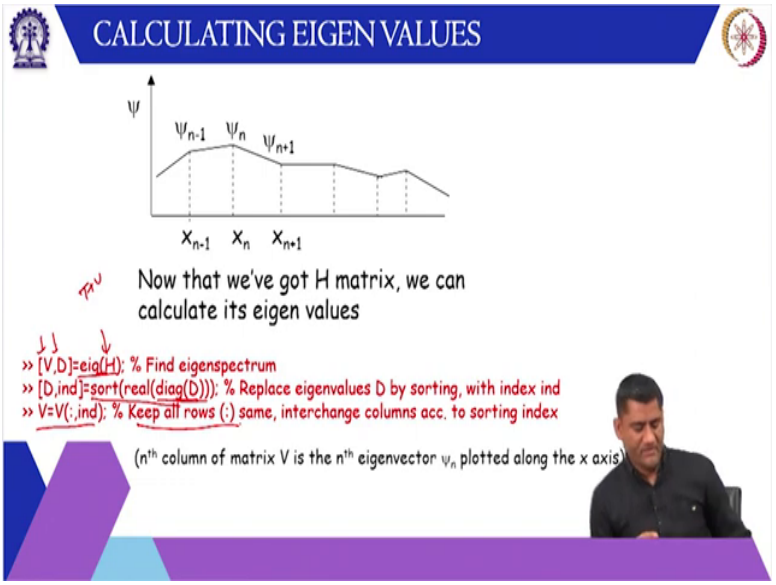

So, in Matlab there is a function called Eigen eig so, just find the Eigen which H is basically T + U these two matrix we have already created. Then we just find the Eigen value of T + U

then that will give you the energies and the corresponding wave functions. So, this V is basically kind of wave functions and this Eigen energies basically and we have to sort it basically.

So, this is basically D is basically kind of diagonal matrix, where only the diagonal elements are non-zero rest are 0. Because these energies are fixed for each wave function. So, what we are doing here, we are sorting it out in terms of energy so that we get the lowest energy then the second higher energy than third higher energy and so on. And then corresponding index is used to calculate the wave function. So then, so that we can plot it, so, this is basically to plot it basically

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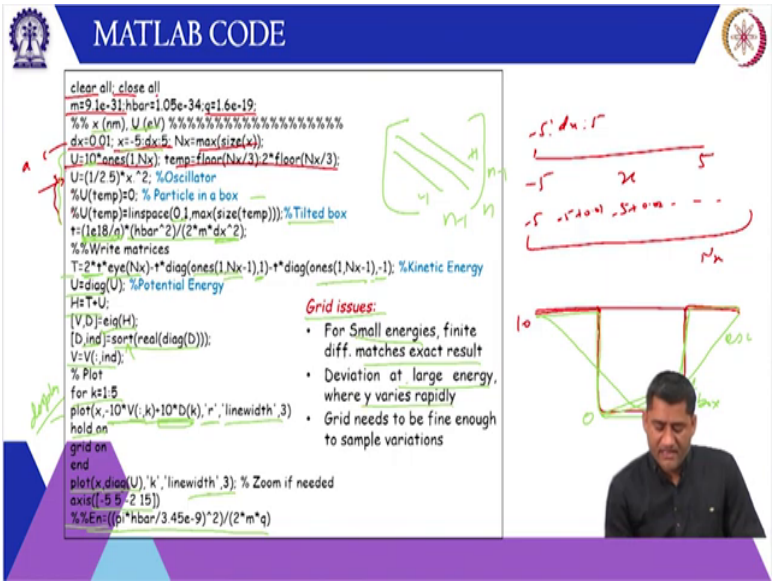

Now, this is the Matlab code, so, maybe just I will. I will describe it briefly so, clear all close all of the Matlab commands to clear everything any the variable if it is there. Then mass is defined here 9.1 10 is to 1 is 31 kg. This is the h bar then q is the charge. Then dx is the a thing that will be defined as a then. We are considering x from – 5 to 5. So, this is your x axis this is from – 5 to 5. Then n x is basically this is a max size X.

So, this is basically from – 5. It goes in the step of dx 2, 5. So, dx is 0.01. So, this is a – 5 point here. Another point next point is – 5 + 0.01 next point will be – 5 + 0.02 and so on. So, these are all the points and we count. How many points are there that is Nx? Then we define U as a potential. So, what we do here. We say that it is U is 10 and once it creates a matrix with size 1, Nx. So, this is basically simply a matrix with value 10.

