Physics of Nanoscale Devices
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Lecture - 03
Basics of Quantum Mechanics

Hello everyone. In our previous discussion we saw that the transistor size is reducing continuously since last 40 years now, and nowadays the channel length in transistors is in few nanometers, few tens of nanometers at max and that is less than the mean free path of the electron and in this situation, in this kind of devices we cannot apply our classical conventional electron transport theory that we derive from Drude's model.

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So, that is why we need to think the electron physics from a fundamentally new perspective and that is what we will begin with from today's class and we saw that nowadays the devices are getting smaller and smaller and if we take an example of two terminal device in which we have a source, a drain and a channel and the channel length is in few tens of nanometers. Generally even in present devices the size of contacts, the size of source and drain their size is larger as compared to the channel.

So, as compared to the channel the source and the drain are considered to be the bulk material ok. So, in this context in these so, to say mesoscopic devices we need to understand the density of states, electron density of states in the channel and Fermi

function of the contacts. So, this is what we also saw in our previous discussion that we in order to properly understand the electronic behavior in now small devices we need to understand the electronic density of states in the channel because the channel is very small.

Now, few tens of nanometers and we need to understand the Fermi function of electrons in the source and the drain and once we understand these two concepts we can we will see in coming classes that we can formulate a new model of transport which is which can characterize the ballistic transport that we saw, that is happening in present day devices and we can also extend that concept to the diffusive transport case.

So, there are two key concepts to understand; one is the density states of electrons in the channel region and second is the Fermi function of the source and the drain contacts. So, the density of states, but what do we mean by density state? So, density of states is the number of energy states, number of electronic energy states per unit volume per unit at a given energy. Sometimes it is also defined as per unit energy, but it is number of electronic states per unit volume at a certain given energy.

And as we as all of us know that electron is a quantum mechanical particle electron is fundamentally a quantum mechanical particle. So, in order to understand the electronic states, we first need to understand the quantum mechanical nature of the electron. So, the first or so to say the stepping stone in understanding the density of state would be to understand the quantum mechanical nature of electrons in solids.

So, that is what we need to do and that is what we will try to develop in coming couple of lectures and once we have the quantum mechanical understanding of electrons in solids, we will see how we can extend that concept to derive the density of states for 0D, 1D, 2D and 3D systems in all kinds of systems basically. Fermi function comes from the statistics and it is relatively easier to understand this we will take up after understanding the density of states.

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So, first thing first. Let us begin with the basic understanding of quantum mechanical nature of electron in solids. So, we will start from the basics and in order to sort of understand the quantum mechanical nature of electron, we first need to understand the postulates of quantum mechanics or the axioms of quantum mechanics on which the entire formulation of quantum mechanics is based.

And, the first postulate of quantum mechanics is that; that every particle on every quantum system can be characterized by a mathematical function called the wave function ok. So, the wave function is a mathematical function and generally the wave function is represented by the symbol psi and it is generally a function of x, y, z and t basically the space and time coordinates. So, the entire nature of a particle or a quantum mechanical system is characterized by the wave function $\Psi(x, y, z, t)$.

And this is purely a mathematical entity. It can be a complex number as well generally it is a complex number, but it contains all the information about the system. So, if we need to understand the nature of electron we need to; we need to basically find out the wave function of the electron in a given condition. So, if you need to understand the electrons in solids, we need to understand the wave function of electrons in solids ok.

So, the first postulate of quantum mechanics says that every system can be characterized by a mathematical function and this mathematical function is known as the wave function.

This is generally a complex function and it belongs to what is known as the Hilbert space of the system.

So, we will not go to the mathematical details of the Hilbert space $\mathcal{H}$ or the linear algebra of quantum mechanics but all the systems or any system can be characterized by a wave function which is which belongs to the Hilbert space of that particular system. It contains every information and interestingly enough it does not we cannot extract physical implication directly from the wave function.

