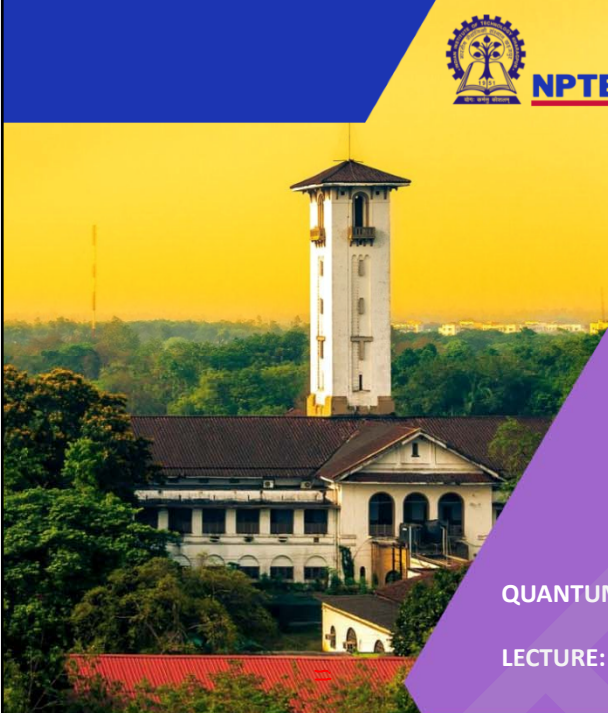




NPTEL ONLINE CERTIFICATION COURSE



SEMICONDUCTOR DEVICE MODELING AND SIMULATION

PROF. VIVEK DIXIT
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QUANTUM MECHANICS

LECTURE: 54



L54 QUANTUM MECHANICS



- *Review Quantum mechanics*

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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 $\rightarrow$ states that can be studied in a laboratory
- accessible information $\rightarrow$ information we can extract from the wave function ψ
- state function $\rightarrow$ 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 c_1 and c_2 are arbitrary complex constants,



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SECOND POSTULATE



- If a system is in a quantum state represented by a state 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).

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SECOND POSTULATE



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

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

- expectation value depends upon the state of the system and can be time-dependent, i.e., $\langle x \rangle = \langle x(t) \rangle$.
- 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 $\langle x \rangle$. Calculate the variance

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

- 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

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

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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.

- 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

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

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

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

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

- If two operators commute $\rightarrow$ simultaneously measurable the observables
- Noncommutivity of the position and the momentum operators is represented with the Heisenberg uncertainty principle,

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

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

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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

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

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SOLVING SCHRODINGER EQUATION



- Using variable separable technique

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

- 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 .

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

- Since V does not depend on time $\rightarrow$ stationary-state wave functions exist for systems with a time-independent potential energy

From the de Broglie-Einstein relation, one has that $E = \hbar\omega = \alpha$

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

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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. $\hat{H}\psi = E\psi$ - eigen equation $\psi(x) \rightarrow E$
- Even if the number of these eigenstates is infinite, the energies of the bound states form a discrete set. $\cancel{V(x)} \quad \left. \begin{matrix} E_1 \rightarrow \psi_1 \\ E_2 \rightarrow \psi_2 \end{matrix} \right\}$
- 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. ψ



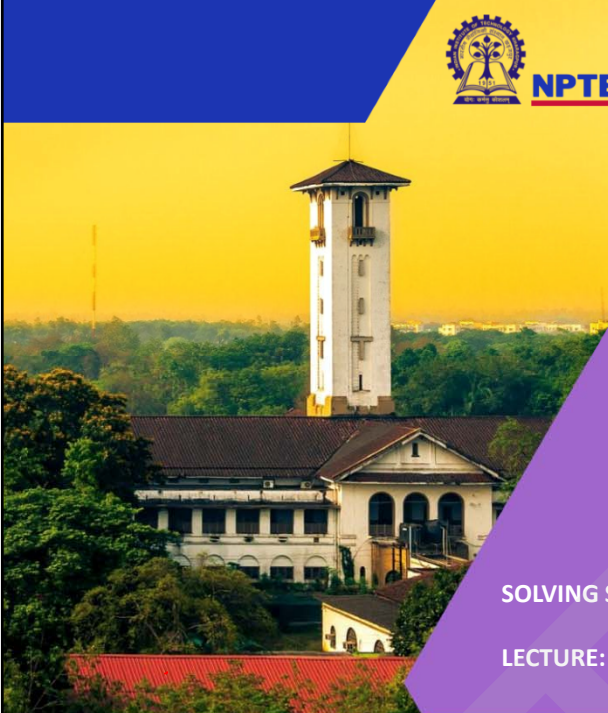
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Thank you



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SOLVING SCHRODINGER EQUATION

LECTURE: 55



L55 SCHRODINGER EQUATION



- Solving Schrodinger Equation
 - Analytically ✓
 - Numerically ✓

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SCHRODINGER EQUATION

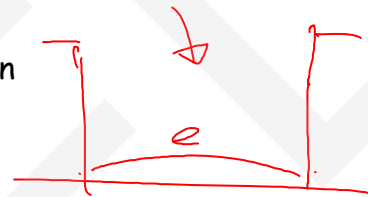


$$\underline{-\frac{\hbar}{i} \frac{\partial}{\partial t} \Psi(x,t) = -\frac{\hbar^2}{2m_0} \frac{\partial^2}{\partial x^2} \Psi(x,t) + U(x) \Psi(x,t)}$$

- this equation was discovered to explain how particles behave when they behave like waves.
- This equation can be solved by using "separation of variables" for static potentials

$$\Psi(x,t) = \underline{\psi(x)} \underline{\phi(t)} = \underline{\psi(x)} \underline{e^{-iEt/\hbar}}$$

$$\text{or } e^{-i\omega t}$$



Electrons can be described by waves,
quantization (boundary condition) and localization (wave packets)

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SCHRODINGER EQUATION



- $\Psi(x,t)$ and its space derivative are continuous, finite and single valued.
- The probability of finding an electron between x and $x+dx$, is:

$$P(x,t) dx = \underline{\Psi^*(x,t) \Psi(x,t)} dx$$

$$\bullet \underline{\int P(x,t) dx = 1}, \text{ Charge density } \rho(x,t) = \underline{qP(x,t)} \times N$$

$$\bullet \text{ Current density } J(x,t) = \underline{qvP(x,t)} \quad \text{or} \quad \underline{qnv}$$

- Average value of any variable Q is:
 - $\langle Q \rangle = \int \Psi^*(x,t) \underline{Q_{op}} \Psi(x,t) dx$
- Classical quantities (Energy and momentum) are related through operator ($\hat{E} = E_{op} = \underline{(-\hbar/j) \partial/\partial t}$ and $\underline{P_{op} = (\hbar/j) \partial/\partial x}$)

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FREE ELECTRON



$$-\frac{\hbar^2}{2m_0} \frac{d^2\psi(x)}{dx^2} + U(x)\psi(x) = E\psi(x)$$

$$\hat{H}\Psi = E\Psi, \hat{H} = -\hbar^2\nabla^2/2m + U$$

$$E = p^2/2m + U \text{ (energy of a particle)}$$

For free electron, $U=0$

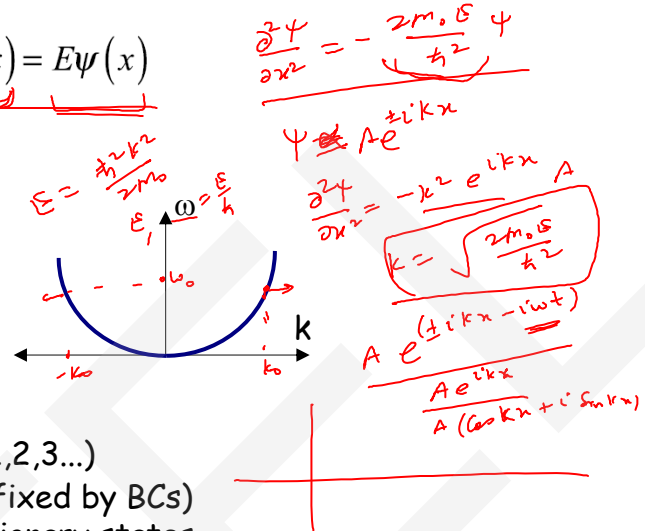
$$\text{Solution } \Psi = Ae^{(\pm ikx - i\omega t)} = Ae^{(\pm ipx - Et)/\hbar}$$

$$E = \hbar\omega = \hbar^2 k^2 / 2m = p^2 / 2m$$

$$\text{BCs: } \hat{H}\psi_n = E_n\psi_n \quad (n = 1, 2, 3, \dots)$$

E_n : eigenvalues (usually fixed by BCs)