Then, this is basically is used to select some portion of it and we define this oscillator particle in the box. So, this code basically there are three types of potential considered here, one is oscillator, others are commented out. This percentage sign is comment. So, if you comment first one and then uncomment the second one then you will simulating particle in the box. So, you see, U Temp is 0.

That means in this region U is 0. So, you will have profiles like this. Let me use different colour. So, you will use some so, for particle in a box the profile will be like this. So, these indexes are written by temp, for the oscillator it is U times 1 by 2.5 times x square x dot means it is a matrix operation. So that means for all the elements of x are squared basically. So, at x equal to 0 this will go to 0 and this is 1 over 2.5.

So, it may be something like this so, here this stamp is not used, so, it is just basically oscillator. This is oscillator and this is box particle in the box and third one is tilted box. So, this is basically U is not 0 here but it is between 0 and 1. So, here it is 0 this is 1 here. So, this is a tilted box basically. So, for all three cases same code will work out basically. So now, T is defined as 1 e 18 by q times h bar square by 2m by dx square.

Then h bar square k square by 2m. So, you see what is a T here? h bar square by 2ma square. So, this is h bar square by 2ma square. Then this factor is there because we are considering this x is in nanometre. And U is in electron volt so, to take care of these values because this quantization will appear when the length scale are appropriate and energy scales are appropriate.

So, to take care of this thing this scaling factor is used so that x can be nanometre. So, you can substitute actual values of x in terms of nanometre. So, this will be multiple over 10 is to – 9 and then electron, volt, 1.6 times 1 – 19. So, to take care of this factor this is basically multiplied here. Because this is 9 so, – 9, so, this is divided by x square now, so, this basically 10 is power –19 times 2.

So, it becomes 10 is power 9 times 2 means times for 18. So, times for 18 and divide by this q because this is electron volt so that has to divide by q. So, this factor you should note down then we are creating the matrix. So, this T is all the diagonal elements are 2T, so, 2T

multiplied by this diagonal matrix This I basically creates a identity matrix with diagonal element equal to 1 so that is multiplied by 2T.

Then T is multiplied by off diagonal element. So, this off diagonal elements are created by this diagonal matrix with 1 to n x – 1 to right side. This is to the left side. So, this now, if you see a matrix here, the length here will be n the length for this diagonal will be n – 1. For this diagonal it will also be n – 1. So that is why we have taken this once n – 1 here and then this is + 1, this is – 1 diagonal. So, these are T matrix then U is basically diagonal U.

So, U is also discretized here is already created here. So, the potential is included here. Now, H is defined as T + U then we calculate the Eigen values of this H. Then we sort this in terms of the energies from low energy to high energy and then corresponding index is here. So, this sort is a function in Matlab. You can write help sort. It will give you the information then V can written a V times colon times index.

So that is this values are arranged in terms of the index basically that we have chosen for these energies. Then, of course we can plot for first five energies. Let us say k = 1 to 5 so, plot x so, x is this we have created here times – 10 times V + 10 times D. So, V is basically the purpose of this thing is basically to plot this wave function at different energies so that we can visualize it.

If we do not use this, we simply write V then what will happen? They all will overlap. So, you cannot distinguish so, this is only for display purpose. What you can do? You can plot for individual waveform, each figure for individual waveform. Here what I am doing, I am plotting all the five wave functions in the same plot. So, I am basically I have plotted at different energy level so that you can see it basically.

So, this is the wave function V and then some offset is added for the display purpose. Then colour is R, line width is 3 and so on the grid on all those things. Then plot x dial U. So, this is also plot of potential profile on the same hold on means it the plot command will be executed at the same diagram. So, it also plot the potential profile along with the wave function. Then x is a limited to – 5 to 5.

And then this for x axis y axis limited from – 2 to 15. Because this value is I think maximum 10 or so and then this value is commented out. But this will give you the energies corresponding to the wave function. So, there are some great issues that need to be considered. So, for a small energy is finite difference matches the exact result and there is a division at large energy where y varies rapidly. So, for that grid needs to be fine enough to sample this variation in the potential.

