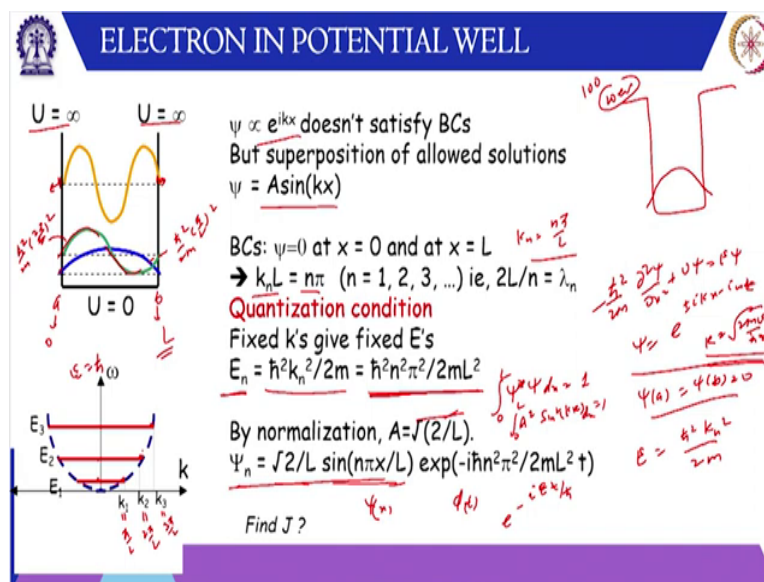


Semiconductor Device Modelling and Simulation
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Lecture – 56
Quantum Correction Models

Hello, welcome to lecture number 56. So, in last lecture we have discussed about the solution to Schrodinger equation. When we solve the Schrodinger equation, we get to know about the quantization effect and the nature of the wave function. So, this electron density corresponding to the wave function, tend to localize in the lowest potential region. Now, we will discuss the quantum well and the corresponding quantum correction models used in Nano MOSFET devices.

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Now, let us revisit this quantum well, so, this is a quantum well with the potential energy infinite outside this well. Now, this is different from the case we consider in the simulation we solved for finite potential this was 10 electron volt here and then we got this waveform like this. We can simulate this also by making it a large value. We cannot write infinite but we can write, it may be, let us say we can write 100 electron volts and so on.

This is as good as you know very large value here. For infinite quantum well of course, this waveform will not go outside. It will be exactly 0 outside because this potential is infinite. So, the difference is $e - U$ is also infinite, so, it will decay with infinite rate, so, e to the

power $-\alpha x$. So, it will go to exactly 0 here. So, this will be exactly 0 at these two boundary conditions.

So, if you solve this Schrodinger equation $\hbar^2 \frac{d^2 \psi}{dx^2} + U \psi = E \psi$. So, U is 0 here so, inside this region your let us say this is a this is b so, between a and b your ψ is $e^{\pm i k x} - i \omega t$ where k is $\sqrt{2mE}$ by \hbar square. Outside this is infinite, so, $e^{-\alpha x}$, so that will anyway 0, so, at ψ at $a = \psi$ at $b = 0$. So, these are the two boundary conditions and this is the expression.

Now, single wave function, $e^{i k x}$ cannot satisfy this boundary condition. So, what we will do a superposition of these waveforms, so, let us say we each one can be called some because this case $\sqrt{2mE}$ by \hbar square $E - U$ is 0 here, so, it will be $\sqrt{2mE}$ by \hbar square. Now, this is in terms of energy then for ψ we can write the summation of these different waveforms $\sum e^{i k x}$.

So, one such solution can be some $\sin kx$. So and this form we can understand that at two point statute 0. You can write cosine kx also with some phase, so that will be same as $\sin kx$. Now, at let us say this a is 0 and b is let us say L . If you use a and b then this expression for k value is slightly complicated because now $\sin ax$ has to be 0 $\sin kx$ has to be 0 $\sin kL$ has to be 0 and so on.

But if you use 0 and L then this \sin is always 0 $\sin 0$ is always 0, so, here \sin is always 0. So, only condition that is remaining is $\sin kL$ has to be 0 so, for kL to be 0 that means $\sin kL$ to be 0 means k also be multiple of π $n \pi$ because $\sin n \pi = 0$. So, this tells you that k is $n \pi$ by L . So, you can say $kn = n \pi$ by L . So, this is same as $\sqrt{2mE}$ by \hbar square. Now, you notice here because of this boundary condition in this case quantized.