$\psi_n(x)$: eigenvectors/stationary states



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FREE ELECTRON UNDER POTENTIAL, $U(x)$



$$\frac{\partial^2 \psi(x)}{\partial x^2} + \frac{2m_0}{\hbar^2} [E - U(x)] \psi(x) = 0$$

$$\text{Case I: } E > U(x), \psi(x) = Ae^{(\pm ikx - i\omega t)},$$

$$k = \sqrt{2m_0[E - U(x)]}/\hbar \Rightarrow E = U + \frac{\hbar^2 k^2}{2m_0}$$

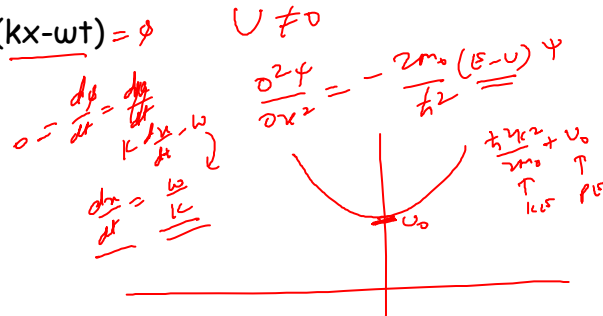
Travelling wave with Phase $= (kx - \omega t) = \phi$

Phase velocity, $v_p = \omega/k$

Wavelength, $\lambda = 2\pi/k$

$$E = U(x) + \hbar^2 k^2 / 2m_0$$

Momentum, $p = \hbar k$



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FREE ELECTRON UNDER POTENTIAL, $U(x)$

$$\frac{\partial^2 \psi(x)}{\partial x^2} + \frac{2m_0}{\hbar^2} [E - U(x)] \psi(x) = 0$$

Case II : $E < U(x)$, $\psi(x) = A e^{(\pm \alpha x - i\omega t)}$, $\alpha = \sqrt{2m_0[U(x) - E]}/\hbar$
 Exponential varying solution

$\Psi(x,t) = \sum_n a_n \psi_n(x) e^{-iE_n t/\hbar}$

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WAVE PACKETS

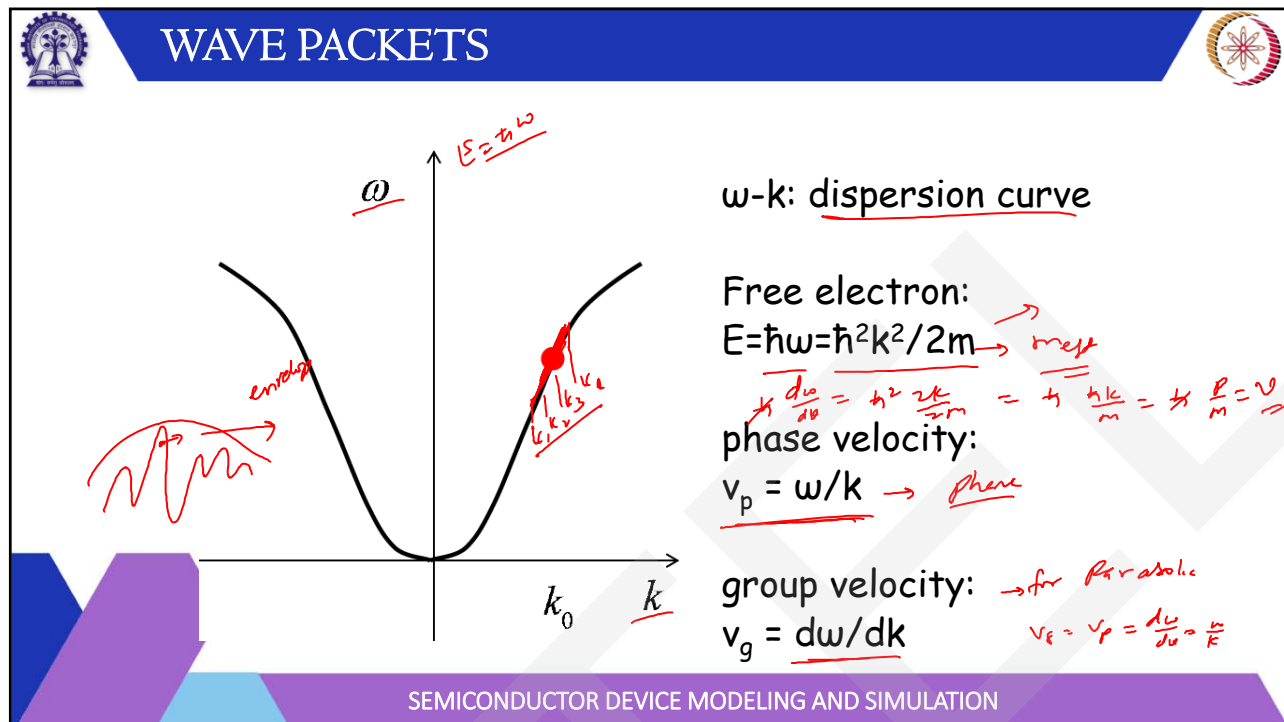
$$\Psi(x,t) = \sum_n a_n \psi_n(x) e^{-iE_n t/\hbar}$$

Particle: $x = x_0$
 Momentum: $p = \hbar k$
 $\Delta x \Delta k \geq 0.5$

Uncertainty relation
 localized in space is spread out in k-space.

sharply defined in time, is spread out in frequency

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NUMERICAL APPROACH



Approximation Techniques

- Graphical solutions (e.g. particle in a finite box)
- Special functions (harmonic oscillator, tilted well, H-atom)
- Perturbation theory (Taylor expansion about known solution)
- Variational Principle (assume functional form of solution and fix parameters to get minimum energy)

Numerical Techniques

- Finite difference
- Finite element

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FINITE DIFFERENCE METHOD

One particular mode

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

$$\psi = \begin{bmatrix} \vdots \\ \psi_{n-1} \\ \psi_n \\ \psi_{n+1} \\ \vdots \end{bmatrix}$$

$$U\psi = \begin{bmatrix} \vdots \\ U_{n-1}\psi_{n-1} \\ U_n\psi_n \\ U_{n+1}\psi_{n+1} \\ \vdots \end{bmatrix} = \begin{bmatrix} \ddots & & & \\ & U_{n-1} & & \\ & & U_n & \\ & & & U_{n+1} \\ & & & & \ddots \end{bmatrix} \begin{bmatrix} \vdots \\ \psi_{n-1} \\ \psi_n \\ \psi_{n+1} \\ \vdots \end{bmatrix}$$

$$= [U][\psi]$$

$$\hat{H} = \frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \psi + U\psi$$

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DISCRETIZING KINETIC ENERGY

$$\frac{\psi_{n+1} - 2\psi_n + \psi_{n-1}}{\Delta x^2} = \frac{d^2\psi}{dx^2} \bigg|_{x_n}$$

$$(d\psi/dx)_n = (\psi_{n+1/2} - \psi_{n-1/2})/a \rightarrow \Delta x$$

$$(d^2\psi/dx^2)_n = (\psi_{n+1} + \psi_{n-1} - 2\psi_n)/a^2$$

$$-\hbar^2/2m(d^2\psi/dx^2)_n = t(2\psi_n - \psi_{n+1} - \psi_{n-1})$$

$$t = \hbar^2/2ma^2$$

$$T\psi = \begin{bmatrix} \ddots & & & \\ & -t & 2t & -t \\ & & -t & 2t & -t \\ & & & -t & 2t & -t \\ & & & & \ddots \end{bmatrix} \begin{bmatrix} \vdots \\ \psi_{n-1} \\ \psi_n \\ \psi_{n+1} \\ \vdots \end{bmatrix}$$

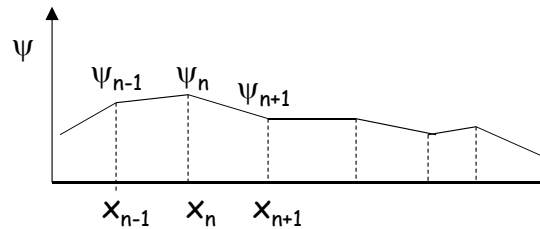
$$U\psi =$$

$$[H] = [T + U]$$

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CALCULATING EIGEN VALUES



Now that we've got H matrix, we can calculate its eigen values

$\downarrow \downarrow$
 $\gg [V,D]=\text{eig}(H);$ % Find eigenspectrum
 $\gg [D,\text{ind}]=\text{sort}(\text{real}(\text{diag}(D)));$ % Replace eigenvalues D by sorting, with index ind
 $\gg V=V(:,\text{ind});$ % Keep all rows (:) same, interchange columns acc. to sorting index

(n^{th} column of matrix V is the n^{th} eigenvector ψ_n plotted along the x axis)

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MATLAB CODE

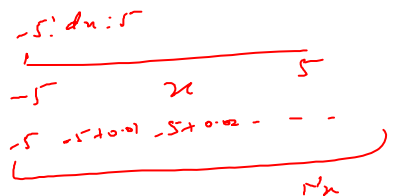
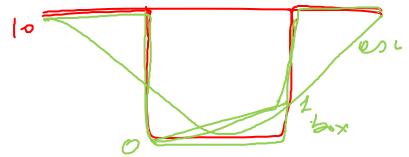


