Green’s Function Approach For MOSFETs

Ramesh Venugopal

School of Electrical and
Computer Engineering
Purdue University

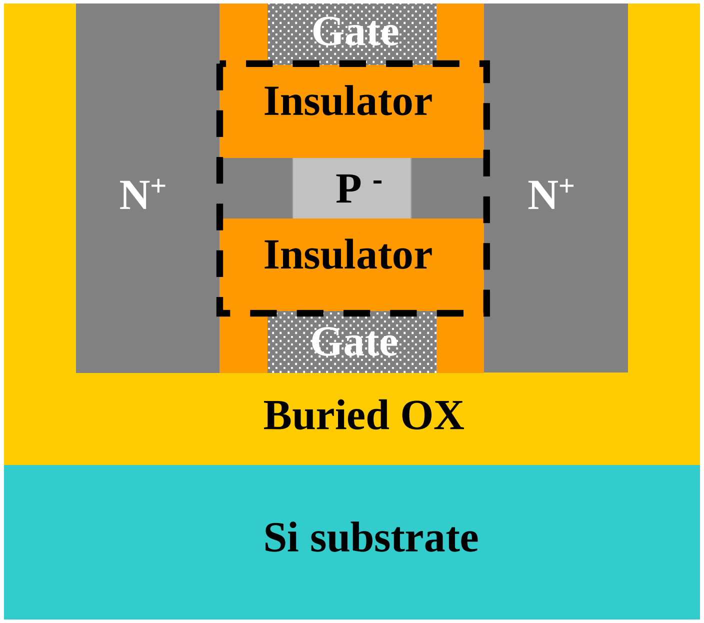
J. Rhew
S. Goasguen
Prof. S. Datta
Prof. M. Lundstrom
CE Group

Outline

- Introduction
- Ballistic Electron Transport: *Real vs. Mode Space*
- Boundary Conditions
- Scattering in n-channel MOSFETs
- Summary

Introduction

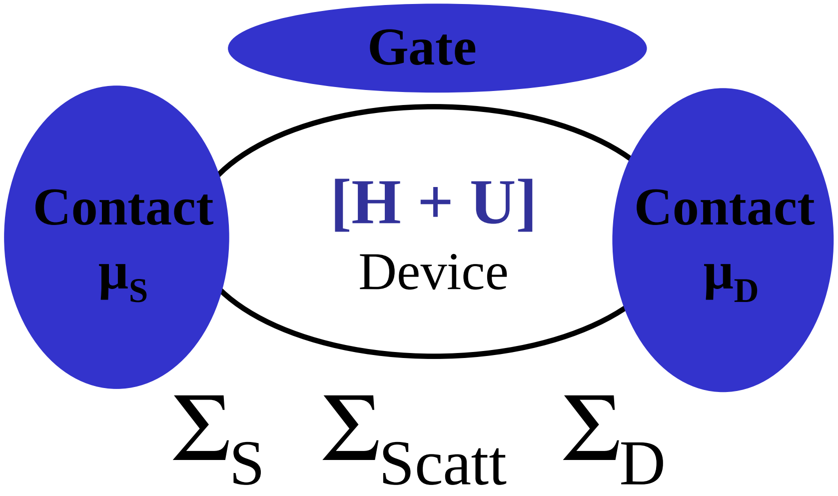
- **Charge Centroid Shift**
  - Decreases the effective gate capacitance
  - Decreases the on-current
- **Thin Body Effects**
  - Increases the threshold voltage (and fluctuations)
  - Decreases the off-current
  - Decreases the on-current
- **Oxide Tunneling**
  - Increases the off-current
- **Source Barrier Tunneling**
  - Increases the off-current (imposes a scaling limit)
- **Quantum Mechanical Treatment of Scattering**
- **Bandstructure(Strain)/ Heterostructures**



Outline

- Introduction
- Ballistic Electron Transport: *Real vs. Mode Space*
- Boundary Conditions
- Scattering in n-channel MOSFETs
- Summary

Real vs. Mode Space



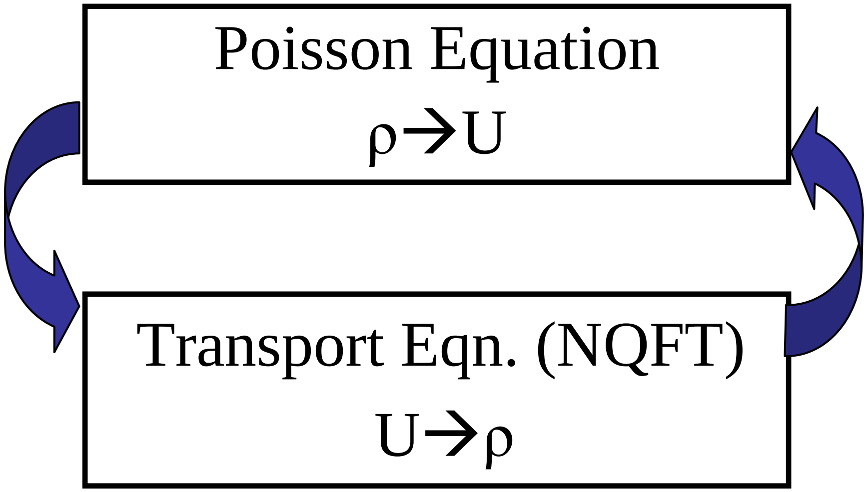
Gate

Contact μ_S

[H + U] Device

Contact μ_D

Σ_S Σ_{Scatt} Σ_D



Poisson Equation

ρ→U

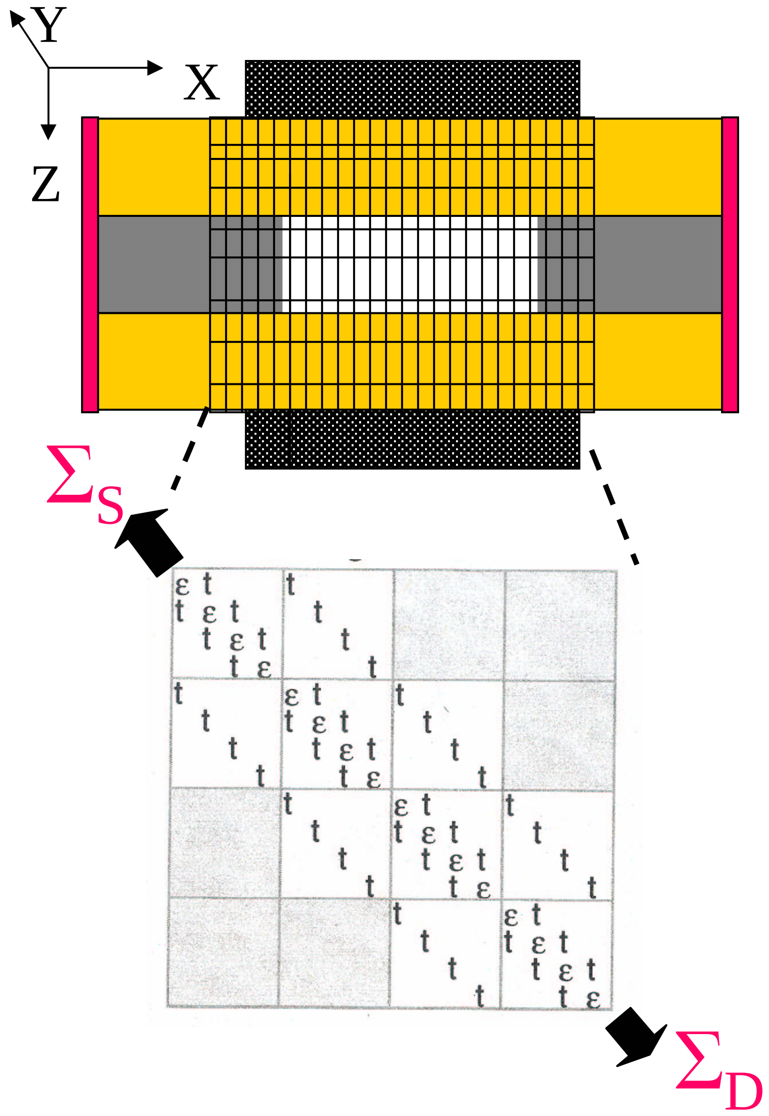
Transport Eqn. (NQFT)

U→ρ

$\Sigma_S , \Sigma_{Scatt} , \Sigma_D , H , U$

- Σ: Self Energy (Describes Coupling)
- G^n, G^p: Correlation Functions (Local Charge Density)
- Σ^{in}, Σ^{out}: The in and out scattering functions (can be related to the state lifetime of electrons and holes)

Real vs. Mode Space



- Basis is $\delta(x-x')\delta(z-z')e^{ik_Y Y/\sqrt{W}}$
- Single band, multi valley effective mass eqn.
- Bandstructure is linked to grid morphology

$$E(k_x)=\frac{\hbar^2}{2m_x}\left(1-\cos(k_x\Delta_x)\right)$$

- Quantum Mechanics (Dyson's eqn.)

$$\left(E[k_x,k_z]I-H-\Sigma^R\right)G^R=I$$

- Non-local Carrier Dynamics

$$G^n=G^R\Sigma^{in}G^A \qquad G^P=G^R\Sigma^{out}G^A$$

- Physical observables along the diagonals
- Block tridiagonal nature of H, permits a recursive calculation of diagonal blocks of G
- Self energy matrices are perturbative elements