So, for $n = 1$ $k = \pi$ by L and that will be waveform like this for $n = 2$ k is 2π by L . So, this will be the corresponding waveform and so on. And if you substitute it here, you will get the expression for energy $E = \hbar^2 k^2$ by $2m$. So, this will be the energy. So, this has energy $\hbar^2 k^2$ by $2m$ times k^2 and k is π by L square. This will be \hbar^2 by $2m$ times 2π by L square, visible energy for the second waveform and so on.

So, this is basically the quantization condition, so that means it only allows energies E_1 , E_2 , E_3 not all the energies are allowed. So, for n th state you can say $E_n = \hbar^2 k_n^2 / 2m$ so, k_n is $n\pi / L$. So, you can write $\hbar^2 n^2 \pi^2 / 2mL^2$. This is energy. Then of course you can normalize. Normalize means $\int_0^L \psi^* \psi dx = 1$.

So that condition, if you do a square \sin^2 so because \sin is complex conjugate will also be \sin , so, this will be $\int_0^L \sin^2 kx dx = 1$. So, this gives you basically $\sin^2 kx$ integral over dx is $L/2$ so, this will be $\sin^2 kx = 1$. So that if you solve it, you get k is equal to $n\pi / L$. Then so, ψ_n can be written as $\sqrt{2/L} \sin n\pi x / L$ so, $n\pi / L$ is k basically.

And this is $\psi(x)$ and this is $e^{-i\omega t}$, so, this is $e^{-iEt/\hbar}$ either this E can be substitute from here $\hbar^2 n^2 \pi^2 / 2mL^2$. So, this is now \hbar will cancel. So, you have $\hbar^2 n^2 \pi^2 / 2mL^2 \times t$. So, this is the overall wave function for this quantum wave. Now, let us look the same thing in the $E-k$ diagram, so, E is $\hbar^2 k^2 / 2m$ versus k .

Now, you notice here this is the $E-k$ diagram the parabolic curve for the free electron. But here all the values are not required but whatever values we have, they are parabolically related. So, let us say even you consider even k is π / L so, this k_1 is π / L , k_2 is $2\pi / L$, this is $3\pi / L$. Then corresponding energy is $\hbar^2 k^2 / 2m$ and so on.

Because it is a single well the mass is basically same mass has not changed. And these are the discrete points. So, if you look at the $E-k$ diagram you will see something like this one point you will see here, one point you will see here, one point you will see here. So, this will not be continuous curve but rather set of points in $E-k$ diagram. So, this discrete point tell you the energies that are available and the corresponding wave vectors.

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ELECTRON IN POTENTIAL WELL

Since Kinetic energy $\sim \frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2}$ Lowest energy wavefunction must have smallest curvature, vanish at ends and be normalized to unity

Ground State $\psi_1(x) \rightarrow$ Smoothest curve with no kinks
 $\psi_2(x)$ orthogonal to the first mode
 \rightarrow Hence the single kink!

If we decrease box size (area under modes is same)
 \rightarrow each mode peak more
 \rightarrow increased curvature, energy levels and their separation
 (Recall, $\Delta k_n = \pi/L$, $\Delta E_n \propto 1/L^2$)
 (Uncertainty: Localizing particle increases its energy!)

$$-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} + U\psi = E\psi$$

$$\frac{d^2\psi}{dx^2} + k^2\psi = 0 \quad \text{for } U=0$$

$$\psi = A \sin kx$$

$$k = \frac{n\pi}{L}$$

$$E_n = \frac{\hbar^2 k^2}{2m} = \frac{n^2 \pi^2 \hbar^2}{2m L^2}$$

Now, you can notice about the physical nature of these wave functions. So, if you look here, let us say this is the $n = 1$. Now, the wave function, if you see here size of wave function, there are two terms $\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2}$ which is kinetic energy. Then $U\psi$ is the potential energy. Now, potential energy U is 0, so, this is anyway 0. Kinetic energy if you see it is related to the derivative of ψ square.

