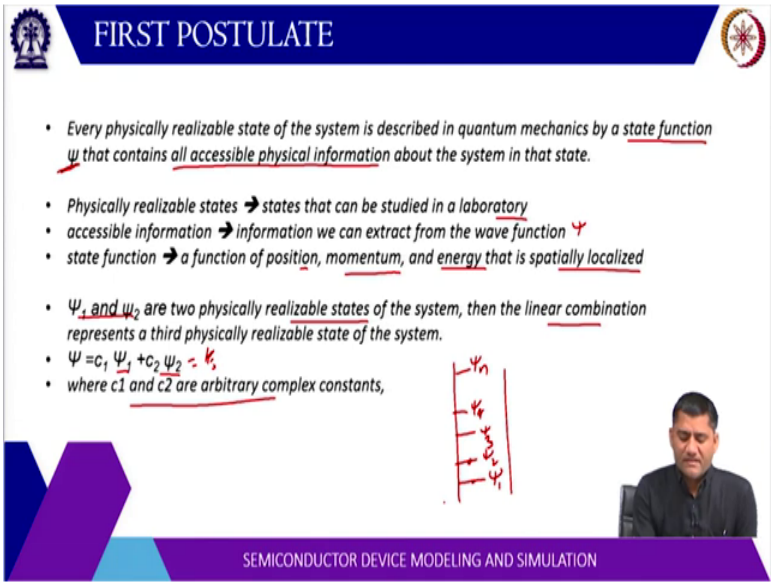
Semiconductor Device Modelling and Simulation
Prof. Vivek Dixit
Department of Electronics and Electrical Communication Engineering
Indian Institute of Technology – Kharagpur

Lecture – 54
Quantum Mechanics

(Refer Slide Time: 00:30)



FIRST POSTULATE

- *Every physically realizable state of the system is described in quantum mechanics by a state function ψ that contains all accessible physical information about the system in that state.*

- *Physically realizable states → states that can be studied in a laboratory*
- *accessible information → information we can extract from the wave function* ψ
- *state function → a function of position, momentum, and energy that is spatially localized*

- *Ψ_1 and ψ_2 are two physically realizable states of the system, then the linear combination represents a third physically realizable state of the system.*
- $\Psi = c_1 \Psi_1 + c_2 \psi_2 = \psi_3$
- *where c1 and c2 are arbitrary complex constants,*

SEMICONDUCTOR DEVICE MODELING AND SIMULATION

Hello, welcome to lecture number 54 in this week we will discuss about the quantum transport and let us begin with reviewing the some basics of quantum mechanics in this lecture. There are four main postulates in the quantum mechanics. The first one is that every physically reliable state of the system is described in quantum mechanics via state function, psi. So, psi state function that contains all accessible physical information about the system in that state.

So, for every state there is a state function psi then, if you look at the keywords here physically realizable states. So that means the states that you can study in the laboratory then the information that you can extract. So, not all the information can be extracted but some information about the position, the momentum, the energy that can be extracted from the wave function psi.

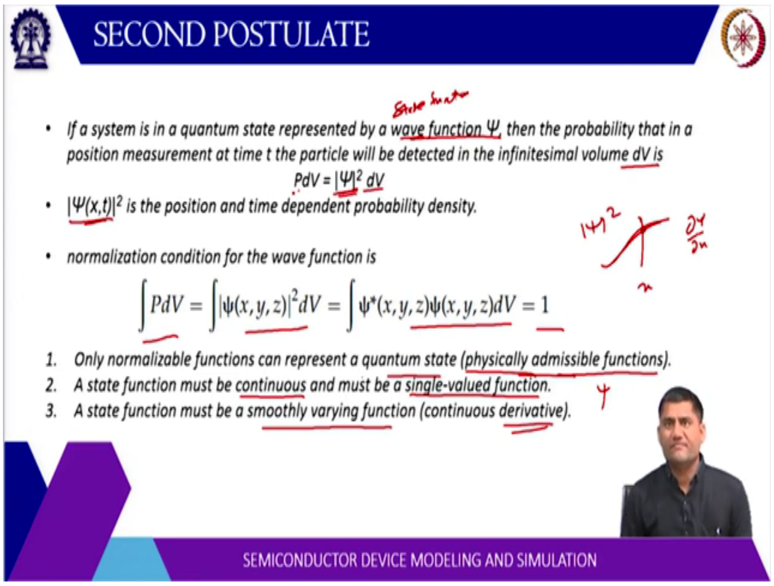
Then this state function psi is a function of position, momentum and energy and which is especially localized. Now, let us consider there can be n number of function, psi 1 psi, 2 psi, 3 and so on. Let us say if there are two physically realizable states psi 1 and psi 2. Then a linear combination which is some constant c 1 times psi 1 + some constant c 2 times psi 2. This will be third state which will also be physically realizable and here c 1 and c 2 can be arbitrary complex constants.