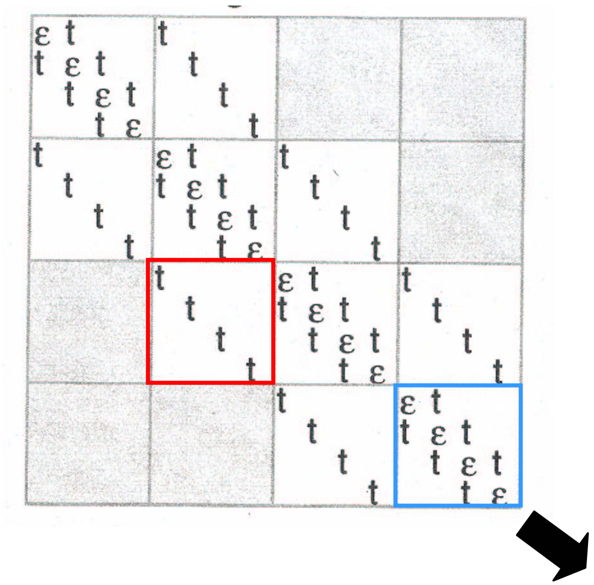
Real vs. Mode Space

$$G = \left[EI - H_{Device+Lead}\right]^{-1} = \begin{bmatrix} EI - H_{Device} & \tau \\ \tau^{+} & EI - H_{Lead} \end{bmatrix}^{-1}$$

$$G_{Device} = \left[EI - H_{Device} - \Sigma_{Lead}(E)\right]^{-1}$$

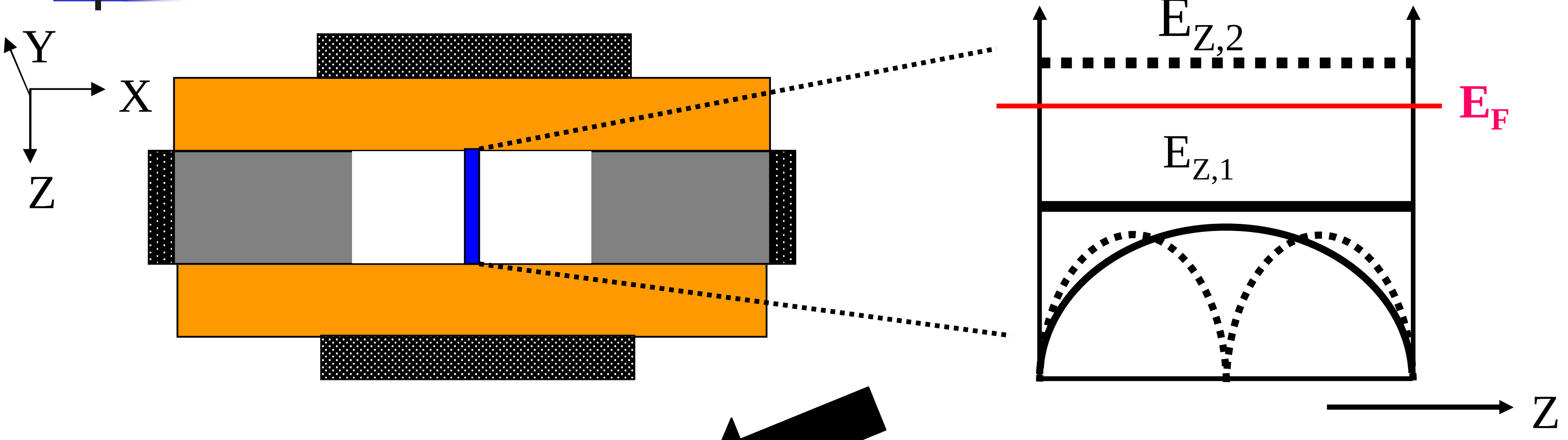
$$\Sigma_{Lead}(E) = \tau G_{Lead}\tau = \tau G^{11}_{Lead}\tau^{+}$$

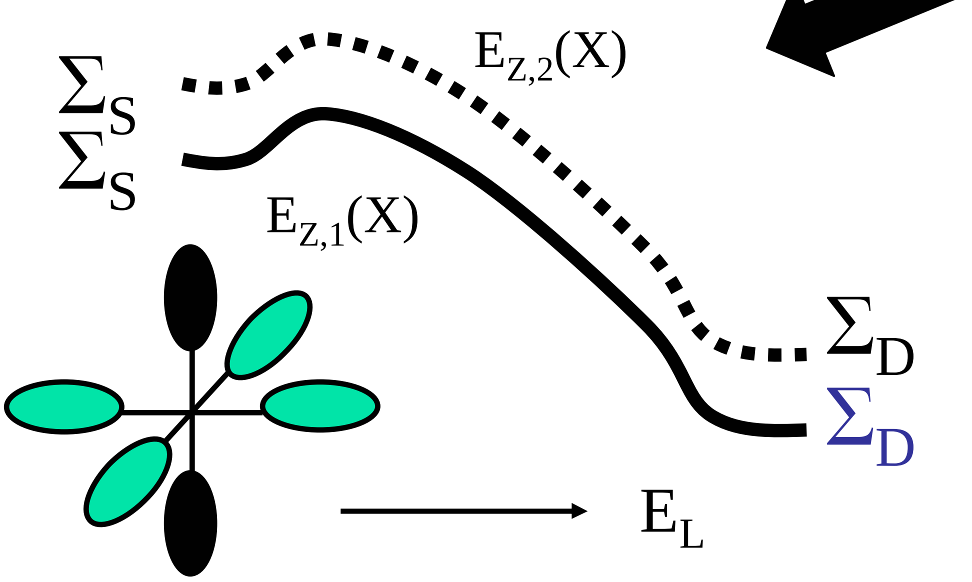
$$I = G^{11}_{Lead}\left[EI - H^{11}_{Lead} - \tau G^{11}_{Lead}\tau^{+}\right]^{-1}$$



- Potential is invariant looking into the lead
- The size of the self-energy matrix is the same as that of the Hamiltonian
- The only non-zero block of the self-energy corresponds to the column of nodes that constitute the boundary between the active device and the lead

Real vs. Mode Space



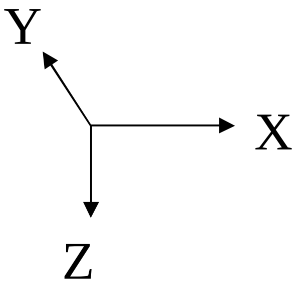


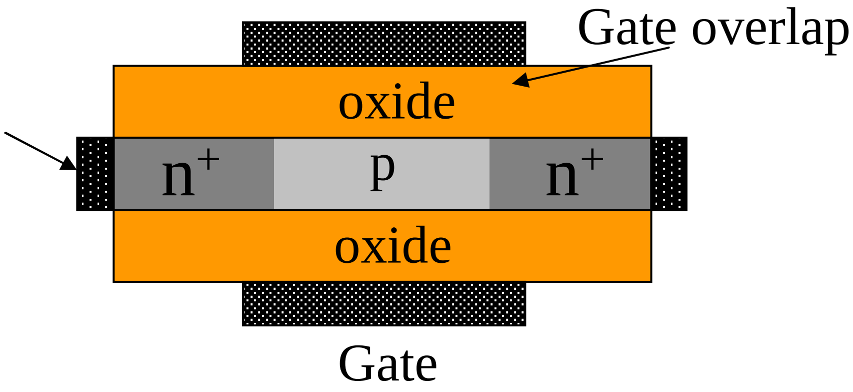
- Mode self-energy is τe^{ika}
- Mode occupancy is limited by the Fermi Function
- Thin body and confinement effects are correctly captured
- Modes can be treated classically or quantum mechanically

Real vs. Mode Space

- Single band, multi valley, effective mass equation.
- Basis is $\delta(x - x')\Psi(x,z)e^{ik_Y Y}/\sqrt{W}$
- The overall wavefunction in the (X, Z) plane is $\Phi(x,z) = \sum_i C_i(x)\Psi_i(x,z)$
- The 1D equation that is discretized, is an equation for $C_i(X)$
- Individual modes are treated independently in the Ballistic limit
- Each mode couples to a contact with its unique self-energy
- Treatment of few, decoupled subbands (occupancy limited) greatly reduces computational cost as compared to real space solution
- The problem size is ~Nx^2 as opposed to ~ $(NxNy)^2$