So, derivative of ψ square means if ψ is varying slowly then the derivative is small double derivative is the curvature. So, if ψ is varying slowly is curvature will be small and therefore, its kinetic energy will also be small. So, if you see $n = 1$ it is a smallest possible curvature in this region within this length 0 to L . Therefore, it is the lowest energy state and it has minimum energy because the curvature is smallest.

Similarly, for $n = 2$ now, the curvature is actually more see what was changing from 0 to L ? Now, same changes available from 0 to half L . So now, curvature is more therefore, its kinetic energy is even more. And you can calculate it basically that $\frac{d^2\psi}{dx^2}$, if you write $\sin A \sin kx$. So, if you take $\frac{d^2}{dx^2}$, you will get $A \times k^2 \sin \cos$, $\cos \sin$ so, it will come $\sin kx$.

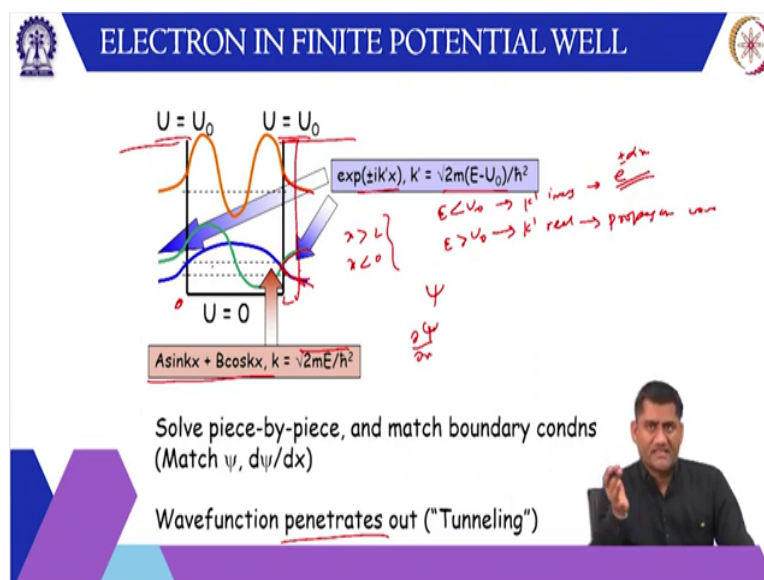
So, this is proportional to k^2 also and that you can see physically also. So that means the lowest energy function wave function should have the smallest curvature because there is a lowest energy and of course, due to the boundary condition it vanishes at ends. And of course, due to normalization condition is normalized to unity. So, ground state function ψ_1 is a smoothest curve with no kinks.

Psi 2 and another thing you can notice here these functions psi 1, psi 2 they are not plane waves. But they are orthogonal to each other basically, so, these are all orthogonal modes basically. So, psi 1, psi 2 are orthogonal to each other and the psi 2 will have single kink and so on. If you go further, number of kinks will increase another thing you can notice let us say you consider 2 box.

So, let us say this is 0 to L and this is 0 + L by 2 so, for the first order mode here which will have more curvature. Of course, this will have more curvature because now length is small. So that means it will have more energy so that means when you decrease the size of the box. So, the energy state will be broadly spaced now. So that means because of the same area under mode, each mode will peak more. So, this peak will be more here.

So, this is, let us say this a is root 2 by n this is a root 2 by half L. So, this will be the peak will be more basically so that there is a broader curvature more curvature is there. So that means their energy levels are have a wider separation. This also tells you that localization because there is a more less uncertainty here about the position because we are more certain about the position. So, it is energy has to increase. So, you can visualize these uncertainty principles using this quantum well example.

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Now, if you consider a finite quantum well, so, let us say this after this 0 to L the potential energy is not infinite but some constant value U naught. So then of course, in this region let us say 0 to L you can write $A \sin kx + B \cos kx$ where k is root $2mE$ by \hbar bar square. But

outside this so, x more than L and x less than 0 you will have e to the power $\pm \text{iota } k \text{ prime } x$. Now, $k \text{ prime}$ is $\sqrt{2mE - U}$.