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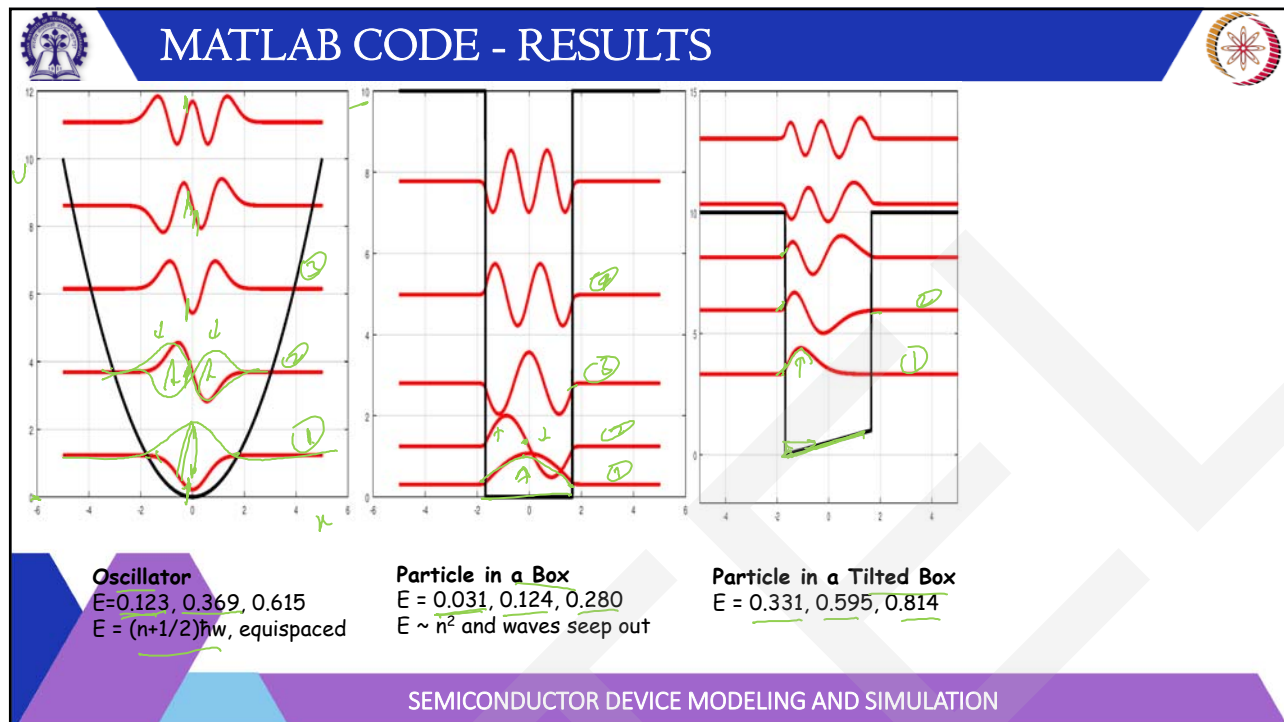
clear all; close all
m=9.1e-31;hbar=1.05e-34;q=1.6e-19;
%% x (nm), U (eV) %%%%%%%%%%%%%%
dx=0.01; x=-5:dx:5; Nx=max(size(x));
U=10*ones(1,Nx); temp=floor(Nx/3); 2*floor(Nx/3);
U=(1/2.5)*x.^2; %Oscillator
%U(temp)=0; % Particle in a box
%U(temp)=linspace(0,1,max(size(temp))); %Tilted box
t=(1e18/q)*(hbar^2)/(2*m*dx^2);
%% Write matrices
T=2*t*eye(Nx)-t*diag(ones(1,Nx-1),1)-t*diag(ones(1,Nx-1),-1); %Kinetic Energy
U=diag(U); %Potential Energy
H=T+U;
[V,D]=eig(H);
[D,ind]=sort(real(diag(D)));
V=V(:,ind);
% Plot
for k=1:5
plot(x,-10*V(:,k)+10*D(k),'r','linewidth',3)
hold on
end
plot(x,diag(U),'k','linewidth',3); % Zoom if needed
axis([-5 5 -2 15])
%% En=((pi*hbar/3.45e-9)^2)/(2*m*q)
  
```

Grid issues:

- For Small energies, finite diff. matches exact result
- Deviation at large energy, where y varies rapidly
- Grid needs to be fine enough to sample variations



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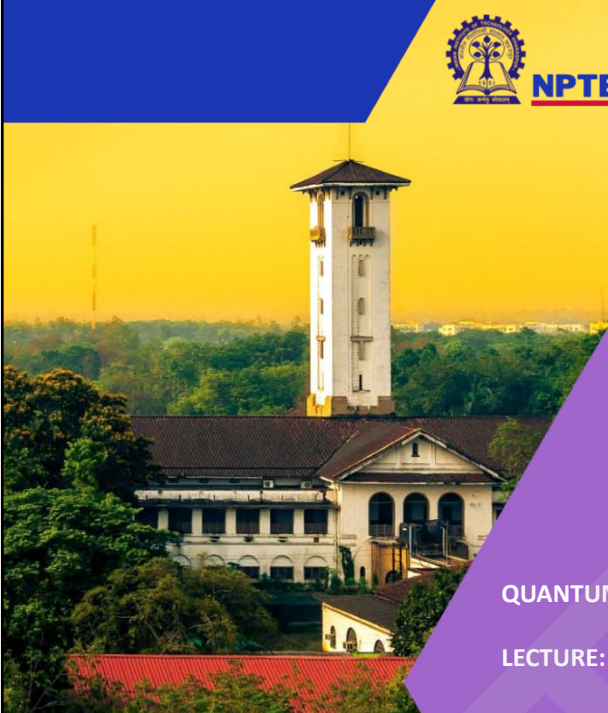


CONCLUSION

- Schrodinger Equation solved with boundary conditions provide wavefunction. Averages of observables can be computed by associating the electron with a probability wave whose amplitude satisfies the Schrodinger equation.
- Boundary conditions imposed on the waves create quantized modes at specific energies. Only a few problems can be solved analytically. Numerically, however, many problems can be handled relatively easily.

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QUANTUM CORRECTION MODEL

LECTURE: 56



L56 QUANTUM CORRECTIONS

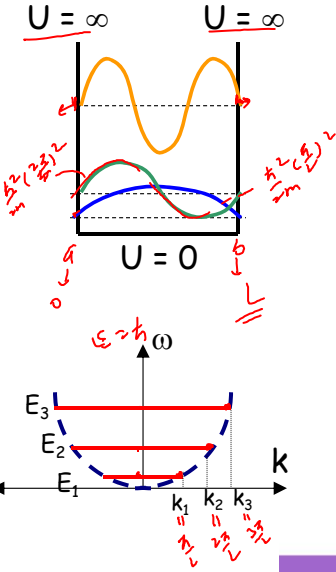


- *Quantum Well*
- *Quantum correction models*

SEMICONDUCTOR DEVICE MODELING AND SIMULATION

ELECTRON IN POTENTIAL WELL



$\psi \propto e^{ikx}$ doesn't satisfy BCs
 But superposition of allowed solutions
 $\psi = A \sin(kx)$

BCs: $\psi=0$ at $x=0$ and at $x=L$
 $\rightarrow k_n L = n\pi$ ($n=1, 2, 3, \dots$) ie, $2L/n = \lambda_n$

Quantization condition
 Fixed k 's give fixed E 's
 $E_n = \hbar^2 k_n^2 / 2m = \hbar^2 n^2 \pi^2 / 2m L^2$

By normalization, $A = \sqrt{2/L}$
 $\Psi_n = \sqrt{2/L} \sin(n\pi x/L) \exp(-i\hbar n^2 \pi^2 / 2m L^2 t)$

Find J ?

SEMICONDUCTOR DEVICE MODELING AND SIMULATION

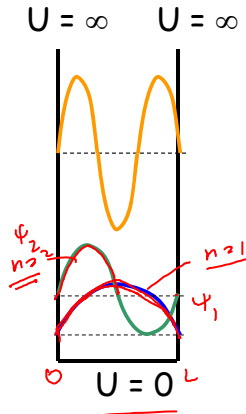
ELECTRON IN POTENTIAL WELL




Since Kinetic energy $\sim \partial^2 \psi / \partial x^2$. 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!

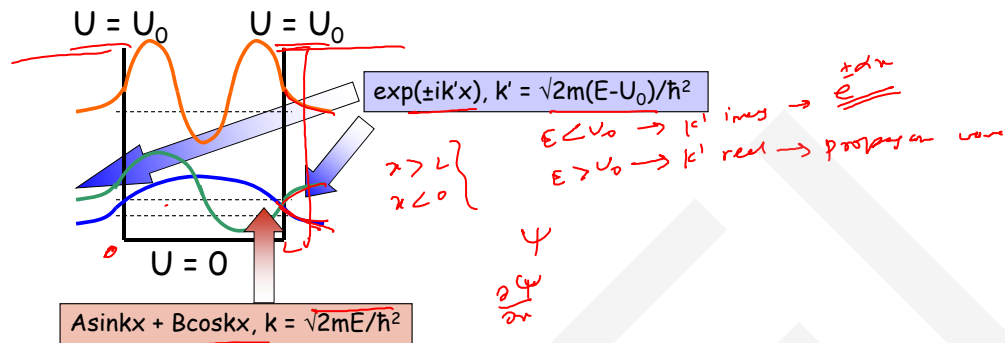
If we decrease box size (area under modes is same)
 $\rightarrow$ each mode peak more