So, that is why this probability density the notion of probability density is defined. The second concept in quantum mechanics is the notion of probability density and the probability density is defined as the multiplication of the complex conjugate of the wave function with the wave function itself $[\,\Psi^*(x,y,z,t).\,\Psi(x,y,z,t) = |\Psi(x,y,z,t)|^2\,]$.

So, it is defined as basically psi star psi or mod psi square. As I just told you psi does not tell us anything physically about the system it is just a mathematical notion it is an abstract concept it is a mathematical notion this probability density function it is actually a physical thing about the system it tells us about.

So, for example, in this case when we are taking psi as a function of x, y, z and t it tells us about the probability of the electron being found or it is the probability density of electron being found in a space time coordinate. So, if we want to find out the probability of electron being found in a certain volume we just need to integrate psi x, y, z t square over that volume at a certain time $\int |\Psi(x,y,z,t)|^2\,dv$.

So, this will give us the probability of the electron or any quantum system being found in the volume dv or in the entire volume if we take the integral, if we do not take the integral it will just give us the probability of the electron being found in the small volume dv and if we integrate it will tell us about the probability of the electron being found in the entire volume ok at an instant t.

So, now we have the wave function of the system, we have the probability density of the system, but how do we measure other things. How do we measure other practical things about this system for example, if we want to measure the position of the electron or momentum of the electron or energy of the electron how do we do that, and for that

quantum mechanics has another has an interesting set of operators these are known as the measurables also and these are the Hermitian operators.

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So, in quantum mechanics corresponding to every physical observable there is an operator an Hermitian operator and if we need to sort of measure any quantity we need to apply the corresponding operator on the wave function ok. So, that will tell us about the. So, for example, the operator corresponding to distance $\hat{x}$ is just the distance x. The operator corresponding to energy is the first derivative of the wave function.

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So, the energy operator is basically $i\hbar\frac{\partial}{\partial t}$ and similarly the momentum operator is $-i\hbar\frac{\partial}{\partial x}$. So, if we apply these operators on the wave function then it will tell us about the corresponding quantity and from the notion of operators we actually have a notion of expectation value corresponding to an operator.

The expectation value of an operator is given as so for example, if we have an operator $\hat{A}$ the expectation value of the operator will be given as the integration of the wave function complex conjugative wave function into operator into the wave function integrated over all parameters dz, where this is the integration is taken over all the parameter $\langle\hat{A}\rangle = \int \Psi^*\hat{A}\Psi \, dxdydz$.

So, this will tell us about the expectation value of an operator. And, but what do we mean by expectation value of an operator? Expectation value of an operator is the average value that we will obtain if we make large number of measurements on the system, if we make large number of measurements corresponding to that operator and this will be the average value that we will obtain.

Please be careful that this is not the actual value that we will obtain if we make one measurement this will be the average value of all the measurements if we make large number of measurements this will be the average value of the outcome after a large number of measurements and this brings us to the notion of measurement in quantum mechanics.

Measurement in quantum mechanics is also an important notion. The measurement in quantum mechanics is unlike quantum mechanics is an application of an operator the measurement is basically application of an operator on wave function and collapse to an Eigen function of that operator.

So, measurement means that the measurement changes the state of the system, it basically collapses the wave function to one of the Eigen functions of the operator measurement operator. So, this is an important notion and this is quite different from classical mechanics in which measurement does not change the system does not change the state of the system.

But in this case the measurement collapses the wave function it changes the wave function to one of the Eigen functions of the measurable operator that we are measuring ok and that is why this notion of expectation value is important because it tells us about the average outcome that we will obtain if we make large number of measurements because different

measurements will give different outcomes and this expectation value will tell us about the average of all those outcomes.

This average is generally weighted by the Eigen values of the operator over the probability density. Another important quantum mechanical idea is that any system evolves according to a specific equation known as the Schrodinger equation a quantum mechanical equation which is also quite different from the classical evolution of systems. So, any system will evolve according to the Schrodinger equation of that particular system.