Real vs. Mode Space





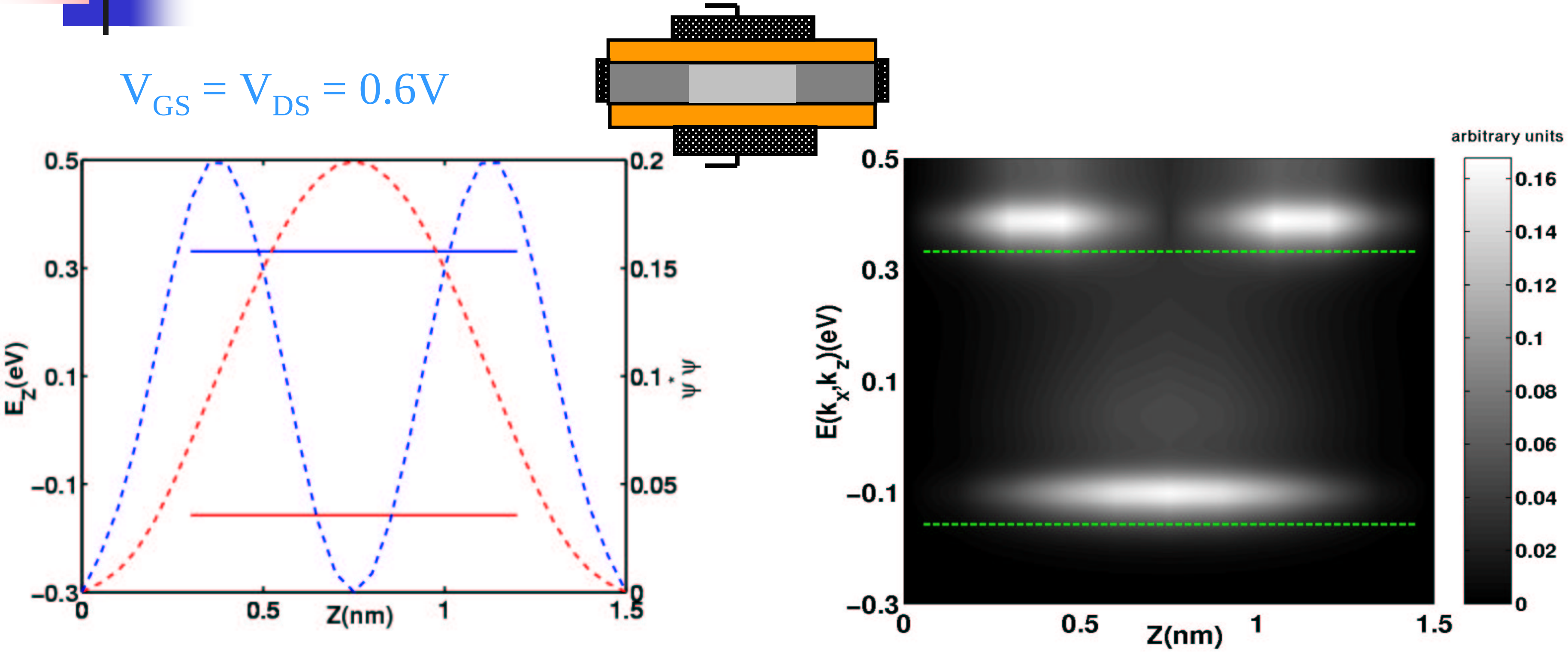
Ideal
absorbing
contact
to flared
out S/D

Single Subband

T_{Si} = 1.5 nm
T_{OX} = 1.5 nm
L_G = 10 nm
V_{DD} = 0.6 V
V_t = 0.15 V
S/D = Abrupt
N(S/D) = $10^{20}/cm^3$

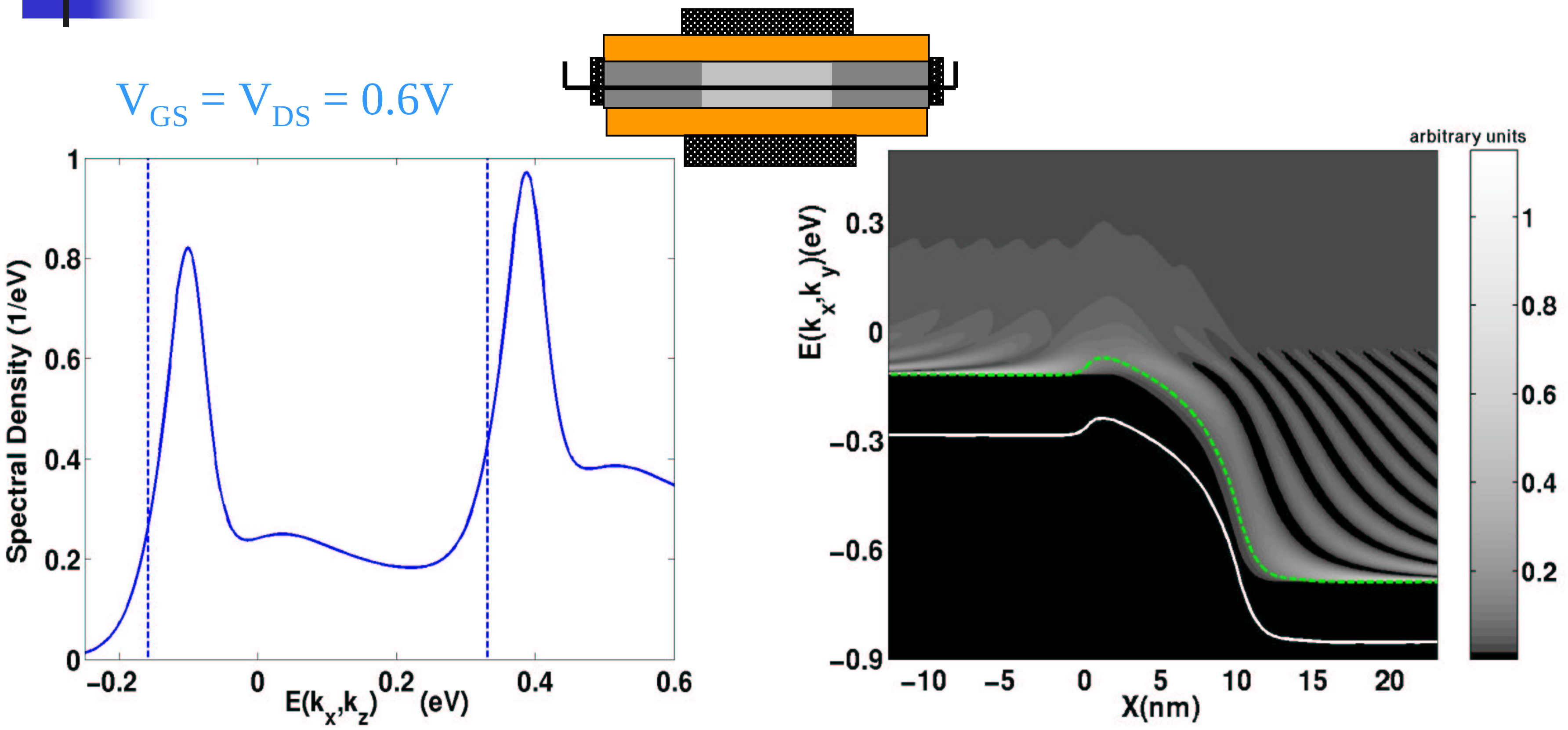
Real vs. Mode Space

$V_{GS} = V_{DS} = 0.6V$



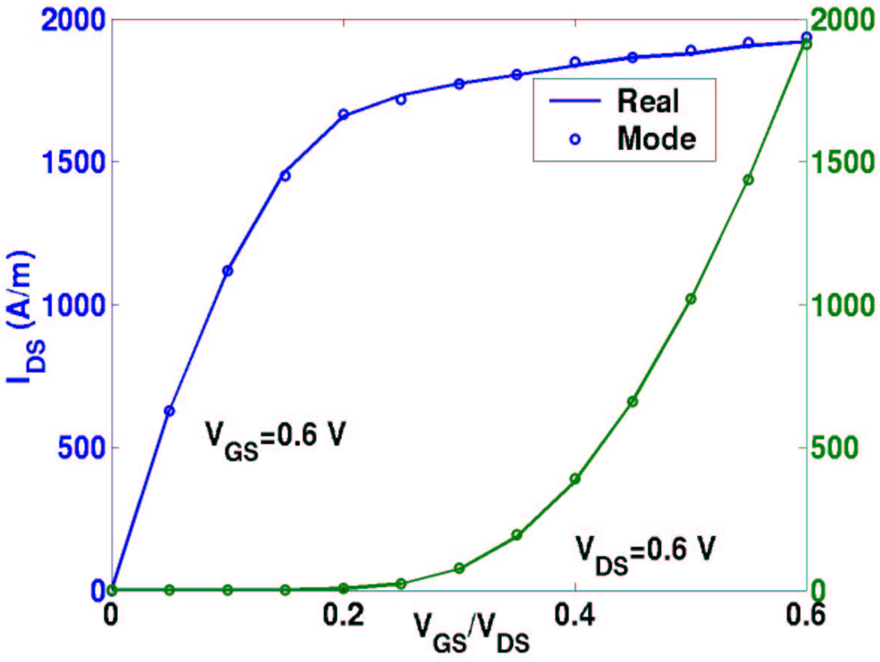
- Mode-Space solutions capture vertical quantum effects
- Quantum effects along the channel are accounted for by coupling modes to contacts
- The 2D spectral function from Real Space simulations includes the mode/subband picture

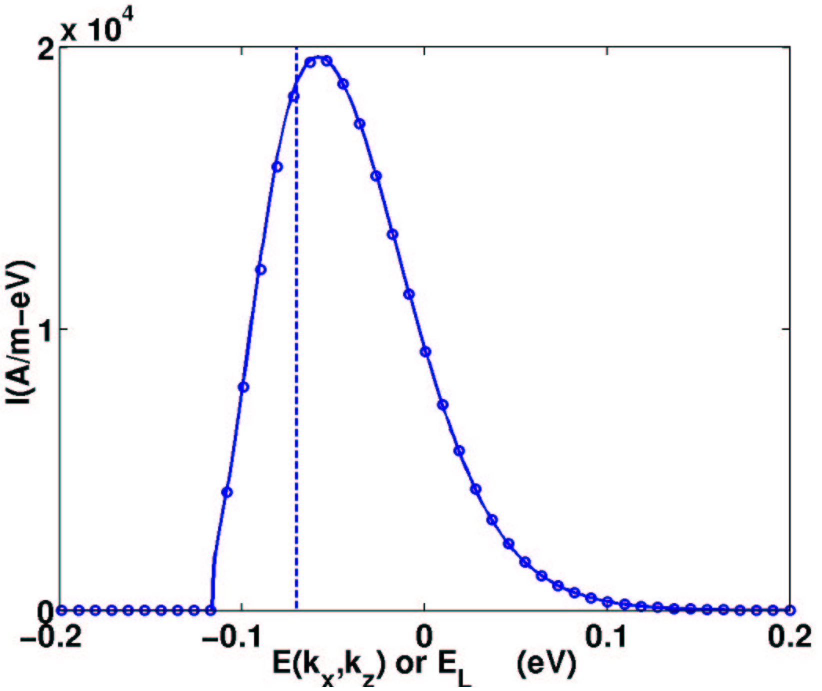
Real vs. Mode Space


$V_{GS} = V_{DS} = 0.6V$

- Coupling to contacts broadens the 2D DOS and shifts the subband energies
- Local oscillations in charge density/DOS are due to quantum interference
- Local oscillations in charge density are washed out when solving Poisson’s eqn.