 $\rightarrow$ increased curvature, energy levels and their separation
 (Recall, $\Delta k_n = \pi/L$, $\Delta E_n \propto 1/L^2$)
 (Uncertainty: Localizing particle increases its energy!)



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ELECTRON IN FINITE POTENTIAL WELL



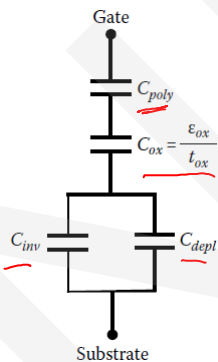
Solve piece-by-piece, and match boundary condns
(Match ψ , $d\psi/dx$)

Wavefunction penetrates out ("Tunneling")

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MOS GATE CAPACITANCE



$$C_{tot} = \frac{C_{ox}}{1 + \frac{C_{ox}}{C_{poly}} + \frac{C_{ox}}{C_{inv} + C_{depl}}} \xrightarrow{\text{Metal gates}} \frac{C_{ox}}{1 + \frac{C_{ox}}{C_{inv}}}$$

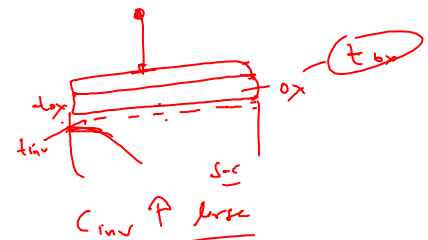
(1) Long channel devices, t_{ox} large

• C_{ox} small, $C_{ox}/C_{inv} \rightarrow 0$, $C_{tot} = C_{ox}$

(2) Nano-scale devices, t_{ox} small

• C_{ox} large, C_{ox}/C_{inv} finite, $C_{tot} < C_{ox}$

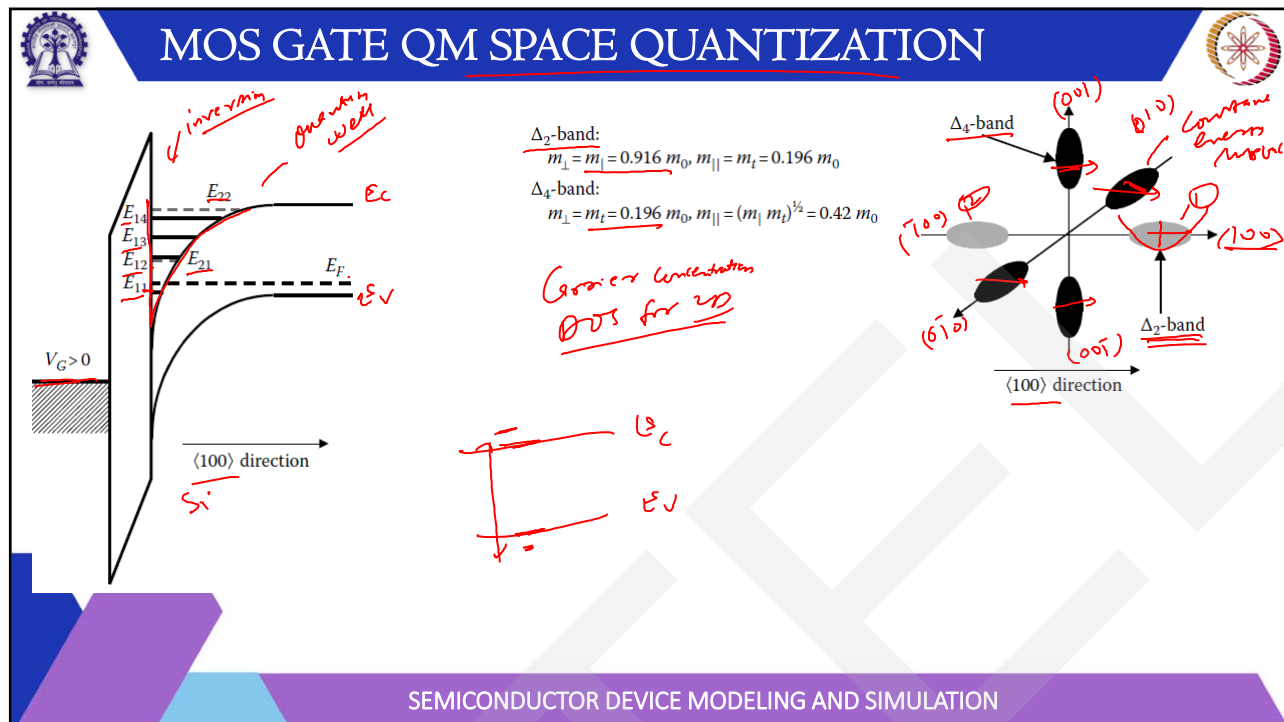
• C_{inv} is always large because the thickness of the inversion layer is small



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

$$C_{tot} = \frac{C_{ox}}{1 + \frac{C_{ox}}{C_{poly}} + \frac{C_{ox}}{C_{inv} + C_{depl}}} \xrightarrow{\text{metal}} \frac{C_{ox}}{1 + \frac{C_{ox}}{C_{inv}}}$$

SEMICONDUCTOR DEVICE MODELING AND SIMULATION



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 the bound state energies or wave functions.

SEMICONDUCTOR DEVICE MODELING AND SIMULATION



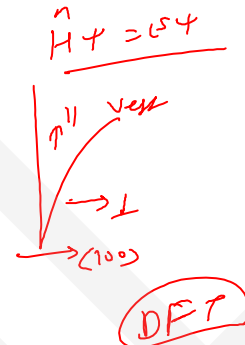
SCHRODINGER+POISSON SOLVERS



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

$$H_o(\mathbf{R}) = -\left(\frac{\hbar^2}{2m_x^*} \frac{\partial^2}{\partial x^2} + \frac{\hbar^2}{2m_y^*} \frac{\partial^2}{\partial y^2} + \frac{\hbar^2}{2m_z^*} \frac{\partial^2}{\partial z^2}\right) + V_{eff}(z) = H_{o\parallel}(r) + H_{o\perp}(z)$$

where
 $\mathbf{R} = (r, z)$
 $V_{eff}(z)$ is the effective potential energy profile of the confining potential
 $H_{o\parallel}$ is the parallel part of H_o



- The transverse part is defined as $H_{o\perp}(z) = -\frac{\hbar^2}{2m_z^*} \frac{\partial^2}{\partial z^2} + V_{eff}(z)$
- 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

SEMICONDUCTOR DEVICE MODELING AND SIMULATION



QUANTUM CORRECTIONS



- 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 capacitances (due to the finite average displacement of the inversion charge from the semiconductor-oxide interface)



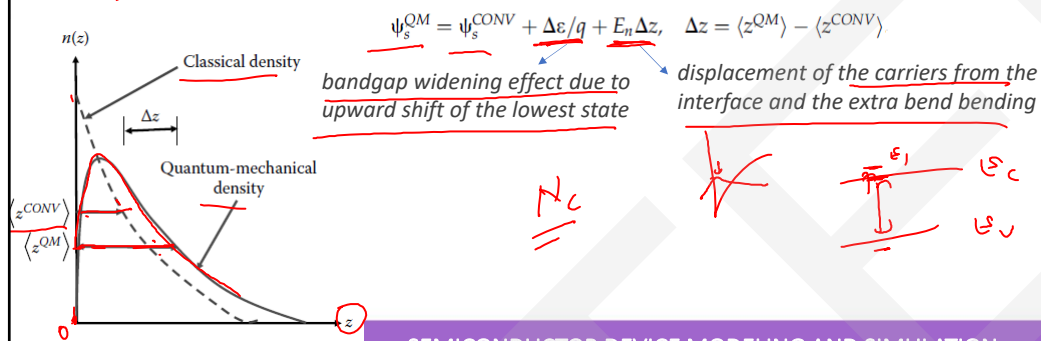
SEMICONDUCTOR DEVICE MODELING AND SIMULATION



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 $N_C^* = N_C [1 - \exp(-z/\text{LAMBDA})]^2$ ↑ Parameter