So, in summary, the first postulate says that state function or the wave function psi for a given state contains all the information about the system in that state. So, given state can have different energies e 1, e 2, e 3 and all these states are represented by some function psi 1, psi 2 psi, 3 and so on. Now, you can visualize it like this. Let us say these are the state psi 1, psi 2, psi 3, psi 4 and let us say psi n.

Electron can be in a state 1 it can mean state 2. And accordingly that wave function will come into the picture. It is possible that half of the time electron is in psi 2 half of the time is it in psi 1. So, your corresponding state will be half psi 1 + half psi 2. So that way, you have multiple combination of these realizable states. So, although there are n number of discrete states but you can have multiple combination of this state combination of 1 state, 2 state, 3 state and so on.

So, this state function or the wave function psi for a given state tells all the information of that particular state. So, this is first post postulate.

(Refer Slide Time: 03:46)



SECOND POSTULATE

- *If a system is in a quantum state represented by a wave function Ψ, then the probability that in a position measurement at time t the particle will be detected in the infinitesimal volume dV is*

$$PdV = |\Psi|^2 dV$$

- *$|\Psi(x,t)|^2$ is the position and time dependent probability density.*
- *normalization condition for the wave function is*

$$\int PdV = \int |\psi(x,y,z)|^2 dV = \int \psi^*(x,y,z)\psi(x,y,z)dV = 1$$

1. *Only normalizable functions can represent a quantum state (physically admissible functions).*
2. *A state function must be continuous and must be a single-valued function.*
3. *A state function must be a smoothly varying function (continuous derivative).*

SEMICONDUCTOR DEVICE MODELING AND SIMULATION

Then the second postulate says given this wave function or the state function psi, so, I will use this one interchangeable, wave function or a state function. Because this wave function is for particular state or combination of state. So, if the particular wave functions then what is the probability density of finding the electron? So, the probability density is psi square that is P. And then what is the probability of finding electron in volume dV that will be probability density psi square multiplied this volume dV.

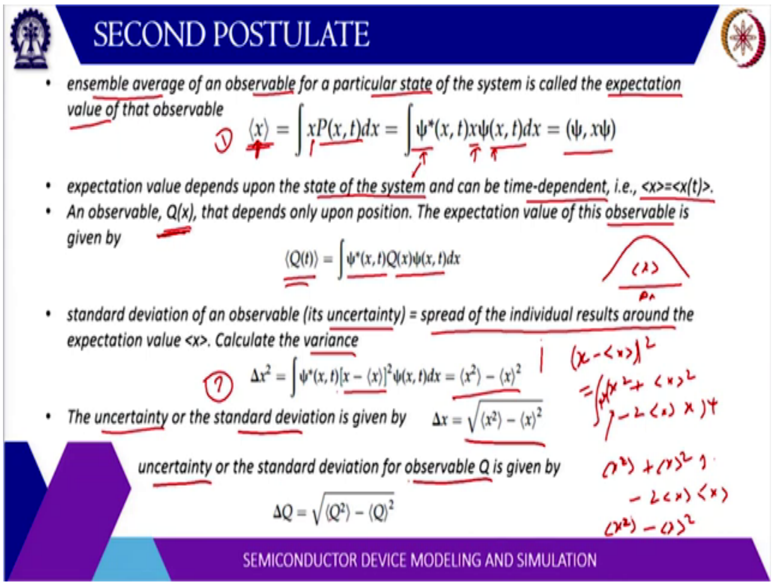
So that will be the probability of finding electron in that particular position. Now, this psi is a function of position and time, so, you can calculate at given time at given position. What is the probability dense probability density function? Now, this wave function has to be normalized. So, this PdV should be equal to 1. And then of course, you can write psi square dV is psi star psi dV that is equal to 1.