Real vs. Mode Space

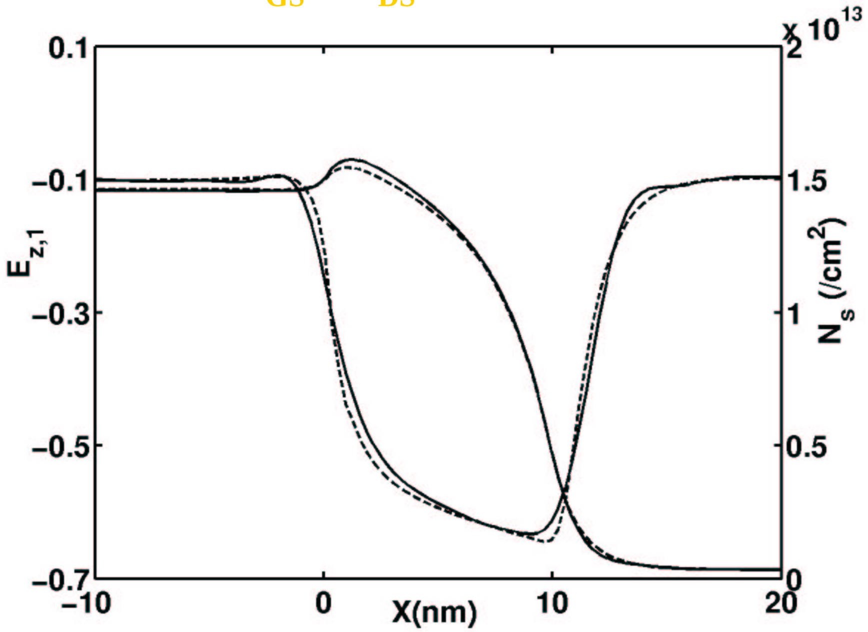


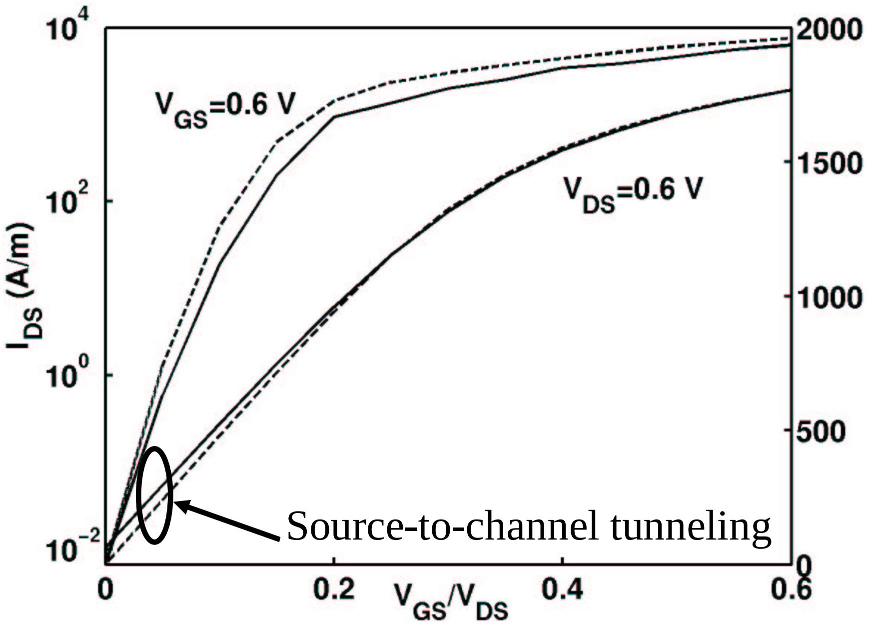


- Mode space solutions are computationally efficient and offer an attractive simulation scheme for modeling SOI devices
- Tunneling affects both the on and the off currents
- ~25% of the on-current is due to tunneling carriers

Real vs. Mode Space

$V_{GS} = V_{DS} = 0.6$ V





- Self-Consistent Boltzmann solutions in Mode space overpredict the on-current as thermionic carriers have a higher velocity than tunneling carriers
- When comparing transport models, Selfconsistency solutions must be considered
- The Mode Space, Boltzmann solution cannot capture source barrier tunneling

Real vs. Mode Space

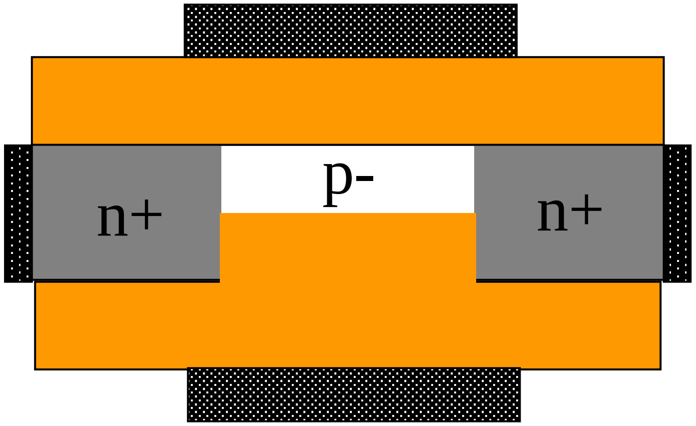
Mode space expansion and approximation

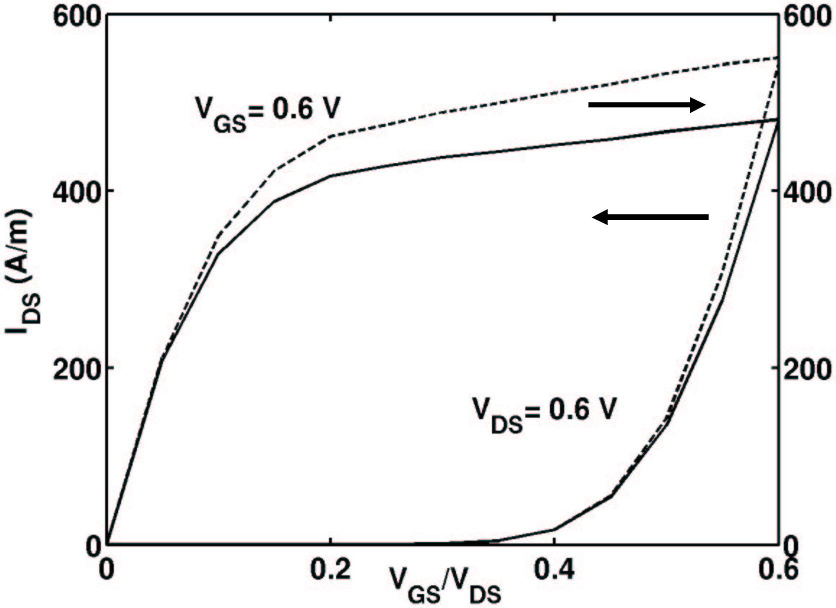
- Basis is $\delta(x-x')\Psi_i(x,z)e^{ik_Y Y/\sqrt{W}}$ and the wavefunction is $\Phi(x,z)=\sum_i C_i(x)\Psi_i(x,z)$
- Expand the 2D Hamiltonian to evaluate $\langle i \mid H \mid \Phi \rangle$

$$\Bigg[\underbrace{-\frac{\hbar^2}{2m_x}\frac{\partial^2}{\partial x^2}}_{\begin{gathered}-\frac{\hbar^2}{2m_x}\frac{\partial^2}{\partial x^2}C_i(x)\\ \Big\Downarrow \\ \frac{\partial\psi_i(x,z)}{\partial x}=0\end{gathered}}\underbrace{-\frac{\hbar^2}{2m_z}\frac{\partial^2}{\partial z^2}+U(x,z)}_{\begin{gathered}C_i(x)E_i(x)\\ \Big\Downarrow \\ \langle i \mid j\rangle=\delta_{ij}\end{gathered}}\Bigg]\Phi(x,z)=\underbrace{E_L\Phi(x,z)}_{E_LC_i(x)}$$

- Final 1D equation for mode "*i*" is $\left[-\frac{\hbar^2}{2m_x}\frac{\partial^2}{\partial x^2}-E_i(x)\right]C_i(x)=E_LC_i(x)$

Real vs. Mode Space





- When modes abruptly change shape the Real and decoupled Mode Space solutions no longer match
- The reduced current from the Real Space solution is due to a quantum mechanical spreading resistance
- Treating the flared out portions of the Source/Drain is challenging

Real vs. Mode Space

The key approximation in the Mode Space Solution:

- The shape of the mode does not vary along the channel, $\frac{\partial \Psi_i(x,z)}{\partial x} = 0$

Implications:

- Different modes are decoupled in the Ballistic Limit
- This solution is justified in case of thin body, fully depleted DG MOSFETs