So, if E is less than U naught, if E is more than U naught, if E is more than U naught then $k \text{ prime}$ is real that means is a kind of propagating wave. So that means it exists in both the regions basically. If E is less than U naught then $k \text{ prime}$ is imaginary, so, this term becomes e to the power $\text{iota } k$ will become α so, e to the power αx . So, this will every exponentially decaying term.

So, you see for these modes which are confined this is exponentially decaying outside. So, what you can do? You can solve it analytically solve the Maxwell equation in these two regions 0 to L and outside one and then match the boundary condition. At the boundary condition ψ and ψ derivative $d\psi$ by dx has to be continuous. So, this is basically kind of phenomena called a penetration of this waveform.

And if this barrier is thin enough then some probability basically comes out of this barrier and that phenomena is called tunneling. So, these two are very important phenomena in quantum transport. We will discuss them in next lecture.

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MOS GATE CAPACITANCE

$$C_{tot} = \frac{C_{ox}}{1 + \frac{C_{ox}}{C_{poly}} + \frac{C_{ox}}{C_{inv} + C_{dep}}}$$

(1) Long channel devices, t_{ox} large
 • C_{ox} small, $C_{ox}/C_{poly} \rightarrow 0$, $C_{tot} = C_{ox}$
 (2) Nano-scale devices, t_{ox} small
 • C_{ox} large, C_{ox}/C_{poly} finite, $C_{tot} < C_{ox}$
 • C_{inv} is always large because the thickness of the inversion layer is small

Handwritten notes:

$$\frac{1}{C_{tot}} = \frac{1}{C_{poly}} + \frac{1}{C_{ox}} + \frac{1}{C_{inv} + C_{dep}}$$

$$C_{tot} = \frac{C_{ox}}{1 + \frac{C_{ox}}{C_{poly}} + \frac{C_{ox}}{C_{inv} + C_{dep}}}$$

SEMICONDUCTOR DEVICE MODELING AND SIMULATION

Now, let us apply this finite size quantization effect to normal MOS capacitor. So, if you consider a typical polysilicon create MOSFET so, this is a structure. So, this is your polysilicon then this is your oxide and this is your semiconductor. When you apply a voltage

here then there is some depletion region is created here, the universal charge is created. So, this is the oxide thickness t_{ox} . This is a poly thickness and then this is the inversion region.

So, inversion region will also have some thickness of inversion region. Then overall capacitance if you look at the capacitance of this MOS gate due to applied wise, this poly may get depleted. So, there may be a poly related capacitance then oxide capacitance is simple ϵ_{oxide} by t_{oxide} so, this is the oxide capacitance. Inside the semiconductor there is a depletion region as well as the inversion region.

So, both these capacitance come in parallel so, $C_{inversion}$ and $C_{depression}$. Now, inversion layer has some finite thickness but that thickness is very small. So, you can say that $C_{inversion}$ is actually quite large is large, very large. So, if you calculate the overall capacitance, so, this will let us say C_{total} $\frac{1}{C_{total}}$ will be $\frac{1}{C_{poly}}$ therein series + $\frac{1}{C_{ox}}$ + $\frac{1}{C_{inversion}}$ + $C_{depletion}$ because they are in parallel, so, they add up.

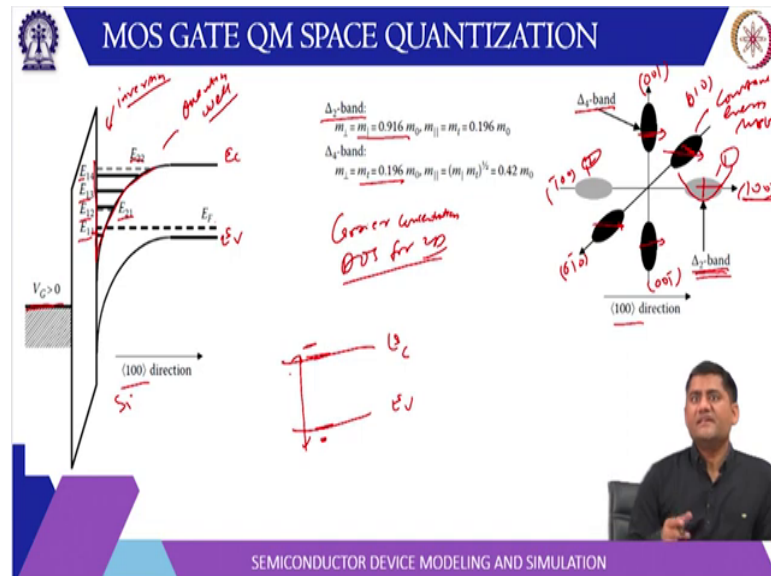
So, if you express in terms of C_{oxide} , so, you can write $C_{total} = C_{oxide}$ can be taken out. So, you can write C_{oxide} then you multiply this thing by C_{oxide} , so, this becomes $1 + C_{oxide} \text{ by } C_{poly} + C_{oxide} \text{ by } C_{inversion} + C_{depletion}$. Then in case of metal gate poly term will disappear so, this will disappear. So, it will not $C_{oxide} \text{ by } 1 + C_{oxide} \text{ by } C_{inversion} + C_{depletion}$. Now, generally inversion capacitance is quite large.