So that will give some normalization condition. So, here there are conditions for this wave function that only normalizable function can represent a quantum state. So that is basically physically admissible functions. If you do not normalize it then they may give an realistic probabilities, basically because probability cannot be more than 1. So, it has to be normalized then about the nature of this wave functions psi this psi must be continuous and must be single valued.

That means there cannot be an abrupt change in the probability basically. So, if you plot psi square it also has to be continuous there cannot be abrupt change. Another one there cannot be two probabilities. Let us say, given position x there can only be 1 value of psi, 1 value side is 1 value of psi square. So that will basically give rise that there is only one probability. There cannot be two probabilities of finding electron.

And then, of course, this function must be smoothly varying. So that means it is derivative that is d psi by dx or d psi by dr is continuous. So, these are the conditions for this wave function.

(Refer Slide Time: 06:23)



SECOND POSTULATE

- ensemble average of an observable for a particular state of the system is called the expectation value of that observable

$$① \quad \langle x\rangle = \int xP(x,t)dx = \int \psi^*(x,t)x\psi(x,t)dx = (\psi, x\psi)$$

- expectation value depends upon the state of the system and can be time-dependent, i.e., <x>=<x(t)>.
- An observable, Q(x), that depends only upon position. The expectation value of this observable is given by

$$\langle Q(t)\rangle = \int \psi^*(x,t)Q(x)\psi(x,t)dx$$

- standard deviation of an observable (its uncertainty) = spread of the individual results around the expectation value <x>. Calculate the variance

$$② \quad \Delta x^2 = \int \psi^*(x,t)[x-\langle x\rangle]^2\psi(x,t)dx = \langle x^2\rangle - \langle x\rangle^2$$

- The uncertainty or the standard deviation is given by $\Delta x = \sqrt{\langle x^2\rangle - \langle x\rangle^2}$

uncertainty or the standard deviation for observable Q is given by

$$\Delta Q = \sqrt{\langle Q^2\rangle - \langle Q\rangle^2}$$

$\langle x\rangle$

$(x-\langle x\rangle)^2$

$= \int \psi^*(x^2 + \langle x\rangle^2 - 2\langle x\rangle x)\psi$

$\langle x^2\rangle + \langle x\rangle^2 - 2\langle x\rangle\langle x\rangle$

$\langle x^2\rangle - \langle x\rangle^2$

SEMICONDUCTOR DEVICE MODELING AND SIMULATION

Now, defining other properties of this wave function; how do we extract out the observable quantities from this wave function? So that is basically done by we can calculate the ensemble averages of an observable for a particular state or a state function. This system of the system this is called expectation value of that observable. So, this is represented by this bracket here, angular bracket.

So, this angular bracket on x. It tells you the expectation value of the position. So, how it is calculated this particular function x is multiplied by the probability density. So, x times probability dx. That is basically psi star x psi dx. So, psi is the state function or the wave function and psi star is the complex conjugate of that wave function. And this x is in between and it can also be written as this in this format which basically shows some kind of inner product the psi x psi.

Now, this expectation value depends on the state of the system that is psi and it can also be time dependent because psi depends on time. So, you can write expectation value of x is same as expectation value of x as a function of time. Now, apart from this position x there can be a function which is dependent on the position let us call Q as a function of x. We can also calculate the expectation value of this Q just substitute this x by Q.

So, you will have psi star Q psi dx. That will be the expectation value of this observable. So, in quantum mechanics we do not have directly these quantities, we have this classical quantities. And then for the classical quantities we define some kind of operator and then from the state function we actually calculate the observable quantities. So, this is one n sample average or the expectation value.