Computational Complexity: N_X x N_Z = 122 x 10, Esteps = 1500

Real Space: 1500*122*$10^{2.7}$ flops * 10 (Poisson iterations) ~ 0.9 Gflops

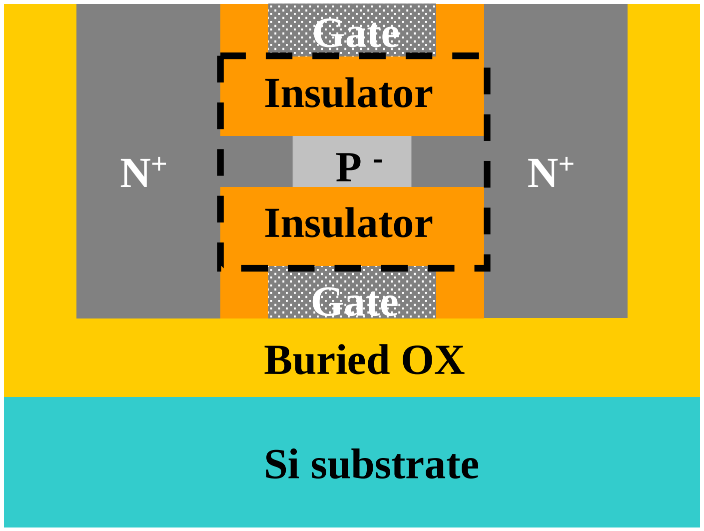
Mode Space (2 modes) = 1500*2*122*log(122) flops* 10 ~ 0.02 Gflops

- Mode space solutions treat few confined modes as higher modes are empty
- Real space solutions implicitly include coupling and all confined modes

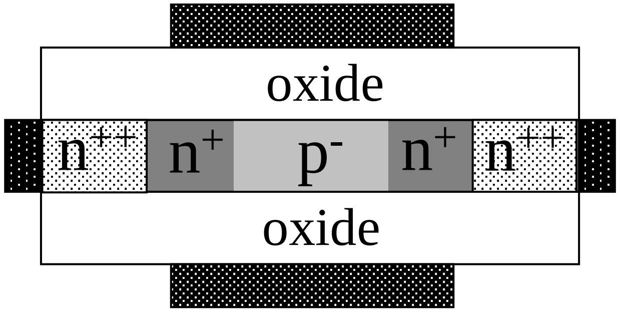
Outline

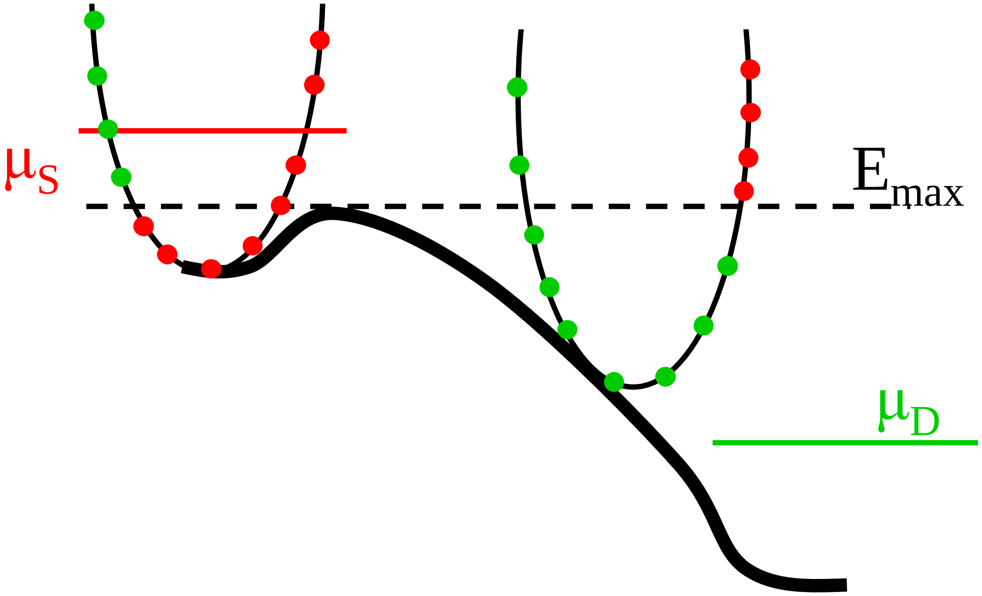
- Introduction
- Ballistic Electron Transport: *Real vs. Mode Space*
- Boundary Conditions
- Scattering in n-channel MOSFETs
- Summary

Boundary Conditions



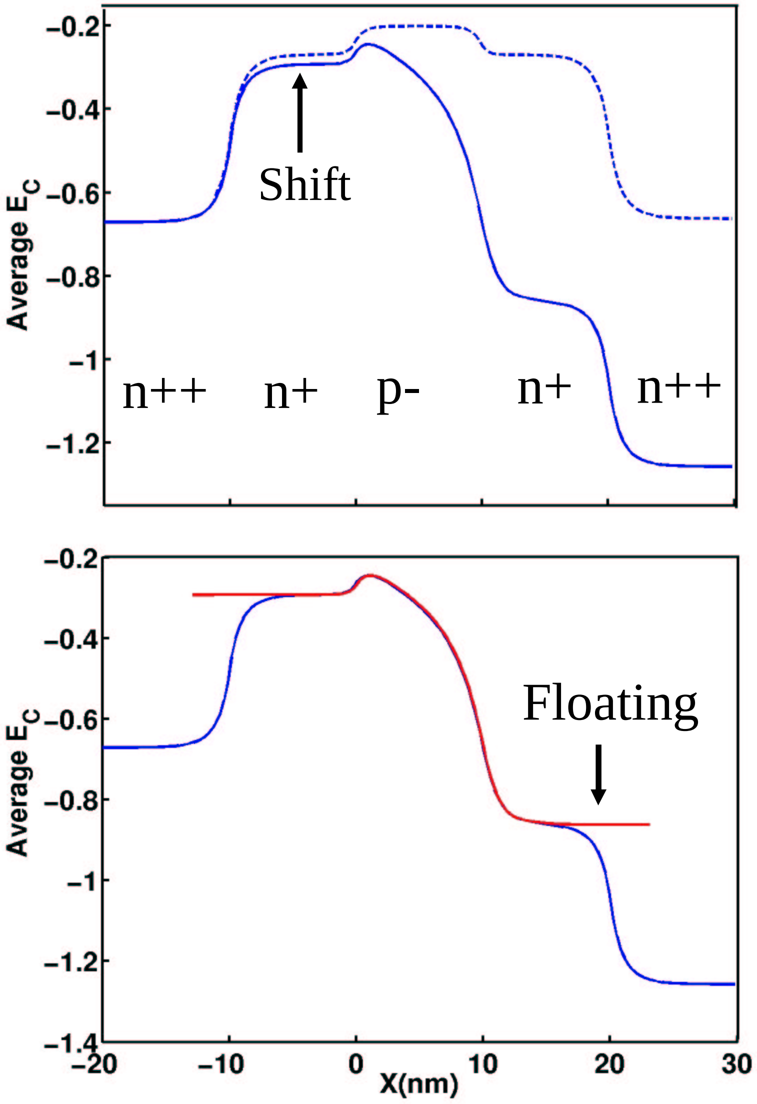
Suppression of the drain injected carriers with increasing drain voltage prevents the source end from attaining charge neutrality in the ballistic limit.

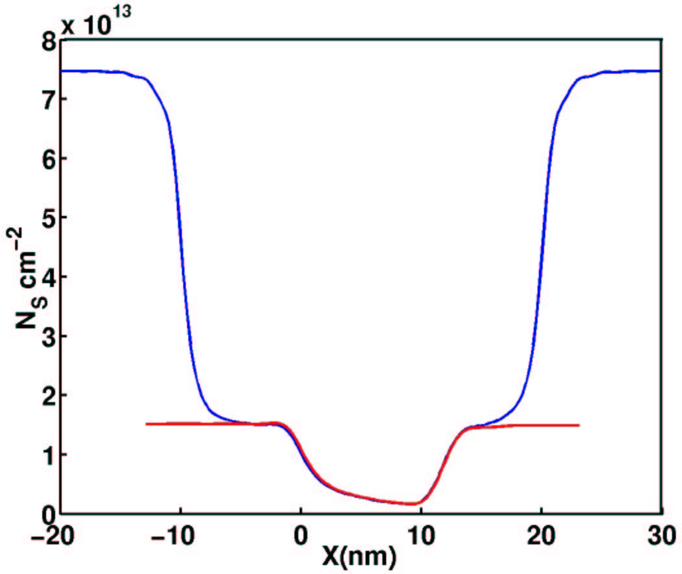




- The artificial n++ region is used to simulate a large scattering contact

Boundary Conditions





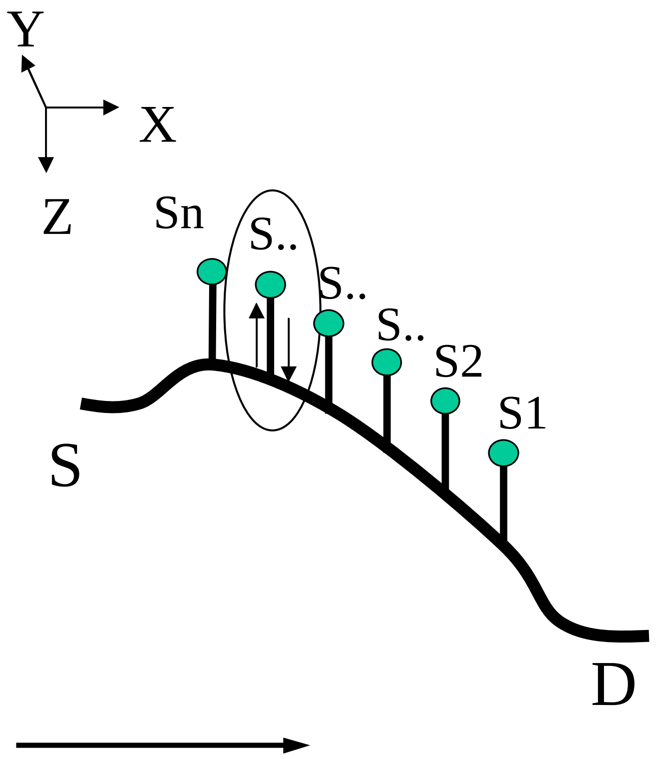
- Floating BC, captures the effect of coupling to a scattering contact
- Floating BC means, $\hat{X} \bullet \vec{\nabla} V = 0$
- Charge neutrality (Integrated doping equals the integrated charge density) is always realized