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So, the Schrodinger equation in very general terms is written as minus h bar square divided by 2 m del 2 plus U psi equals psi $\left[\left(\frac{-\hbar^2\nabla^2}{2m} + \widehat{U}\right)\Psi = i\hbar\frac{\partial}{\partial t}\Psi\right]$. So, this is the Schrodinger equation of any system. On the left hand side we have this U is the potential energy of the system potential energy of any particle that we are trying to understand or so to say potential energy operator which is equal to the potential energy itself.

This is the kinetic energy operator and this on the right hand side is the energy operator total energy operator that we saw few minutes ago. Now, we have the wave function which basically contains all the information about the system we have the probability density correspond of that particle which gives us a physical sense where the particle is more likely to be found we have measurable operators we have operators by which we can measure physical things physical parameters of a system.

We have an evolution equation corresponding to a system which is the Schrodinger equation and finally we have a few conditions that this wave function needs to satisfy in order to be a valid quantum mechanical wave function. So, the first condition that it needs to satisfy is the square integrability of the wave function $\int |\Psi^2| dv = finite$.

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So, the wave function corresponding to a quantum mechanical particle should be square integrable and by square integrable we mean that the square of the wave function basically psi square should be the integral of this square should be finite. Moreover there is another condition that is known as the normalizability and according to normalizability the integration over entire space should be 1 $[\int |\Psi^2| dv = 1]$.

It basically means that the probability of the particle being found in the entire universe should be 1 basically so this condition is it is related to square integrability this is known as the normalizability of the wave function. The second condition that the wave function needs to satisfy is the continuity of the wave function and as you might have already guessed the continuity of the wave function we need the continuity of wave function because the wave function corresponds to a physical system.

And if the wave function is discontinuous at any point then its derivative will be infinite at that point and as you can see the derivative corresponds to the physical operators. So, those operators will be infinite which could be a nonphysical situation ok. So, the wave function should be continuous and in by same logic the first order derivatives of the wave

function should also be continuous because if there is a discontinuity in the first order derivative it will mean that the second order derivative will be infinite at those points.

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Which basically will say that that the kinetic energy of the system which is given by this operator will be will blow up and that is an unphysical situation there is a small caveat here if the if at any point.

So, for example, if you are considering a delta function as the potential energy of the system if the potential energy of the system is given by the delta function in that case there is at x equal to 0 the potential energy will be a delta function, if we plot potential energy versus x it will be a delta function and in that case the wave function will have a discontinuity at this point and its second order derivatives will not be properly defined.

But this is a special situation and these situations we can easily understand if we understand the Schrodinger equation and all other conditions that the wave function need to satisfy, but in generally when the energy is properly defined, when the electronic energy or any energy of the quantum mechanical particle is properly defined in those cases the wave function and its first order derivatives should be continuous ok.

So, these are few basic postulates I would say that any quantum system need to satisfy and once we have these things properly defined for a system we can study that system in a proper way. So, now, with this basic knowledge of quantum mechanics we are now ready

to understand the nature of electrons. So, please keep this thing in mind our ultimate aim is to understand the nature of electrons in solid.

And as we know the solids are extremely complex objects. So, first we will start with the free electron, first we will take a very simple system in which electron is free it is not basically bound by any system.

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And we will see how the electron behaves when it is entirely free, free means in a way that the electron is alone in the entire universe. It is again highly unphysical situation it does not happen, but this is a good starting point you know to understand the quantum mechanical nature of electron.

So, if the electron is completely free what it means is that there is no interaction that the electron is undergoing. So, there is no interaction which basically means that the potential energy of the electron will be 0 and in this condition we can write down the Schrodinger equation by taking with potential energy to be 0.

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There is another important thing about the Schrodinger equation and that is if you recall the Schrodinger equation reads as minus h bar square divided by 2 m del 2 plus U psi equals i h bar del by del t psi.