- Van Dort model modifies the intrinsic carrier concentration by taking into account the effective bandgap increase due to quantum-mechanical size quantization effects



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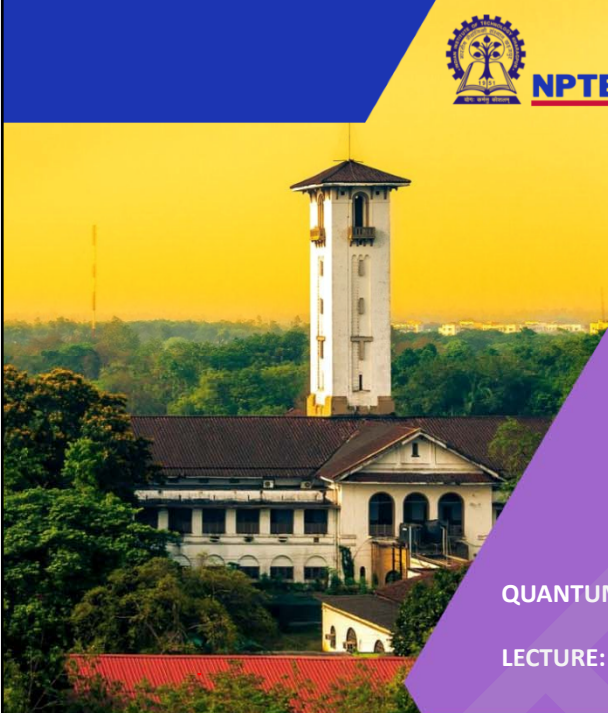
CONCLUSION



- Discussed Quantum Mechanical Confinement and
- Quantum correction modelling approach

SEMICONDUCTOR DEVICE MODELING AND SIMULATION





NPTEL ONLINE CERTIFICATION COURSE



SEMICONDUCTOR DEVICE MODELING AND SIMULATION

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QUANTUM TRANSPORT

LECTURE: 57



L57 QUANTUM TRANSPORT



- *Carrier concentration in a quantum well*
- *Quantum transport*
 - *Potential step penetration and*
 - *Tunneling through potential barrier*

SEMICONDUCTOR DEVICE MODELING AND SIMULATION



CALCULATE CARRIER CONCENTRATION



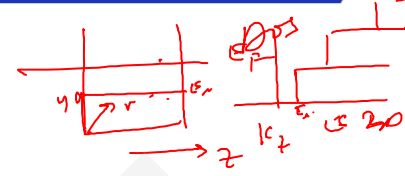
- Calculate carrier concentration in a quantum well
- 2D DOS = $\frac{m}{\pi\hbar^2} dE$
- Given: g_i = valley degeneracy factor, E_F = Fermi energy

$$N_i = g_i \int_{E_i}^{\infty} \frac{m}{\pi\hbar^2} \cdot \frac{1}{1 + \exp\left(\frac{E - E_F}{k_B T}\right)} dE$$

$$= g_i \frac{m}{\pi\hbar^2} k_B T \int_{(E_i - E_F)/k_B T}^{\infty} \frac{1}{1 + \exp(x)} dx = g_i \frac{m}{\pi\hbar^2} k_B T \cdot \log \left[1 + \exp\left(\frac{E_F - E_i}{k_B T}\right) \right]$$

$$I = \int_{\alpha}^{\infty} \frac{1}{1 + e^x} dx = \int_{\alpha}^{\infty} \frac{e^{-x}}{1 + e^{-x}} dx = \left[-\log(1 + e^{-x}) \right]_{\alpha}^{\infty} = \log(1 + e^{-\alpha})$$

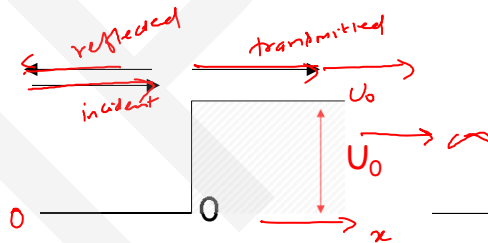
SEMICONDUCTOR DEVICE MODELING AND SIMULATION



$$\frac{\partial \psi}{\partial x} = \frac{q}{\epsilon} (N_A - N_D)$$



POTENTIAL STEP



$$-\frac{\hbar^2}{2m_0} \frac{d^2\psi(x)}{dx^2} + U(x)\psi(x) = E\psi(x)$$

$$\psi = A e^{ikx} + B e^{-ikx}$$

$$\psi(x) = e^{ikx} + r e^{-ikx}, x < 0$$

$$= t e^{ik'x}, x > 0$$

$$k = \sqrt{2mE}/\hbar \rightarrow \text{left}$$

$$k' = \sqrt{2m(E - U_0)}/\hbar \rightarrow \text{right}$$

Boundary Conditions:

$$\psi(0^-) = \psi(0^+)$$

$$d\psi/dx|_{0^-} = d\psi/dx|_{0^+}$$

$$1 + r = t$$

$$k(1 - r) = k't \rightarrow 2r = t - \frac{k'}{k} t \rightarrow t = \frac{1}{1 - \frac{1}{2}(1 - \frac{k'}{k})}$$

$$r = \frac{\frac{k'}{k} t}{1 + r} \rightarrow r = \frac{\frac{k'}{k} t}{1 + \frac{k'}{k} t} = \frac{k' t}{k + k' t}$$

SEMICONDUCTOR DEVICE MODELING AND SIMULATION



POTENTIAL STEP



Case-1: $E > U_0 \rightarrow k, k'$ real

Boundary Conditions:

$$1 + r = t$$

$$k(1-r) = k't$$