Outline

- Introduction
- Ballistic Electron Transport: *Real vs. Mode Space*
- Boundary Conditions
- Scattering in n-channel MOSFETs
- Summary

Scattering

Büttiker probes



E_L, (electron energy along the channel)

- Electrons are scattered, thermalized, and re-injected.
- Current is conserved through the entire channel.
- The interaction energy between the probe and the device can be related to a mobility

Energy Relaxation: Electron energies are fully randomized at each probe (energy relaxation) $\int I(E_L)dE_L = 0$

Phase Breaking: Complete loss of coherence $I(E_L) = 0$

Scattering

$\Sigma(E_L)$, describes the coupling between the probe and the device and can be related to a low field mobility

$\Sigma^{in}(E_L)$, and $\Sigma^{out}(E_L)$, are the in and out scattering strengths. They are expressed in terms of $\Sigma(E_L)$ and the Fermi-level, μ, of each probe (includes degeneracy)

Current at each probe is constrained to be zero by adjusting Fermi energies of all probes

$$H = -\frac{\hbar^2}{2m^*}\nabla^2 + U$$

$$G(E_L) = [E_L I - H - \Sigma(E_L)]^{-1}$$

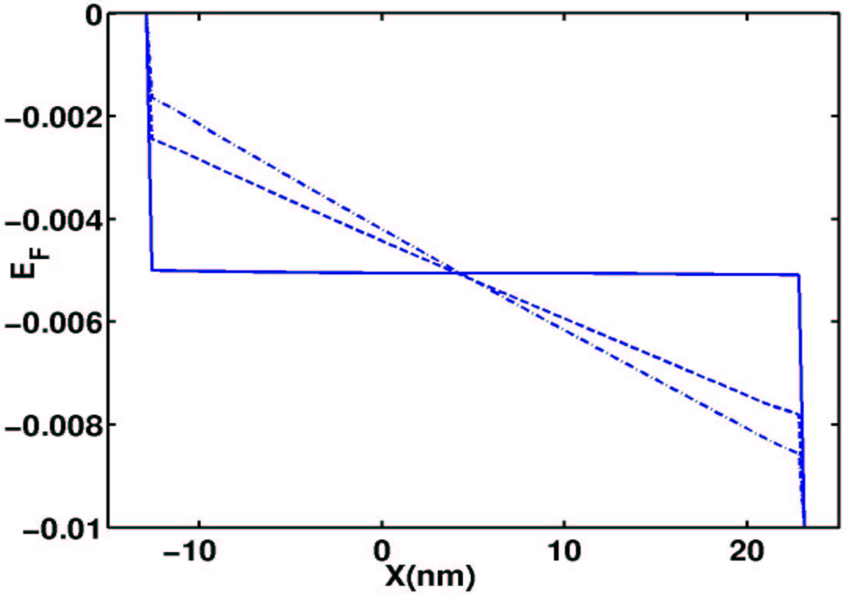
$$G^n(E_L) = G(E_L)\Sigma^{in}(E_L)G^+(E_L)$$

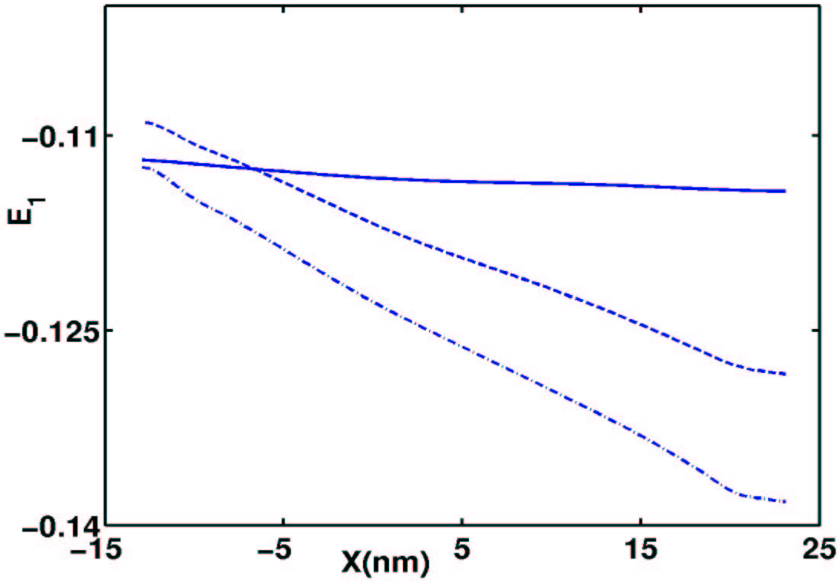
$$G^p(E_L) = G(E_L)\Sigma^{out}(E_L)G^+(E_L)$$

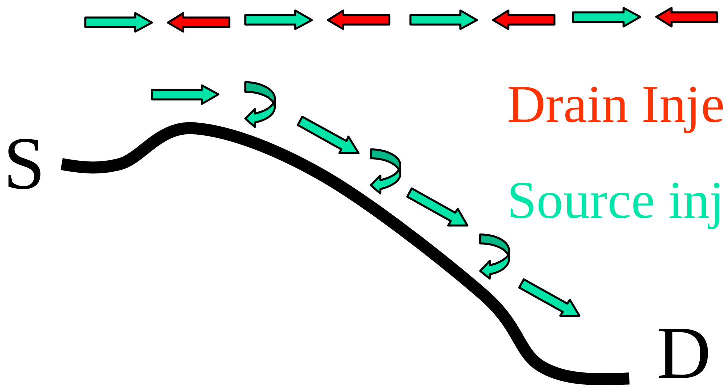
$$I_m(E_L) = \frac{q}{h}Trace[\Sigma_m^{in}G^p - \Sigma_m^{out}G^n]$$

Scattering

How does the voltage drop?





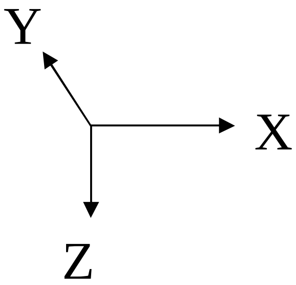


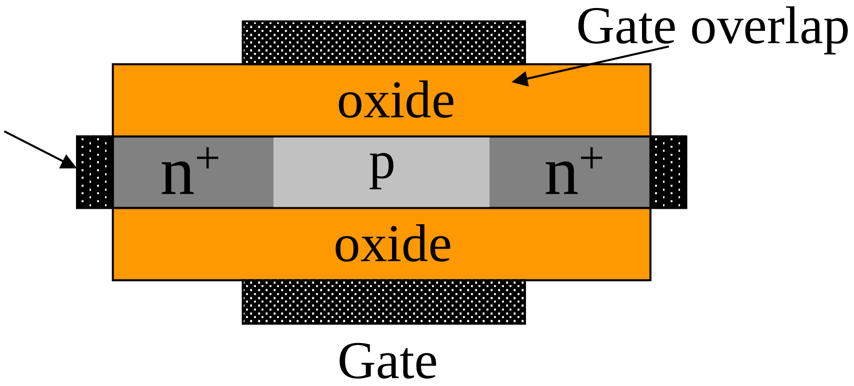
Drain Injected

Source injected

- Uniformly doped (1 x $10^{20}\mathrm{cm}^{-3}$), semiconductor, 10 mV bias
- The scattering model smoothly scales to the Ballistic Limit

Scattering





Ideal absorbing contact to flared out S/D

Single Subband

T_{Si} = 1.5 nm
T_{OX} = 1.5 nm
L_G = 10 nm
V_{DD} = 0.4V
S/D = Abrupt
N(S/D) = $10^{20}/cm^3$

Multiple Subband

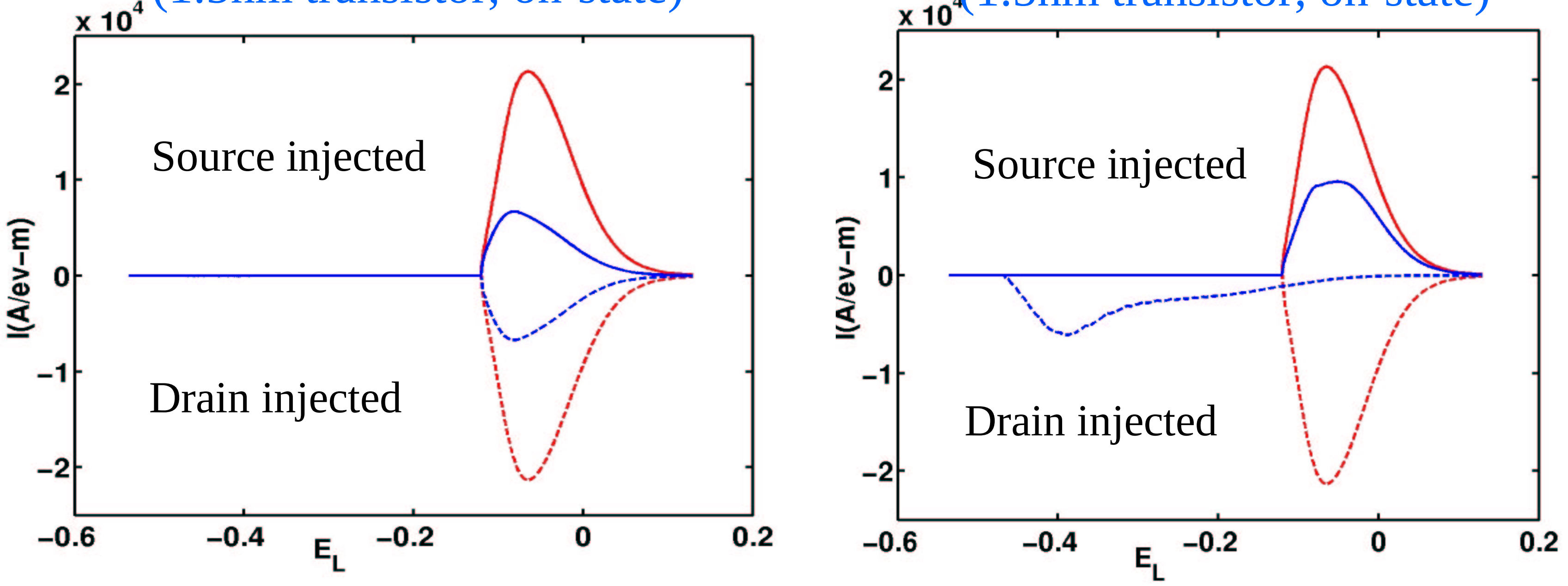
T_{Si} = 3 nm
T_{OX} = 1.5 nm
L_G = 10 nm
V_{DD} = 0.4 V
S/D = Abrupt
N(S/D) = $10^{20}/cm^3$