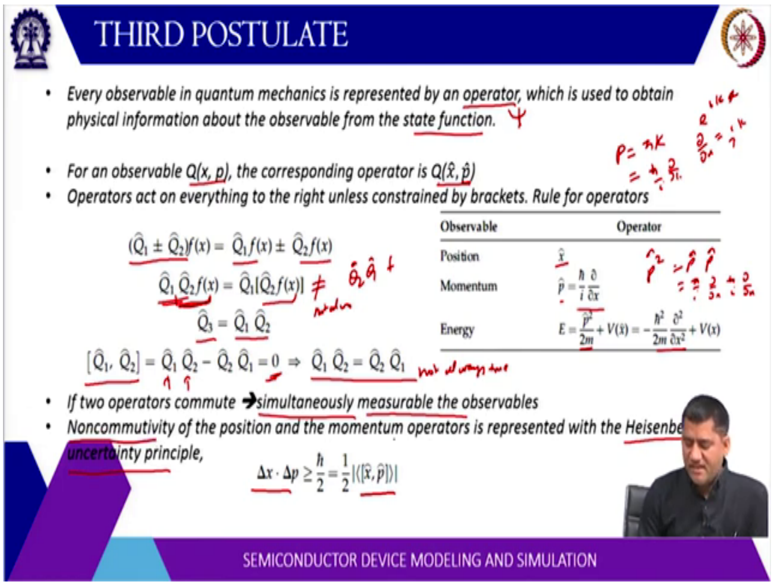
So, this is one and another quantity that is of interest is the standard deviation or it is uncertainty. So that is second basically so, this is basically let us say you calculate the average position then you would like to find out this average position and what is the deviation? So, that will be delta x basically. So that is a spread of individual observable around the expectation value. So, for that we calculate the variance which is delta x square.

So, delta x square is basically calculated as expectation value of x – average x square. So, if you put it here, it is basically like x – average x square = x square + average x square – 2 average x times x. Then, if you integrate it for psi star psi, what you will get? The first term will give you x square average value of x square. Secondly, x square times psi star psi which will be 1 – 2 times average value of x times psi star x psi which will also be average value of x.

So, this is basically x square average value + x average square – 2 x average square. So, that will be x average square. So that is what you have here. So, variance is basically average value of x square or the expectation value of x square – square of expectation value of x. So that is the variance and from the variance you can calculate the uncertainty or the standard deviation which is the square root of variance basically.

And now, we can replace this x by any observable Q here and that will give you the uncertainty or the standard deviation for observable Q which is delta Q is equal to average value of Q square minus square of average value of Q and then whole square root.

(Refer Slide Time: 11:05)



THIRD POSTULATE

- Every observable in quantum mechanics is represented by an operator, which is used to obtain physical information about the observable from the state function. Ψ
- For an observable Q(x, p), the corresponding operator is $Q(\hat{x}, \hat{p})$
- Operators act on everything to the right unless constrained by brackets. Rule for operators

$$(\hat{Q}_1 \pm \hat{Q}_2)f(x) = \hat{Q}_1 f(x) \pm \hat{Q}_2 f(x)$$

$$\hat{Q}_1 \hat{Q}_2 f(x) = \hat{Q}_1[\hat{Q}_2 f(x)] \neq \hat{Q}_2\hat{Q}_1$$

$$\hat{Q}_3 = \hat{Q}_1 \hat{Q}_2$$

$$[\hat{Q}_1, \hat{Q}_2] = \hat{Q}_1 \hat{Q}_2 - \hat{Q}_2 \hat{Q}_1 = 0 \Rightarrow \hat{Q}_1 \hat{Q}_2 = \hat{Q}_2 \hat{Q}_1$$

not always true

Observable	Operator
Position	$\hat{x}$
Momentum	$\hat{p} = \frac{\hbar}{i}\frac{\partial}{\partial x}$
Energy	$E = \frac{\hat{p}^2}{2m} + V(\hat{x}) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)$