So, you can ignore the depletion capacitance, so, you can just write $C_{oxide} \text{ by } C_{inversion}$. Now, for long channel devices t_{ox} is fairly thick. So, C_{oxide} is small and $C_{inverse}$ in largely quite large, so, this term goes to 0. So, your C_{total} is basically C_{oxide} so, for both the case accumulation, as well as the inversion region. For nano-scale device, your t_{ox} is quite a small basically.

So, typically when it is order of 10 nanometre or small. This is comparable to the $C_{inversion}$ because your inversion thickness is also order of few nanometre. So, this $C_{ox} \text{ by } C_{inversion}$ is not 0 now, it is finite. So that means your C_{total} will be C_{ox} divided by $1 + \text{some finite number}$. So, this will be less than C_{oxide} , so that means C_{total} becomes less than the C_{oxide} that happens in case of nano-scale devices.

So now, reduction in the C_{total} so, this C_{total} reduction in C_{total} decreases the drive capability of this MOSFET because now less charge will be accumulated there under the immersion region and less current will flow basically.

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Another thing you can see here because of this there is a there is some band bending here. So, if you see this is a gate structure here and this is the conduction band you see, this is a balance band E_v . This is a Fermi level. So, when we apply a positive gate bias, so, these bands will bend accordingly and this is the reason where inversion layer is created. Now, let us consider, unless we are considering silicon in 100 direction which is perpendicular to this plane.

Now, you see this potential profile does it resemble some kind of well, quantum well that means energy is really quantized here. That means not all the energies are allowed that we have already seen through the example of quantum well. Now, it will have only the allowed energies, some quantized energies and that will depend on the mass of the electron. Now, we can also recall our knowledge of the band structure.

In case of silicon the band structure is basically there are six phases of the cube basically, so, these are the 100 and equivalent directions. So, along which at I think 3 by 4th length these are the constant energy surfaces. So, let's you consider this 100 direction. So, if you consider band this band 1 and this band 2 their mass will be the longitudinal mass. So, longitudinal C if you see here this is the longitudinal mass this will be the transverse mass.

So, longitudinal mass will be this is more broad so, this mass will also be more. So, this is m a longitudinal mass. So, these are $\Delta 2$ bands is written here these are the $\Delta 2$ bands. So, this is in 100 direction, others which are in 010 or 001 direction. So, let us say this is 100 this will be, let us say, 010 and this will be 001 and the opposite will be 001 bar. This will be bar 100 and so on 01 bar 0 and so on.

So, these four if you see in x direction, their corresponding mass will be the transverse mass. So, the transverse mass is small $0.196 m$ naught. So, there are 2 $\Delta 2$ bands there are 4 $\Delta 4$ bands. So, corresponding quantized energy will also be small. Now, if you see corresponding to which band the smallest quantization energy will exist. The electron with higher mass will have a small energy.