Scattering

Phase Breaking vs. Energy Relaxing

Reduced Current, Momentum Relaxation (1.5nm transistor, on-state)

Reduced Current, Energy Relaxation (1.5nm transistor, on-state)

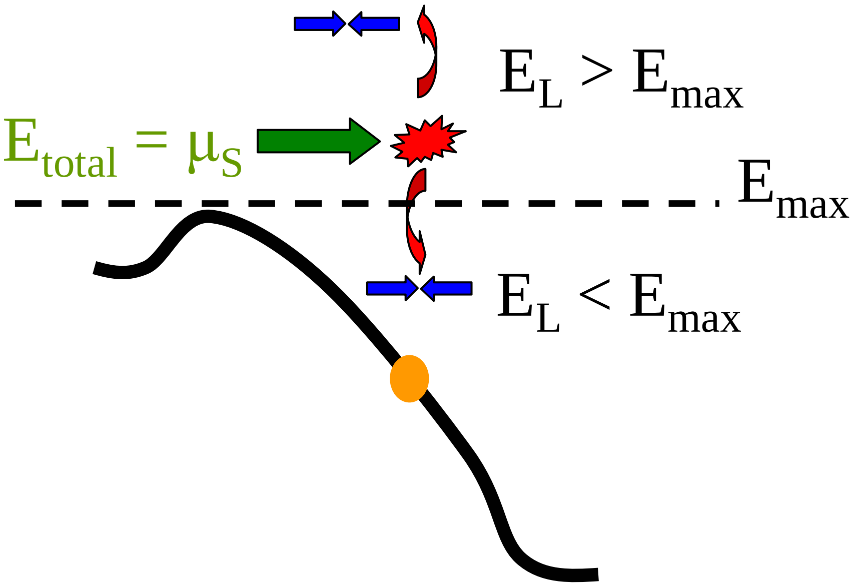


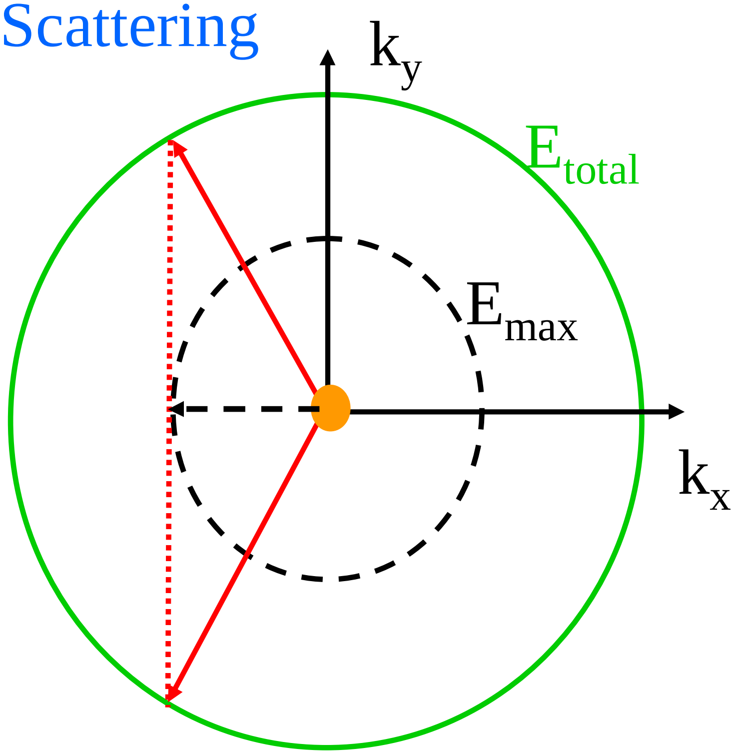
Ballistic Components, Scattering Components

- Phase breaking scattering does not relax the directed longitudinal carrier energy

Scattering

Essential Physics of Scattering



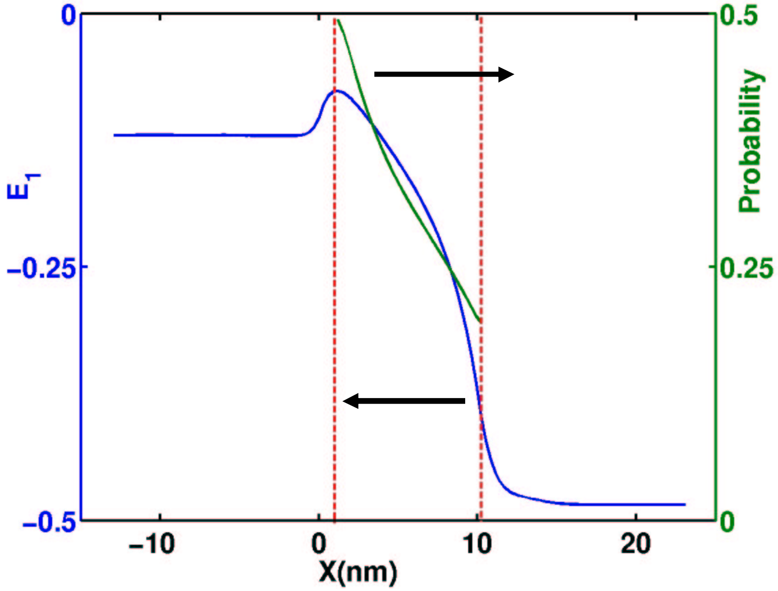


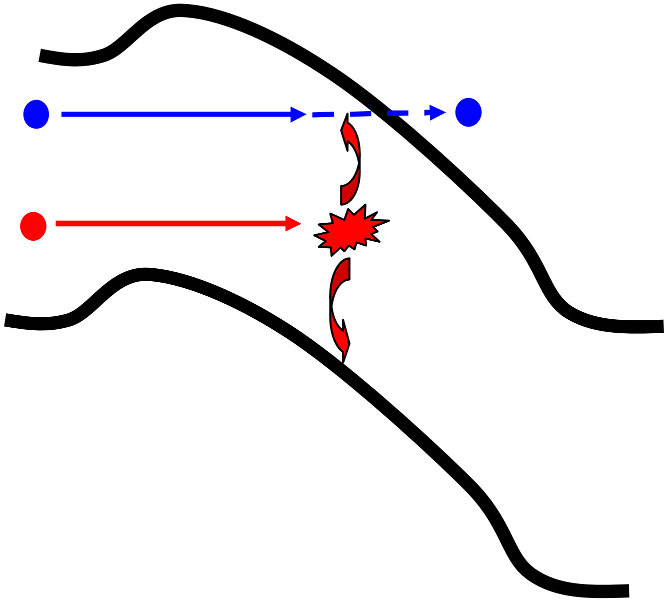
- Only a small cone of carrieres with enough longitudinal energy can make it back to the source
- This cone reduces as one progresses towards the drain thus reducing the probability of backscattering into the source

Ref. Lundstrom, *TED*, p. 133, 2002

Scattering

Essential Physics of Scattering





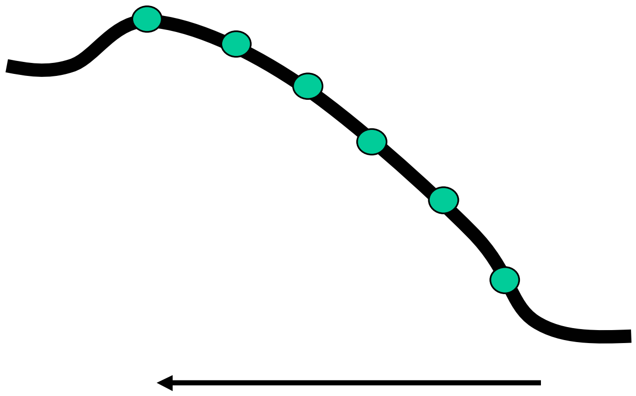
- The probability of backscattering from the channel into the source reduces towards the drain

- The high 1D density of states below the source barrier aids downscattering as opposed to upscattering in longitudinal energy