$$\begin{aligned} \psi(x) &= e^{ikx} + re^{-ikx}, x < 0 \rightarrow e^{ikx} + \frac{k-k'}{k+k'} e^{-ikx} \\ &= te^{ik'x}, x > 0 \rightarrow \frac{2k}{k+k'} e^{ik'x} \end{aligned}$$

$$\begin{aligned} t &= 2k/(k+k') \\ r &= (k-k')/(k+k') \end{aligned}$$

Transmission = current transmitted/current incident

Reflection Coeff = current reflected/current incident

$$J = \text{Re}(\hbar k/m |\psi_0|^2) \text{ and } T = \text{Re}(k'|t|^2/k), R = |r|^2$$

$$\begin{aligned} T &= \text{Re}(k'|t|^2/k) = \frac{4kk'}{(k+k')^2} \\ R &= |r|^2 = \frac{(k-k')^2}{(k+k')^2} \\ T + R &= 1 \end{aligned}$$

SEMICONDUCTOR DEVICE MODELING AND SIMULATION



POTENTIAL STEP



Case-2: $E < U_0 \rightarrow k'$ imaginary = $i\eta$

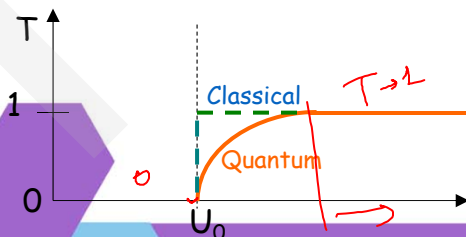
$$\begin{aligned} \psi(x) &= e^{ikx} + re^{-ikx}, x < 0 \\ &= te^{ik'x}, x > 0 \end{aligned}$$

$$k = \sqrt{2mE}/\hbar$$

$$\eta = \sqrt{2m(U_0 - E)}/\hbar$$

$$\begin{aligned} t &= 2k/(k+i\eta) \\ r &= (k-i\eta)/(k+i\eta) \end{aligned}$$

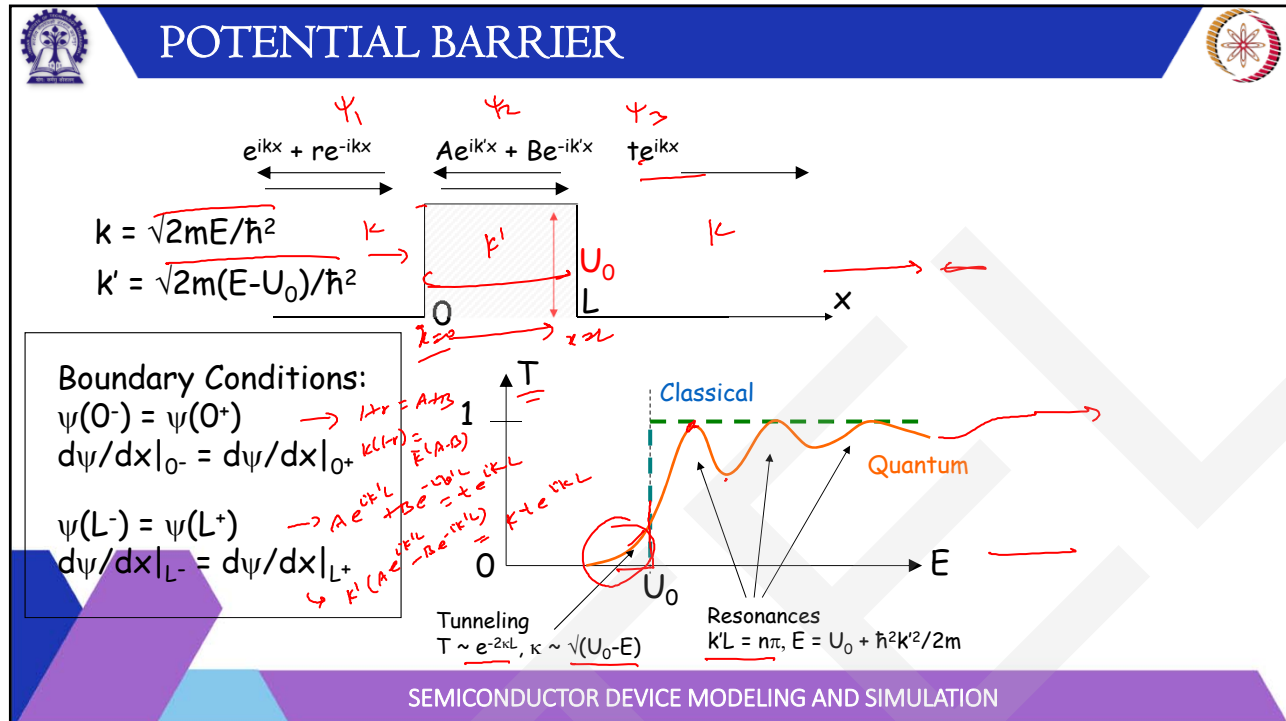
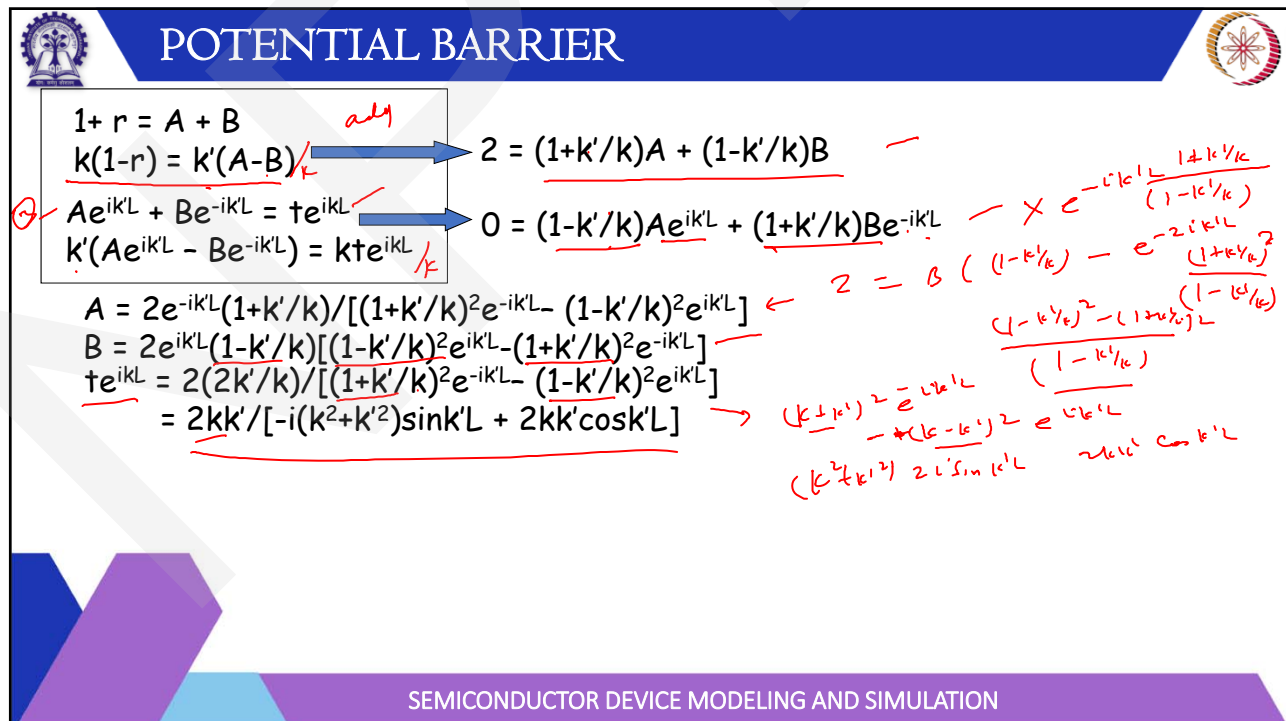
$$\begin{aligned} T &= \text{Re}(i\eta |t|^2/k) = 0 \\ R &= |r|^2 = |k-i\eta|^2/|k+i\eta|^2 = 1 \end{aligned}$$



$E \gg U_0 \rightarrow k_1 \approx k_2$
 $\rightarrow$ classical result $T = 1, R = 0$

there is a finite probability for a particle with an energy, $E > U_0$, step height to be reflected.

SEMICONDUCTOR DEVICE MODELING AND SIMULATION



POTENTIAL BARRIER

$1 + r = A + B$
 $k(1 - r) = k'(A - B) \rightarrow 2 = (1 + k'/k)A + (1 - k'/k)B$
 $Ae^{ik'L} + Be^{-ik'L} = te^{ik'L}$
 $k'(Ae^{ik'L} - Be^{-ik'L}) = kte^{ik'L} \rightarrow 0 = (1 - k'/k)Ae^{ik'L} + (1 + k'/k)Be^{-ik'L}$

$A = 2e^{-ik'L}(1 + k'/k) / [(1 + k'/k)^2 e^{-ik'L} - (1 - k'/k)^2 e^{ik'L}]$
 $B = 2e^{ik'L}(1 - k'/k) / [(1 - k'/k)^2 e^{ik'L} - (1 + k'/k)^2 e^{-ik'L}]$
 $te^{ik'L} = 2(2k'/k) / [(1 + k'/k)^2 e^{-ik'L} - (1 - k'/k)^2 e^{ik'L}]$
 $= 2kk' / [-i(k^2 + k'^2)\sin k'L + 2kk'\cos k'L]$

For $E > U_0$: $T = 4k^2k'^2 / [(k^2 + k'^2)^2 \sin^2 k'L + 4k^2k'^2 \cos^2 k'L]$
Or $T = 4k^2k'^2 / [(k^2 - k'^2)^2 \sin^2 k'L + 4k^2k'^2] \rightarrow T_{max}$
Resonances (T_{max}): $\sin k'L = 0, k'L = 0, n\pi$
For $E < U_0$: $k' = i\alpha, T = 4k^2\alpha^2 / [(k^2 + \alpha^2)^2 \sinh^2 \alpha L + 4k^2\alpha^2]$
Wide barriers: $\alpha L \gg 1, \sinh(\alpha L) \sim \cosh(\alpha L) \sim e^{\alpha L}/2$
 $T \approx 16k^2\alpha^2 e^{-2\alpha L} / (k^2 + \alpha^2)^2 \sim [16E(U_0 - E)/U_0^2] e^{-2\alpha L} \rightarrow$

$T = |t|^2$

$k = \sqrt{2mE}/\hbar$
 $k' = \sqrt{2m(U_0 - E)}/\hbar$

$\sinh x = \frac{e^x - e^{-x}}{2}$
 $\sin x = \frac{e^{ix} - e^{-ix}}{2i}$

SEMICONDUCTOR DEVICE MODELING AND SIMULATION

MATLAB/OCTAVE CODE