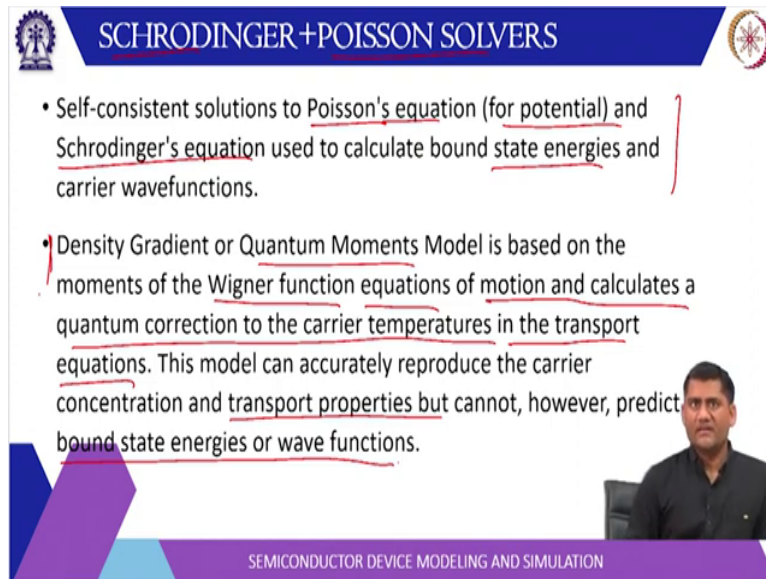
So, if you consider this $\Delta 2$ band its mass is more. So, the smallest energy will correspond to the $\Delta 2$ band. So, $\Delta 2$ it has how many such bands are there? There are two such bands. So, this will be basically two such energy levels will exist at the same position because they will concert basically. So, this is let us equal E_{11} then E_{12} , E_{13} , E_{14} . These are quantized then corresponding to $\Delta 4$ point there will be E_{21} E_{22} and they will get a high energy levels.

So, these are the quantized energy levels that exist inside this potential well. So now, if you see, if you calculate the carrier concentration so that carrier concentration has to be calculated with respect to the DOS for 2D system because there is a seat of current density here. And with this Fermi level, you have to calculate the carrier concentration here, so, the expression for carrier concentration will change expression for energy is now different.

And if you notice here if both the electron and holes they are inside some kind of quantum well. Then the band gap they see will also be more now because this is a conduction band is a balance band. So now, the lowest energy is not at the band x but somewhere here, lowest energy is not easier somewhere here. So now, effective band gap is actually more, so, the electron concentration is actually slightly less.

So, this is the MOS gate that quantum mechanical space quantization effect is there and that is how this is basically analyzed.

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SCHRODINGER+POISSON SOLVERS

- Self-consistent solutions to Poisson's equation (for potential) and Schrodinger's equation used to calculate bound state energies and carrier wavefunctions.
- Density Gradient or Quantum Moments Model is based on the moments of the Wigner function equations of motion and calculates a quantum correction to the carrier temperatures in the transport equations. This model can accurately reproduce the carrier concentration and transport properties but cannot, however, predict bound state energies or wave functions.

SEMICONDUCTOR DEVICE MODELING AND SIMULATION


Now, how do we solve this scenario? We have to solve both the Schrodinger equation and the Poisson equation simultaneously or self consistently. So, the self consistent solution to the Poisson equation from which we obtain the potential profile. And the Schrodinger equation from where we get the carrier wave functions and the bound state energies they have to be solve self consistently.

Now, this is basically just to find out what are the potential profiles? And what are the wave functions? We can use this equation solve these equations self consistently. Another method is basically people use, they use density gradient or quantum moment model which is based on the moment of Wigner function equation of motion and calculate a quantum correction to the carrier temperature in the transport equation.


So, these equations, we have discussed the transport equations there are the carrier temperature, there is a lattice temperature. So, they are also corrected based on this quantization condition. So, this can produce the carrier concentration and the transport properties. But the boundary state energy or the wave functions are not so, accurate in this method density gradient method.

So, there are multiple models are there in especially in the commercial tools. There are multiple models are there. So, when we discuss the commercial tool, we will consider one or two model and how to invoke? And how to get these profiles we will discuss?