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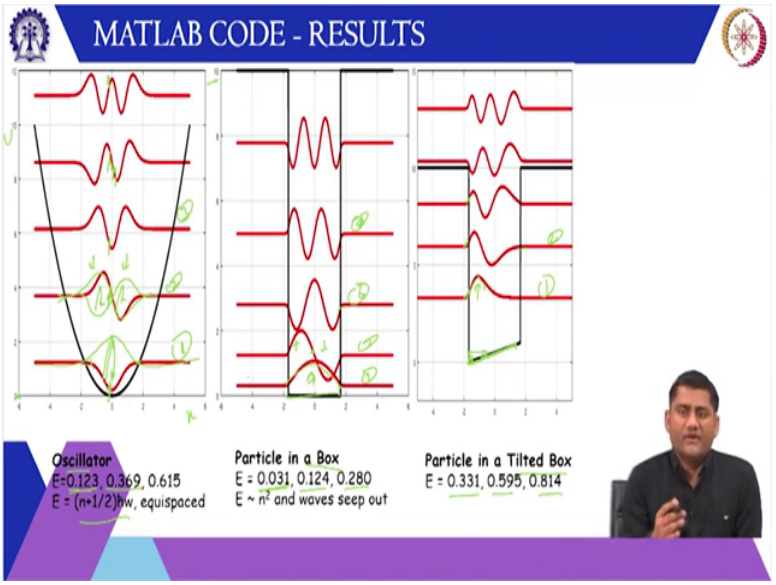

So, here, these three cases, oscillator particle in a box and particular tilted box are considered here. So, for oscillator you see this is first waveform. So, it is plotted here and basically, whether you plot it like this or you plot it like this. It does not really matter you can you just as a sign difference, basically because this wave is basically oscillating like this. It goes up, goes down like this it is oscillating.

And the energy is corresponding with this one is 0.123. So, this is 0 here and it is basically some parabolic potential profile. So, this is U versus x and if you relate it with the analytical solution for harmonic oscillator quantized energy is given by n + half times h bar omega. So, for first state n is 0. It is simply half h bar omega. Then second will be 1 + r h bar omega, so, the difference will be h bar omega. So, this0.123 it moves 0.369.

So, this is second and this is third and so on and you see here, this waveform is like this or you can also assume this is like this. So, it is basically as oscillating like this, so, there are one minima here, 1, 0 crossing. Then there are 230 crossing here and so on. And you can notice

one more thing here it is symmetric, so, this see it is symmetric around symmetric, is symmetric here is around symmetric here. It is symmetric here.

You can see symmetric here symmetric here, so, this is basically symmetric. Then particle in a box that is also symmetric, so, lowest is 0.031 and you notice the value here. This value is small compared to this one because the value is kind of narrow here. So, when it is constrained in position then in a momentum space, it will be broadly spaced. So, this energy will be larger here.

Same thing you can see here these are tilted, so, it is a narrow here that we see that this should be more. So, you see 0.03 is 0.331. The next is 0.5, 0.8 here 0.124, 0.28. This is a one waveform, so, this is only one maxima here. This is a second so, third, this is a 4 and so on. This is the 1, this is 2 and for the tilted waveform you can see this maxima occurs somewhere here. For a normal box it appears exactly in the middle.

Because this is symmetric. It is asymmetric, so, here is a lower potential, so, probability is supposed to be maximum here but it is slightly away from the surface. So, these results you can find out for any arbitrary potential profile. You can solve the Schrodinger equation and use this real to analyse, what happens with the energy? And the wave function because energy tells you the ground state energy.

And this wave functions tell you what is the probability of finding electron here? So, you see there is a maximum probability in the middle here for first one. Second one it is exactly 0, so, maximum probability is somewhere here for rectangular is in the middle then for the second one is 1 by fourth from either side and so on. Here for tilted one it is close to the lower potential side but not at the boundary because boundary has to be 0.

And another thing you can notice here, these values are not this is not infinite potential is a finite potential value. So that is why there is some leakage. You see there is some leakage to the outside, see there is some leakage. It is not exactly 0 here, so, there is some leakage to the side also. Because of this finite potential barrier but this 10 electron will volt is already quite high. So, you can see this leakage is small here.

If you, let us say, rerun the simulation with a small value, let us say 4 or something then you will see a bigger leakage or a more leakage to the sides where the potential energy is lower.

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So, in this lecture, we have discussed how to solve the Schrodinger equation with boundary conditions, so, this boundary condition give rise to the particular shape to the wave function and now wave function is not e to the power iota kx +– omega T but It is a combination of these waves to give certain shape which satisfy the boundary condition and again I am reiterating that boundary condition lead to the quantization of these energy states and the localization. So, thank you very much.