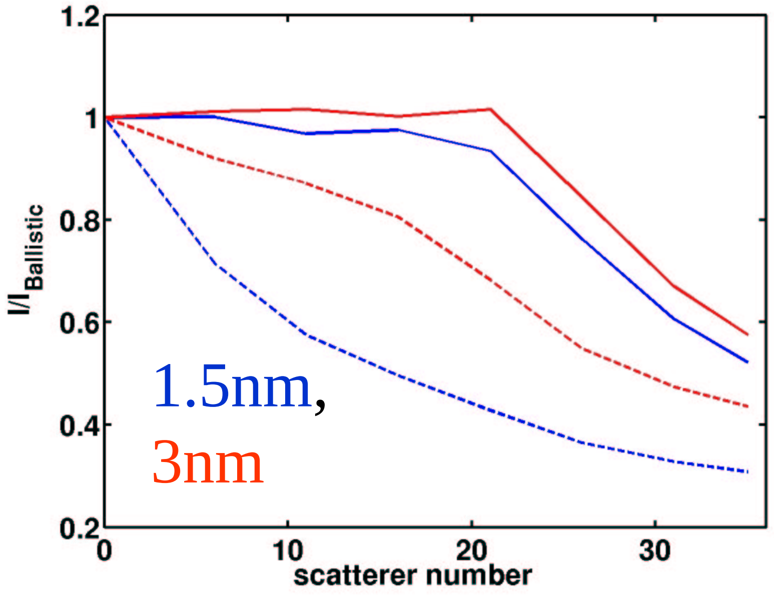
- As the number of subbands increases, band to band coupling causes the backscattering probability is reduced even more

Scattering

Phase Breaking (--) vs. Energy Relaxing



Direction of increase in the scatterer number



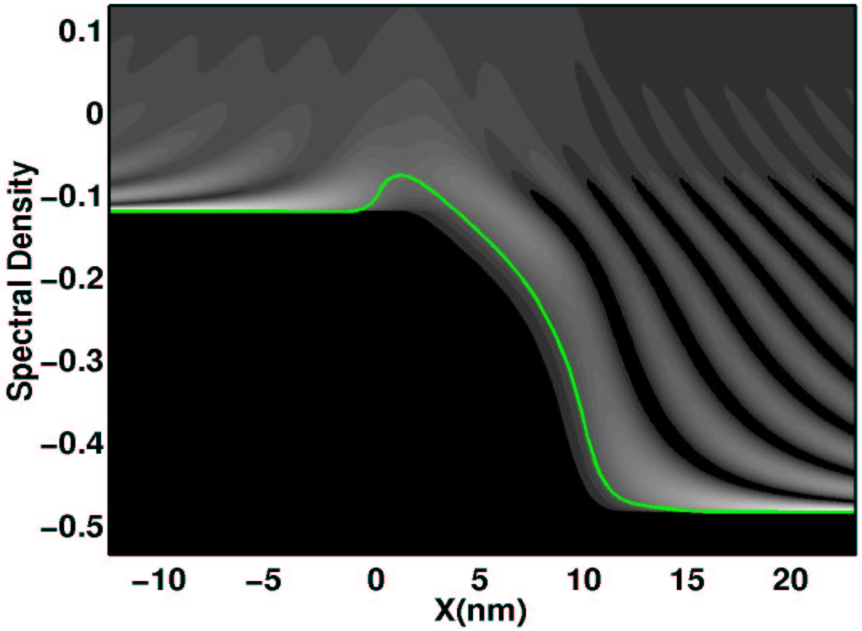
- The phase breaking model exhibits no critical scattering region. Scattering occurring in the entire channel equally affects device performance.

- The energy relaxing model exhibits a critical scattering region wherein scattering strongly affects device performance (Captures the Essential Physics).

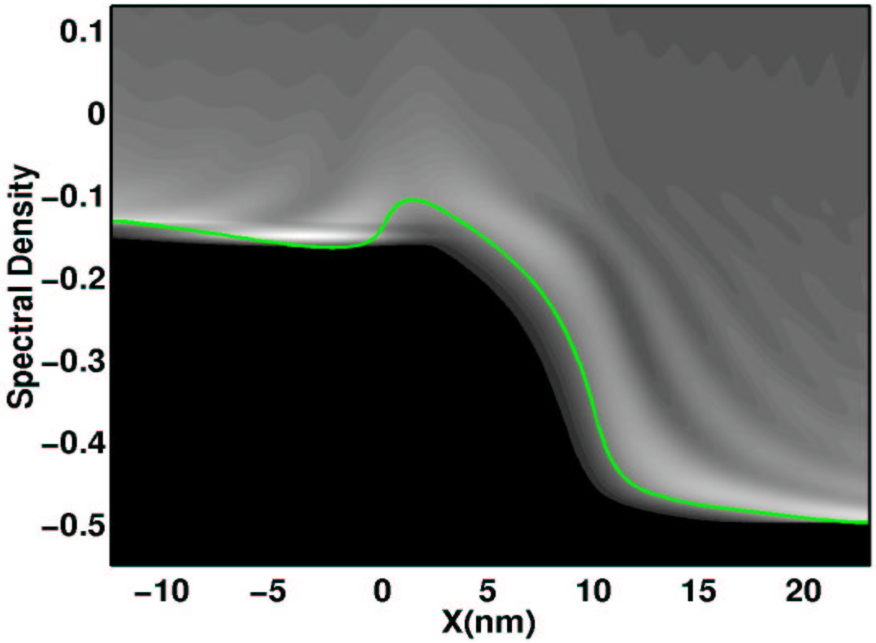
Scattering

Coherent vs. Incoherent Transport

Ballistic (on-state), 1.5 nm body



Scattering everywhere, 1.5 nm body



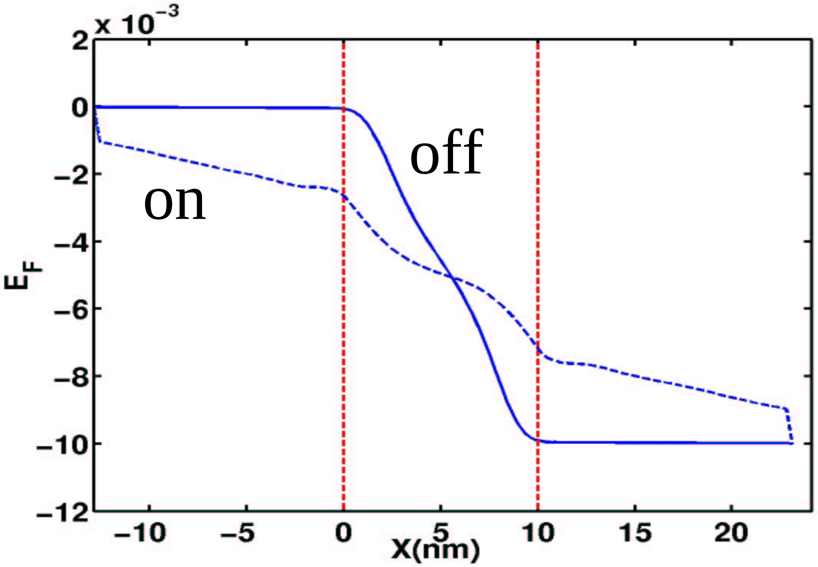
- Coherent oscillations in the Local Density of States is washed out due to scattering

- The probe self-energy cuts off below the band edge and there is very little increase in tunneling current due to scattering

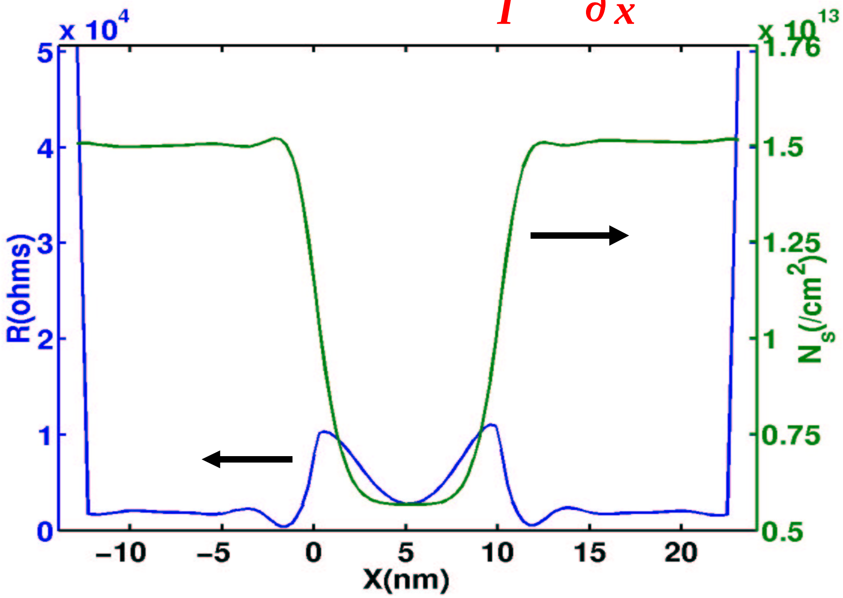
Scattering

Potential Drop and Resistance

10mV drain bias 1.5 nm body



$$R(\Omega / sq) = \frac{1}{I}\frac{\partial F_{Probe}}{\partial x}$$



- The total resistance is the area under the resistance/square curve
- There are five components to the overall intrinsic device resistance: Source, Drain, Tip, Channel and the Quantum Contact resistance
- In short channel MOSFETs, the tip resistance dominates the overall resistance, although the junctions are abrupt

Summary

- The Mode Space approach is a computationally efficient and accurate method for simulating quantum transport
- The decoupled Mode Space method is limited to simulating transport in uniform SOI geometries
- When coupled with a Büttiker probe based scattering model, the Mode Space solution clearly captures the essential physics of scattering including Fermi degeneracy effects
- This tool can be used to examine design issues which affect the performance of nanoscale transistors operating in the quasi ballistic limit