$p = \hbar k = \frac{\hbar}{i}\frac{\partial}{\partial x}$

e^{ikx}

$\hat{p}^2 = \hat{p}\,\hat{p} = \frac{\hbar}{i}\frac{\partial}{\partial x}\frac{\hbar}{i}\frac{\partial}{\partial x}$

- If two operators commute → simultaneously measurable the observables
- Noncommutivity of the position and the momentum operators is represented with the Heisenbe uncertainty principle,

$$\Delta x \cdot \Delta p \geq \frac{\hbar}{2} = \frac{1}{2}|\langle[\hat{x}, \hat{p}]\rangle|$$

SEMICONDUCTOR DEVICE MODELING AND SIMULATION

So, we have discussed two postulates that psi tells us about the state of a system from which we can estimate all the observables and the second postulate tells that psi square gives you the probability density and then using these expectation values. We can calculate these observable quantities. Now, third postulate every observable in quantum mechanics is represented by an operator.

So, position x there will be operator, momentum there will be operator, energy level operator. And which is used to obtain the physical information about the observer from the state function psi. So, we do not use directly this equation but we use these operators on the state functions psi to calculate the observable values. So, for any observable Q which is a function of position and momentum, the corresponding operator can be written as Q of x cap P cap.

So, here, x and P are represented by replaced by their operators x cap and P cap. So, for position, let us say this is x cap for momentum P cap. Now, you know that P is equal to h bar K. And if you have function E to the power iota Kx this type of function then d by dx will give you iota K times this function. So, this can be written as H bar times d by dK divided by I. So that K comes here basically.

So, this h bar by I d by dx, so that is operator for momentum. Similarly, for energy is given by P square by 2m + the potential energy. So, the kinetic energy + the potential energy. And then, of course, you replace this p and x by their operators like here x and P are represent replaced by their operators. So, p is this, so, P square will be P operator, P square operator is basically P operator again P operator.

So, this is h bar by I del by del x h bar of I del by del x. So, h bar I is independent of x can be taken here. So, h bar square by I square, so that is –h bar square d 2 by dx square. So, h bar square d 2 by dx square, divided by 2m. And I square is minus so, there is a minus sign here. And + V x. So, this is the operator for energy. Now, there is properties of these operators. If there are multiple operators in addition, subtraction and multiplication.

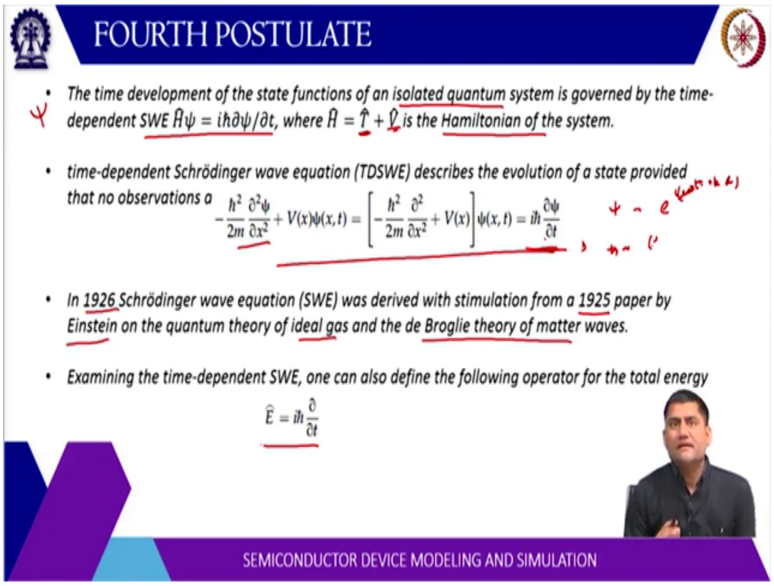
Then how do we use them? How they act on the function? So, if there is a summation operator 1 +– operator 2 on state function f will be operator 1 operating on the function f +– operator 2 independently operating on the function f. So, this is the addition property and the subtraction property multiplication it depends on the order. So, Q 1, Q 2 f means first Q 2, Q 2 will operate on f.