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SCHRODINGER+POISSON SOLVERS



- Hamiltonian for an electron residing in one of the valleys is

$$H_e(\mathbf{R}) = -\left(\frac{\hbar^2}{2m_x^*} \frac{\partial^2}{\partial x^2} + \frac{\hbar^2}{2m_y^*} \frac{\partial^2}{\partial y^2} + \frac{\hbar^2}{2m_z^*} \frac{\partial^2}{\partial z^2} \right) + V_{eff}(z) = H_{eff}(r) + H_{tr}(z)$$
 where $\mathbf{R} = (r, z)$
 $V_{eff}(z)$ is the effective potential energy profile of the confining potential
 H_{eff} is the parallel part of H_e
- The transverse part is defined as

$$H_{tr}(z) = -\frac{\hbar^2}{2m_z^*} \frac{\partial^2}{\partial z^2} + V_{eff}(z)$$
- Where, $V_{eff}(z) = V_H(z) + V_{xc}(z)$
- Hartree term obtained from the solution of the 1D Poisson equation
- exchange–correlation correction to the ground state energy of the system

$\hat{H}\psi = E\psi$

DFT

SEMICONDUCTOR DEVICE MODELING AND SIMULATION

Now, just to give us some information about the Schrodinger Poisson solver. So, if you consider the Hamiltonian because we know that $H\psi = E\psi$ is the Schrodinger equation. So, the Hamiltonian evenly $H = \frac{\hbar^2}{2m} \nabla^2 + V$, so that is in 1 dimension. But in 3 dimension $\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$ and corresponding mass m_x, m_y, m_z , \hbar^2 included then plus effective potential.

Now, we can divide this Hamiltonian into a parallel part and the perpendicular part. So, quantization effect is only in the parallel perpendicular part which is perpendicular to the 100 direction. So that is of interest and this parallel part, will give you regular values of k_x and k_y . So, ∇^2 parallel to part of the H and V_{eff} is the effective potential energy profile of the confining potential. So, this is basically your V_{eff} .

Now, it basically contains two things basically, one is what term which is obtained from the solution of Poisson equation? Now, this also called Hartree term and the method that is used is called density function theory. That is another course basically, if you want to learn about DFT that we will not go into it. So, this potential is obtained from the density function theory and there is another term called exchange correlation correction.

So, this is basically some kind of correction term which include the electron interaction and so on. So, this is the total potential and these are solved using the density function theory or some approximation is made to this exchange correlation function. What is done basically? Some ground state energy is considered and correction term is applied to that energy. And it is basically substitute back to the Hamiltonian and then Schrodinger equation is solved.

So, this is the process for the solving the Schrodinger and Poisson equation. This is just a basically preview that I have given but there are more details about how to do DFT calculations?

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The slide is titled "QUANTUM CORRECTIONS" and features a blue header with logos on either side. The main content consists of four bullet points, each with handwritten red annotations. The first bullet point is "Quantum correction to Semiclassical transport models", with a red checkmark to its left. The second bullet point is "Analytical and macroscopic (i.e. classical transport framework by adding correction terms to account for the quantum-mechanical effects) models", with a red checkmark to its left. The third bullet point is "problems associated with these approaches are directly related to the nonstationary nature of the carrier transport (velocity overshoot) in deep submicron devices", with a red checkmark to its left. The fourth bullet point is "MOSFETs scaling requires thinner gate oxides and higher doping levels to achieve high drive currents and minimized short channel effects", with a red checkmark to its left. The fifth bullet point is "For oxide thickness 10 nm and below, the total gate capacitance is smaller than the oxide capacitance due to the comparable values of the oxide and the inversion layer capacitance (due to the finite average displacement of the inversion charge from the semiconductor interface)", with a red checkmark to its left. Below the text, there are two hand-drawn diagrams in red ink. The first diagram shows a potential well with a red curve representing the wave function. The second diagram shows a potential well with a red curve representing the wave function. A small inset image of a person is visible in the bottom right corner of the slide.

- Quantum correction to Semiclassical transport models
- Analytical and macroscopic (i.e. classical transport framework by adding correction terms to account for the quantum-mechanical effects) models
- problems associated with these approaches are directly related to the nonstationary nature of the carrier transport (velocity overshoot) in deep submicron devices
- MOSFETs scaling requires thinner gate oxides and higher doping levels to achieve high drive currents and minimized short channel effects
- For oxide thickness 10 nm and below, the total gate capacitance is smaller than the oxide capacitance due to the comparable values of the oxide and the inversion layer capacitance (due to the finite average displacement of the inversion charge from the semiconductor interface)

SEMICONDUCTOR DEVICE MODELING AND SIMULATION

Now, in the quantum corrections the analytical and the microscopic models they basically what they do? In the classical transport equation, they add a correction term to account for this quantum mechanical effects. Now because we assumed that the potential V is not changing with time that gave rise to stationary states, stationary solutions. So that may give some kind of nonstationary nature to the carrier transport.