```

close all; clear all
m=9.1e-31; hbar=1.05e-34; q=1.6e-19;
L=1e-9; %length
U0=1; %potential, Volts
Ne=511; E=linspace(0,5,Ne);
k=sqrt(2*m*E*q/hbar^2);
eta=sqrt(2*m*(E-U0)*q/hbar^2);
T=4.*k.^2.*eta.^2./((k.^2+eta.^2).^2.*sin(eta.*L).*sin(eta.*L)+4.*k.^2.*eta.^2.*cos(eta.*L).*cos(eta.*L));
figure(1); plot(E,T,'r','linewidth',3)
title('L = 1 nm','fontsize',15)
grid on
hold on
tcl=2.*k./(k+eta); tcl=tcl.*conj(tcl);
Tcl=real((eta./k).*tcl);
plot(E,Tcl,'k--','linewidth',3)
plot(E,Tcl,'k--','linewidth',3)

```

$E=1.3725$ $E=2.49$
 $K'L=3.14$ $K'L=6.28$

SEMICONDUCTOR DEVICE MODELING AND SIMULATION

TUNNELING

$T \approx [16E(U_0 - E)/U_0^2] e^{-2\alpha L}$ Even though $E < V_0$, $L > 0$

More generally, WKB approximation

$$T \sim \exp\left[-2 \int_{x_1}^{x_2} \sqrt{2m[U(x) - E]}/\hbar dx\right]$$

$\downarrow$ as barrier $L \uparrow$, $U_0 \uparrow$ and mass $\uparrow$
 Cases: Source-Drain tunneling in MOSFETs
 Resonant Tunneling Devices (RTDs)

SEMICONDUCTOR DEVICE MODELING AND SIMULATION

TUNNELING - DEVICES

resonant tunneling diode From Lake, R. and J.J. Yang,
 IEEE Transactions on Electron Devices, 50(3), 785, 2003

Scanning tunneling microscope uses
 quantum-mechanical tunneling

SEMICONDUCTOR DEVICE MODELING AND SIMULATION



CONCLUSION



- Discussed quantum transport through a potential step and a potential barrier.



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SEMICONDUCTOR DEVICE MODELING AND SIMULATION

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TRANSFER MATRIX APPROACH

LECTURE: 58



L58 TRANSFER MATRIX APPROACH



- *Transfer Matrix approach*
- *Matlab code*
- *Transmission through a double barrier*

SEMICONDUCTOR DEVICE MODELING AND SIMULATION

TRANSFER MATRIX APPROACH

- A generalized procedure for calculating the transmission coefficient
- many piece-wise constant segments with arbitrary potential barrier
- propagation matrix P_i through the segment
- Boundary matrix B_i applies at the boundary between segments i and $i+1$

Consider two consecutive segments

$$\psi(x) = Ae^{ik_i x} + Be^{-ik_i x}$$

$$\psi(x) = Ce^{ik_{i+1} x} + De^{-ik_{i+1} x}$$

$$\begin{bmatrix} C \\ D \end{bmatrix} = B_i \begin{bmatrix} A \\ B \end{bmatrix}$$

$$B_i = \frac{1}{2} \begin{bmatrix} 1 + \frac{k_i}{k_{i+1}} & 1 - \frac{k_i}{k_{i+1}} \\ 1 - \frac{k_i}{k_{i+1}} & 1 + \frac{k_i}{k_{i+1}} \end{bmatrix}$$

$$B_i^{-1} = \frac{1}{2} \begin{bmatrix} 1 + \frac{k_{i+1}}{k_i} & 1 - \frac{k_{i+1}}{k_i} \\ 1 - \frac{k_{i+1}}{k_i} & 1 + \frac{k_{i+1}}{k_i} \end{bmatrix}$$

Handwritten notes for B_i^{-1} :

$$A+B = C+D$$

$$k_i(A-B) = k_{i+1}(C-D)$$

$$A = \frac{1}{2} \left(C \left(1 + \frac{k_{i+1}}{k_i} \right) + D \left(1 - \frac{k_{i+1}}{k_i} \right) \right)$$

SEMICONDUCTOR DEVICE MODELING AND SIMULATION

TRANSFER MATRIX APPROACH

- A generalized procedure for calculating the transmission coefficient
- many piece-wise constant segments with arbitrary potential barrier
- propagation matrix P_i through the segment
- Boundary matrix B_i applies at the boundary between segments i and $i+1$

$$\psi(x) = ae^{ikx} + be^{-ikx}$$

$$\psi_l = \begin{bmatrix} A \\ B \end{bmatrix}$$

$$P_i = \begin{bmatrix} e^{ik_i l_i} & 0 \\ 0 & e^{-ik_i l_i} \end{bmatrix}$$

$$B_i = \frac{1}{2} \begin{bmatrix} 1 + \frac{k_{i+1}}{k_i} & 1 - \frac{k_{i+1}}{k_i} \\ 1 - \frac{k_{i+1}}{k_i} & 1 + \frac{k_{i+1}}{k_i} \end{bmatrix}$$