Then Q 1 will operate on the result of this Q 2 operator f. So that is Q 1 then bracket Q 2 f. So, this Q 1, Q 2 may not be equal, is known necessarily or not always is equal to Q 2, Q 1, f. In fact, Q 1, Q 2 can be defined as another operator called Q 3. So, this Q 1, Q 2 bracket is written as Q 1, Q 2 – Q 2, Q 1. And if this is 0 then these two operators are equal. So, this is not always true. So, if Y two operator commutes that means this is 0.

Then that means both Q 1 and Q 2 there are corresponding observables are measurable simultaneously they can be simultaneously measured. And if this is not 0 then these two observables corresponding to Q 1 and Q 2 cannot be observed measured simultaneously. And for this there is a famous Heisenberg uncertainty principle which says delta x delta p is greater than equal to h bar by 2 and which characterize half x cap, P cap.

So, this is basically coming from the non-commutativity of the position and momentum operator.

(Refer Slide Time: 15:57)



FOURTH POSTULATE

- The time development of the state functions of an isolated quantum system is governed by the time-dependent SWE $\hat{H}\psi = i\hbar\partial\psi/\partial t$, where $\hat{H} = \hat{T} + \hat{V}$ is the Hamiltonian of the system.
- time-dependent Schrödinger wave equation (TDSWE) describes the evolution of a state provided that no observations a $-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V(x)\psi(x,t) = \left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right]\psi(x,t) = i\hbar\frac{\partial\psi}{\partial t}$
- In 1926 Schrödinger wave equation (SWE) was derived with stimulation from a 1925 paper by Einstein on the quantum theory of ideal gas and the de Broglie theory of matter waves.
- Examining the time-dependent SWE, one can also define the following operator for the total energy

$$\hat{E} = i\hbar\frac{\partial}{\partial t}$$

SEMICONDUCTOR DEVICE MODELING AND SIMULATION

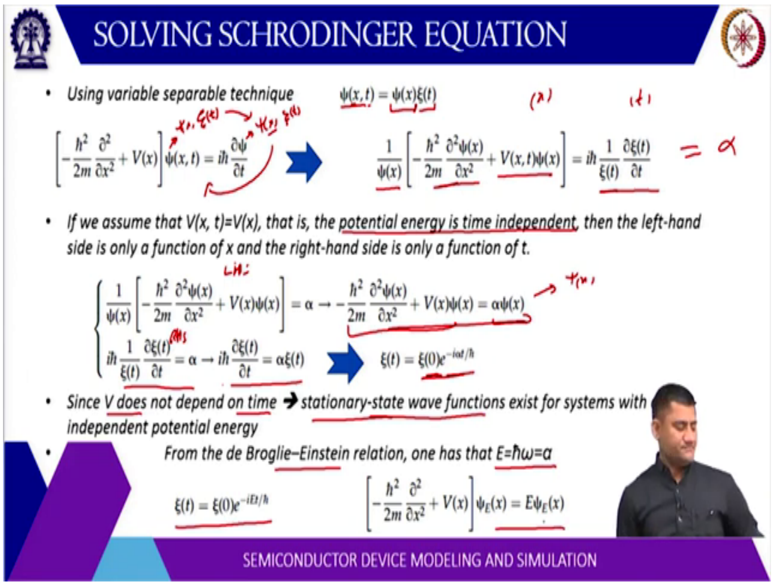
Now, the fourth postulate the time development of the state function. That means how this state function of the wave functions psi evolves with time. So, the time development of a state function of an isolated quantum system is governed by the time dependent, Schrodinger wave equation. So that is H psi is equal to iota H bar D psi by dt. So, H is basically Hamiltonian of the system.

So, this is basically for the potential energy this for the potential energy, this for the kinetic energy. And this time, dependent Schrodinger wave equation, is written as –H bar square by 2m d 2 psi by dx square, as you can see in the previous slide. This is the energy operator so that we have used + V psi. So that is, the energy operator is equal to the time domain, iota H Bar d psi by dt. So because psi is e to the power iota omega t – kx.