So, the kind of velocity overshoot or so, in deep submicron devices. So, this correction have to be applied in case of MOSFET when they are scaled to a thinner gate oxide or higher doping levels to achieve high drive current or minimized the short channel effect. So, this we have already discussed in case of class on MOSFET and so on. Now, the criteria for quantum correction is that when oxide thickness is below 10 nanometre.

Then the gate capacitance is smaller than the oxide capacitance, as already discussed. Then the inversion layer capacitance due to the finite average displacement of the inversion charge from the semiconductor oxide interface. Because you see here this is the potential profile. And then if you recollect that for a tilted quantum well, the wave function was something like this.

So, it was not exactly here but slightly away here. So, same thing will appear here. So, this peak will appear somewhere here. It will not exactly at the edge of this region, so, this is oxide, this is silicon, so, it will slightly away. The peak will be slightly away from the interface, so, this inversion thickness inversion layer will have certain thickness. And that will give you inversion capacitance that will be finite.

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QUANTUM CORRECTIONS

- Quantum correction models incorporate quantum-mechanical description of carrier behavior via modification of certain device parameters within the standard drift-diffusion or hydrodynamic model
- Hansch model modifies the effective DOS function $N_c^* = N_c [1 - \exp(-z/\Lambda_{BDA})]^2$ *Protona*
- Van Dort model modifies the intrinsic carrier concentration by taking into account the effective bandgap increase due to quantum-mechanical size quantization effects

$\psi_c^{QM} = \psi_c^{CONV} + \Delta E_c/q + E_g \Delta z$, $\Delta z = (z^{QM}) - (z^{CONV})$

Classical density
Quantum-mechanical density
bandgap widening effect due to upward shift of the lowest state
displacement of the carriers from the interface and the extra bend bending

N_c

SEMICONDUCTOR DEVICE MODELING AND SIMULATION

Now, one or two correction term that I will discuss here. One is the model by Hansch model which modifies the effective density of a state function. So, we have calculated that N_c is the density of state, so, this N_c is modified in terms of position z . So, z is this position from this, so, N_c is modified N_c^* is given as N_c times $1 - \exp(-z/\lambda^2)$ square.

So which λ is a parameter that can be set in the calculation, so, $z = 0$ you see it is going to 0 here. So, it is number of state is 0 here you see according to this model, number of state is 0 and then it basically increases. So, this is one model which modifies a density of state. Another model is called Van Dort model which modifies the intrinsic carrier concentration by taking into account the effective bandgap.

Because effective bandgap is now has increased because of this quantization. You see this is the conduction band this is the balance bandage. So now, bandgap is not exactly easy but the first energy is slightly above easy. So now, bandgap is slightly more basically, so that is take into account. So, this is basically ΔE is a bandgap binding effect due to upward step to the lowest state because lowest stage is not as easy is slightly away let us say E_1 .

So that has to be added then plus the displacement of the carriers from the interface. So because this is the wave function and it the peak appears slightly away from the interface. So, this is $E \times \Delta z$ another potential basically. So, this is the overall potential, so, the quantum mechanical potential is conventional potential plus potential due to the bandgap, binding plus potential due to the displacement of carriers.

So, you see here there is a classical density of a state. This is a quantum mechanical, so, quantum mechanical is slightly shifted. So, corresponding displacement for the peak is this is here, this is the for conventional, this is for quantum mechanical. So, this is basically bigger basically. So, these are the different quantum corrections model there are more number of models are there.

So, those who want to go deep into it they can refer the textbook computational electronics.

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CONCLUSION

- Discussed Quantum Mechanical Confinement and
- Quantum correction modelling approach

SEMICONDUCTOR DEVICE MODELING AND SIMULATION

So, with this we have discussed the quantum mechanical confinement and the corresponding quantum correction modelling approach. Thank you very much.