$$\psi_r = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

$$\psi_r = P_1 B_1 P_2 B_2 \dots P_m B_m \psi_l$$

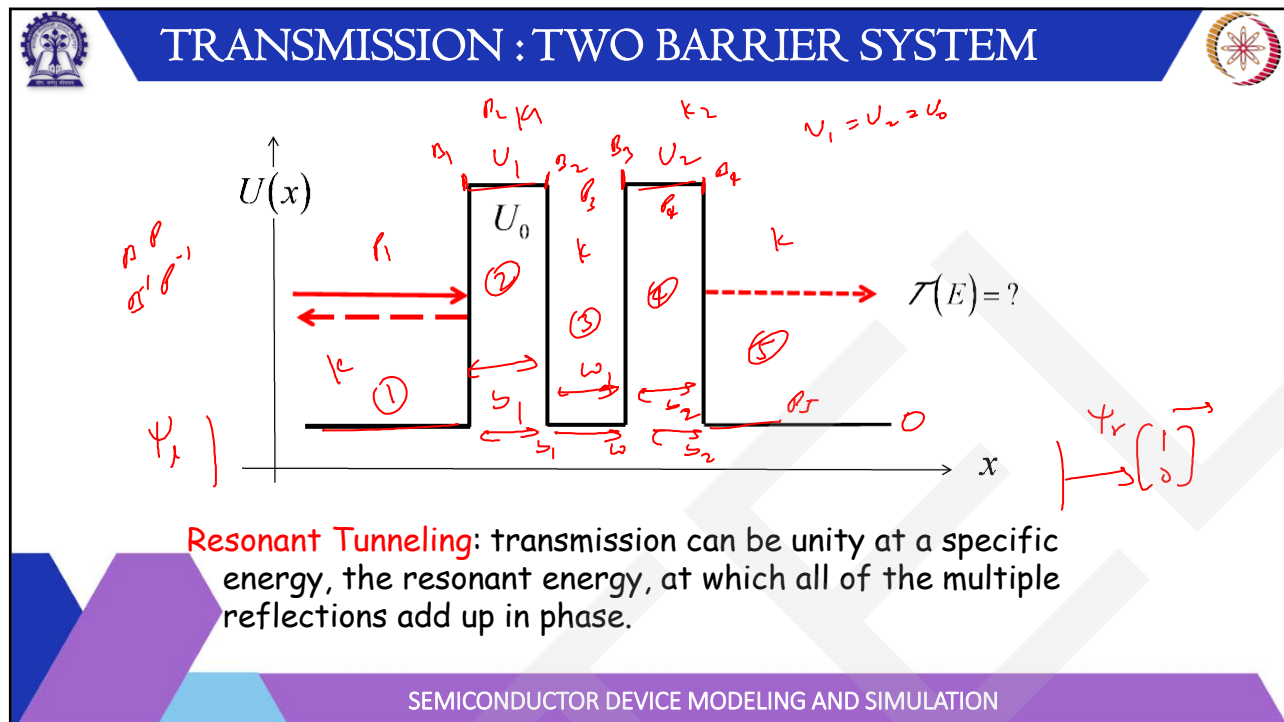
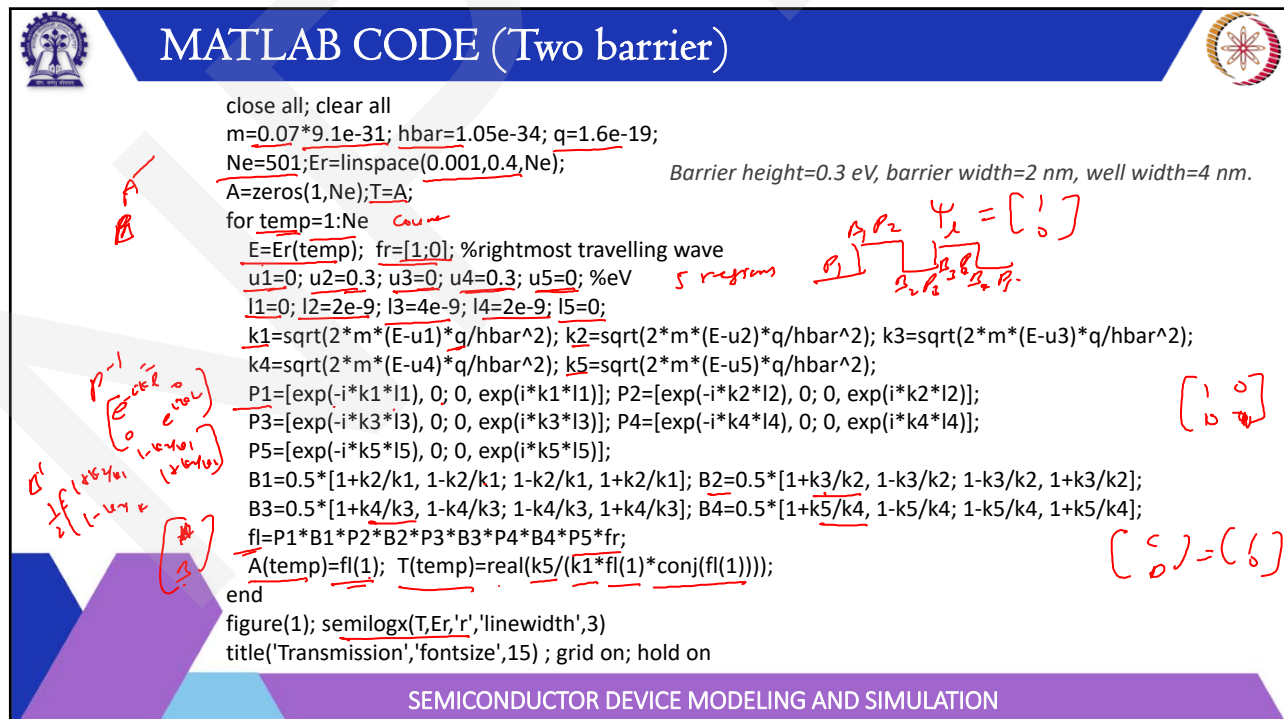
Handwritten notes for B_i :

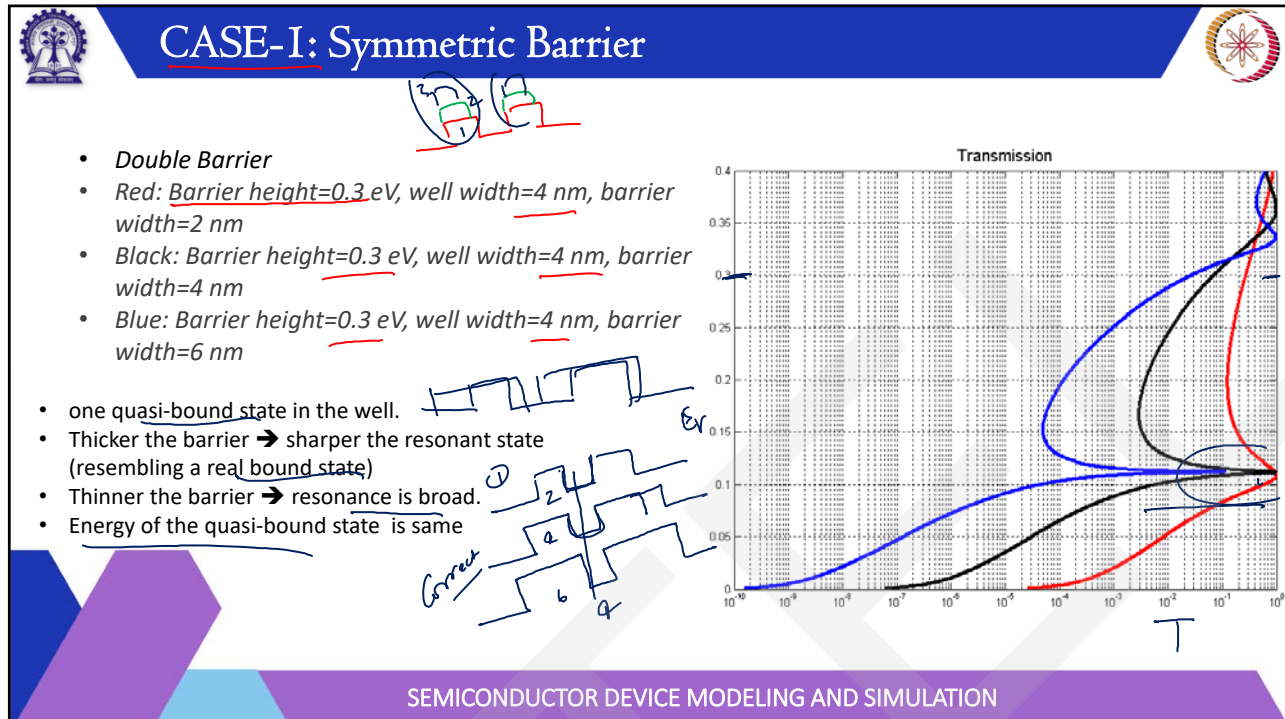
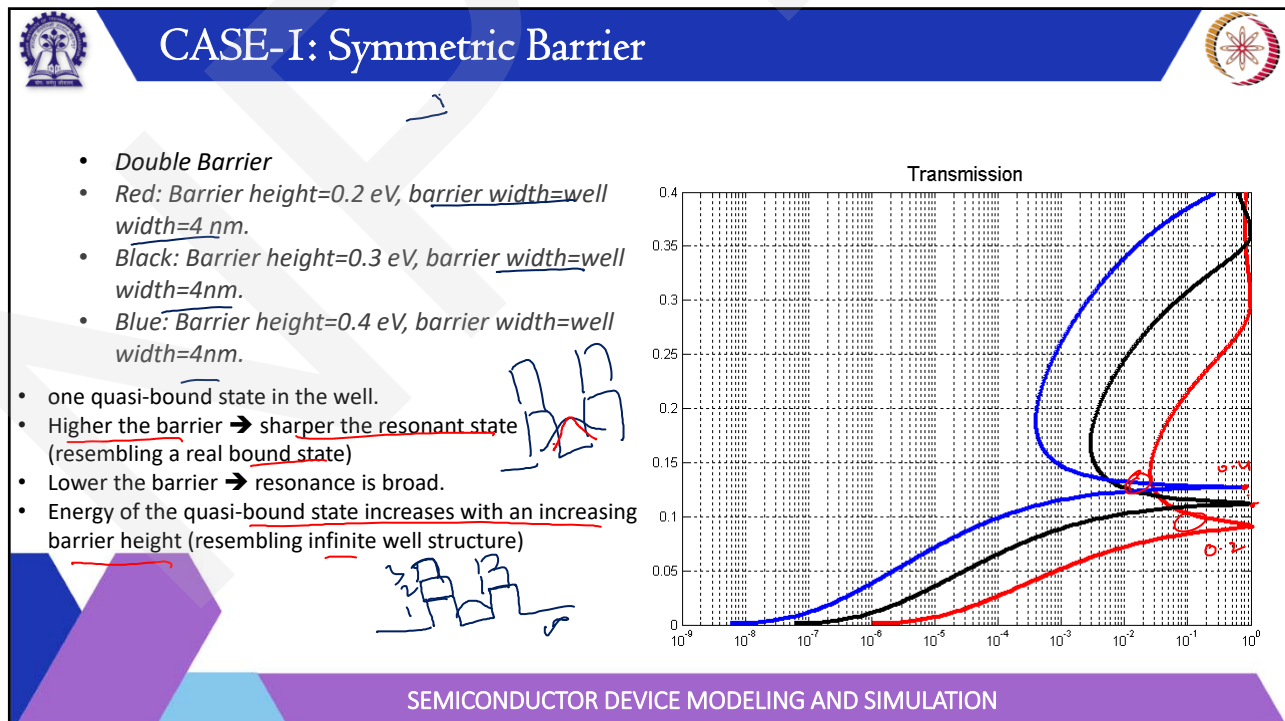
$$r = \frac{k_{i+1}}{k_i} \Rightarrow B_i = \frac{1}{2} \begin{bmatrix} 1+r & 1-r \\ 1-r & 1+r \end{bmatrix}$$

Handwritten notes for ψ_r :

$$\begin{bmatrix} e^{ik_{i+1} l_i} & 0 \\ 0 & e^{-ik_{i+1} l_i} \end{bmatrix} \begin{bmatrix} Ae^{ik_{i+1} l_i} \\ Be^{-ik_{i+1} l_i} \end{bmatrix} = \begin{bmatrix} e^{ik_{i+1} l_i} \\ 0 \end{bmatrix}$$

SEMICONDUCTOR DEVICE MODELING AND SIMULATION



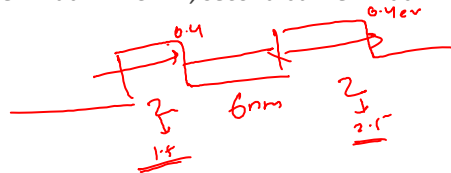




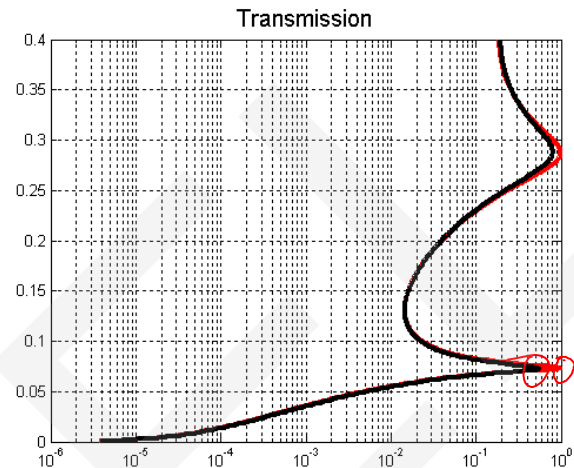
CASE-2: Asymmetric Barrier



- Double Barrier
- Red: Barrier height = 0.4 eV, well width = 6 nm, first barrier width = 2 nm, second barrier width = 2 nm
- Black: Barrier height = 0.4 eV, well width = 6 nm, first barrier width = 1.5 nm, second barrier width = 2.5 nm



unequal barrier widths there is no perfect transmission



SEMICONDUCTOR DEVICE MODELING AND SIMULATION



LIMITATIONS OF TRANSFER MATRIX APPROACH



- Prone to arithmetic overflow
- For regions where the wave function is evanescent, the P matrices contain real elements equal to the attenuation of the region and its inverse. The inverse is likely to be a very large positive number and if several evanescent regions are cascaded, the numbers in the matrix will rapidly exceed the dynamic range of floating point variables.
- When transmission matrix scheme is applied to multiband models, because at any given energy, many of the bands will be evanescent. Overflow is more severe.
- Other popular approach include the scattering matrix approach and Green's function method to calculate the quantum transport properties, with the coupling to the leads being introduced via the self-energy. The advantage of this approach is the well-developed theory of the Green's functions that also allows one to consider inelastic scattering within the nonequilibrium Green's function formalism.

$$e^{-\alpha L} e^{-\alpha L}$$

Nobody knows

SEMICONDUCTOR DEVICE MODELING AND SIMULATION



LIST OF TRANSPORT MODELS



MODEL	Application/ Limitation
Compact models	Appropriate for circuit design <i>Spiral</i>
<u>Drift-diffusion model</u>	Good for devices down to <u>0.5 μm</u> , include <u>$\mu(E)$</u> $\rightarrow$
<u>Hydrodynamic model</u>	<u>Velocity overshoot effect</u> can be <u>treated properly</u> $\rightarrow$
<u>Boltzmann transport equation</u>	Accurate up to the classical limits
<u>Monte Carlo methods</u>	
<u>Quantum hydrodynamics</u>	<u>Classical hydrodynamic features</u> + <u>quantum corrections</u>
<u>Quantum Monte Carlo methods</u>	all classical features + quantum corrections
<u>Green's functions method</u>	Includes <u>correlations in both space and time domain</u>
<u>Direct solution of the n-body Schrödinger equation</u>	Can be solved only for <u>small number of particles</u>

SEMICONDUCTOR DEVICE MODELING AND SIMULATION



CONCLUSION



- Discussed quantum transport through Transfer Matrix Approach

SEMICONDUCTOR DEVICE MODELING AND SIMULATION