So, if you take derivative, it will be iota omega or kx – omega you can write whatever. Then it will be – iota minus, minus will become plus. So, it this will basically be H bar omega times your psi. So, this is basically, you can say this another operator for energy, so, e cap is iota H bar del by del t. So, this equation basically was introduced by Schrodinger in 1926 and it was the idea he got was from a 1925 paper by Einstein on quantum theory of ideal gases.

And the de Broglie theory of matter waves. So, this Schrodinger equation a time dependent Schrodinger equation, basically governs the evolution of this state function of the wave function psi.

(Refer Slide Time: 17:57)



SOLVING SCHRODINGER EQUATION

- Using variable separable technique $\psi(x,t)=\psi(x)\xi(t)$ (x) (t)

$$\left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+V(x)\right]\psi(x,t)=i\hbar\frac{\partial\psi}{\partial t} \Rightarrow \frac{1}{\psi(x)}\left[-\frac{\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2}+V(x,t)\psi(x)\right]=i\hbar\frac{1}{\xi(t)}\frac{\partial\xi(t)}{\partial t} = \alpha$$

- If we assume that V(x, t)=V(x), that is, the potential energy is time independent, then the left-hand side is only a function of x and the right-hand side is only a function of t.

$$\begin{cases}\frac{1}{\psi(x)}\left[-\frac{\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2}+V(x)\psi(x)\right]=\alpha\rightarrow-\frac{\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2}+V(x)\psi(x)=\alpha\psi(x)\\ i\hbar\frac{1}{\xi(t)}\frac{\partial\xi(t)}{\partial t}=\alpha\rightarrow i\hbar\frac{\partial\xi(t)}{\partial t}=\alpha\xi(t)\Rightarrow\xi(t)=\xi(0)e^{-i\alpha t/\hbar}\end{cases}$$

- Since V does not depend on time → stationary-state wave functions exist for systems with independent potential energy
- From the de Broglie–Einstein relation, one has that $E=\hbar\omega=\alpha$

$$\xi(t)=\xi(0)e^{-iEt/\hbar} \qquad \left[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+V(x)\right]\psi_E(x)=E\psi_E(x)$$

SEMICONDUCTOR DEVICE MODELING AND SIMULATION

Now, how do we solve the Schrodinger equation? There is a general procedure for solving the Schrodinger wave equation. What we do? There are two variables here, one is the position which is x and other is time which is T. So, we use a method of separation of variables. So, this psi x, t can be written as a product of two functions, one is dependent on x other is dependent on T. So, let us say we write at psi x times theta t.

And then, if you substitute this one to the Schrodinger equation. So, this becomes psi x this is zeta t, this is also psi x, this is zeta t. Now, here we are operating with respect to x only. So, zeta T can be separate out here we are taking derivative. So, psi x can be tabulate out and we can change the side and zeta t can be taken here. So, when it is taken to the left hand side, it become 1 over psi x and this becomes 1 over zeta t.

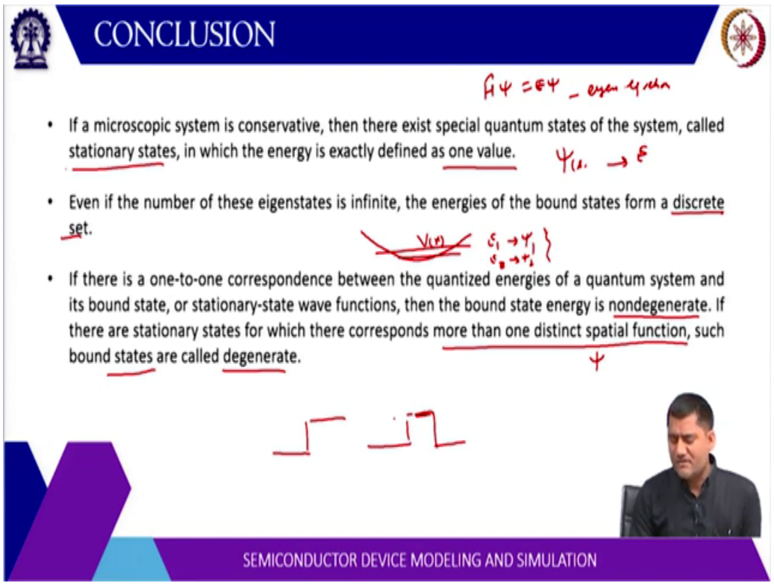
And then we operate it over psi x and zeta t. Now, if you notice here this H bar square by 2m d 2 psi by dx square, it does not depend on T. It only depends on x this d by dt. This also depends only on T but the potential may depend on x and t. So, if potential is varying as a function of time then of course these are coupled equation. We can do nothing about it but if the potential we assume that potential energy is position dependent only or it is time independent.