So, this is the time dependent Schrodinger equation, but if the total energy of the system is fixed if the total energy of the system under consideration is fixed it is not changing with time in that case this equation in this equation the time dependent part and the time independent part the spatial part and the time part of the wave function they can be separated, and the time dependent part does not change it is properly defined.

So, what we basically mean by solving a Schrodinger equation in this case that we can solve just the time independent Schrodinger equation which basically looks like this equals E psi where E is the total energy of the electron.

So, in case so, in this case in the case of free electron the total energy of the electron is fixed. In fact, the potential energy is also 0. So, in this case by solving the Schrodinger equation we can or by solving the time independent Schrodinger equation we can completely characterize the electronic wave function.

We can completely deduce the electronic wave function and this transformation from time dependent Schrodinger equation to time independent Schrodinger equation is a simple derivation I would recommend all of you to go back and please do this after the class.

So, in this case the Schrodinger equation will read as minus h square by 2 m h bar square by 2 m del 2 psi x, y, z plus U psi x, y, z equals E psi x, y, z. For a free electron as we saw that it is free from any interaction the potential energy is 0. So, in this case this equation basically boils down to h square by 2 m del 2 psi x, y, z with the minus equals E times psi x, y, z... $\left[\left(\frac{-\hbar^2\nabla^2}{2m}\right)\Psi(x,y,z) = \hat{E}\Psi(x,y,z)\right]$

And if we for simplicity if we consider only one dimensional case in that case this equation further simplifies to h bar square by 2 m del 2 psi x plus E psi x equals to 0 or del 2 psi by del x square plus k square psi equals to 0, but psi is now just the function of x and k is now 2 m E divided by h bar square square root ok. So, now, the Schrodinger equation boils down to a second order differential equation a simple second order differential equation, whose solution we can easily do from a basic calculus course.

So, the solution of this equation would be as you might have already guessed the solution of this second order differential equation are either there are multiple ways of writing the solution of this equation we can write the write down the solution of this equation in the form of exponentials we can also write down the solution of this equation in form of sines and cosines we can also write them down in form of hyperbolic functions.

So, for simplicity we will write the solutions in the form of sines and cosines. So, as you can check sorry this should be k x here as you can check psi x equals A sin k x plus B cos k x is a valid solution of this equation the Schrodinger equation of the free electron. $\Psi(x) = Asin(kx) + Bcos(kx)$

Now where k is square root of 2 m E divided by h bar square. $k = \sqrt{\frac{2mE}{\hbar^2}}$ So, as you can see we have obtained the wave function of the free electron and the wave function is represented in terms of a new parameter the parameter k which is basically which comes with sines and cosines which comes as a parameter of sines and cosines. So, that is why this parameter is known as the wave number corresponding to the electronic wave function ok.

And here apart from this we do not have any other condition because this function is continuous its derivative is continuous it can be normalized if we want. So, it satisfies all

valid conditions that a wave function needs to satisfy and so, that is why we have completely characterized a free electron.

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So, as we can see if we represent energy as a function of the wave number this is how it would look like and generally it is an in quantum mechanical systems specially in solid states it is it simplifies our understanding of things if we plot the relationship between the energy of the system and the wave number of the wave function of the system wave number of the wave function of the system. So, basically the E k relationship and in this case this is a straight forward parabolic relationship. $E = \frac{\hbar^2 k^2}{2m}$

So, as you can see the relationship between E and k is a parabolic relationship and there are no other restrictions electronic energy can take any value k can take any value, but this will not hold true as you will see in coming classes as we will see, as we will derive in the next lecture this simplified or this elegant relationship between E and k will no longer hold true if we go beyond a free electron system ok.

So, in the coming class we will see how the electron behaves when it is confined in a certain space when it is for example, confined by a potential. So, we will study electron in a potential well and then we will see how the electron behaves in a natural solid ok. So, see you in the next class.