Then the left hand side is a function of x and the right hand side is a function of time. So, we can represent both by some constant let us say alpha. So, left hand side is equal to alpha and the right hand side is also equal to alpha because they are independent, so, they have to be some constant which is equal. Then, if you see here, if you equate this one then you can write H bar square root 2m d 2 psi by dx square + V psi is equal to alpha psi that is one equation.

And for time dependent d zeta by zeta is equal to alpha t by iota H bar. So, it will have simple solution. The zeta t evolves as a time is equal to zeta t = 0 times e to the power – alpha t by iota h bar or you can write e to the – iota alpha t by h bar. So, this is zeta t and so and here from here you can get psi x and you can get the total function. Now, since potential does not depend on time.

That means these are stationary state wave function exist for the system with time, independent potential energy. And then, of course, if you look at this relationship so, from the de Broglie Einstein relationship, we can say that e is equal to h bar omega and which is basically alpha here. So now, zeta T candidates zeta at t = 0 times e to the power – iota e t by h bar. And similarly, this h psi is equal to E psi for the position dependent function.

(Refer Slide Time: 21:28)



CONCLUSION

- If a microscopic system is conservative, then there exist special quantum states of the system, called stationary states, in which the energy is exactly defined as one value.
- Even if the number of these eigenstates is infinite, the energies of the bound states form a discrete set.
- If there is a one-to-one correspondence between the quantized energies of a quantum system and its bound state, or stationary-state wave functions, then the bound state energy is nondegenerate. If there are stationary states for which there corresponds more than one distinct spatial function, such bound states are called degenerate.

SEMICONDUCTOR DEVICE MODELING AND SIMULATION

So, in conclusion, if a microscopic system is conservative then there exists a special quantum state of the system and these states are called stationary state in which energy is exactly defined as one value. So, for given psi x which is conservative in nature, you will have particular energy. And in fact, if you look at this 1 h psi is equal to E psi. Where H is operator is energy, so, this is basically kind of Eigen equation.

So, E is the Eigen value of this operator when operated on a psi wave function. So, E is the Eigen value and psi is the Eigen wave function. Now, even if the number of these Eigen state is infinite, the energies of the bound state form a discrete set. So, this energies will be discrete in number. So, for a given potential profile because here, of course, we know that V is only function of position. It is not changing with time.

So that is why it is conservative and you will have different energies even corresponding psi 1 will be there. So, this is E 1. This is psi 1 then there is a E 2. There will be corresponding psi 2 and these are basically kind of principle values and corresponding to that we can have multiple combination. So, there can be E 1 + E 2 corresponding to psi 1 + psi 2, wave function and so on.

Now, if there is one to one correspondence between the quantized energy of quantum system and it is bound state or the stationary state wave function then bound state energy is non degenerate. So that means, there is at most one wave function corresponding to the one energy level. But if there are stationary state for which there are more than one special function. So, there are more than, this wave functions.

More than one wave functions then of course, for a given energy we have two wave functions. So then we call these states are degenerate states. These are called this bound state circle degenerate states. So, with this background information about the basics of quantum mechanics postulates we will continue our discussion and find out how the wave particles of this electron in quantum state they move because the quantum transport for different types of quantum scenarios?

So, firstly, we will discuss about the potential barrier then the tunnel through a step junction and the potential barrier. And then, of course, we will also look at the quantum corrections that are used in modern most devices and with that we will conclude our discussion on quantum transport, so, thank you very much.