From Quantum Theory to Nanodevices

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This talk is based on our following papers

J. P. Sun, G. I. Haddad, P. Mazumder and J. Schulman, "Resonant Tunneling Diodes: Device and Modeling," ***Proceedings of the IEEE,*** Apr. 1998, pp. 641-663.

S. Mohan, J.P. Sun, P. Mazumder and G. I. Haddad, "Device and Circuit Models for Resonant Tunneling Devices for Circuit Simulation," ***IEEE Transactions on Computer-Aided Design of Integrated Circuits and Systems,*** Vol. 140, No. 6, June 1995, pp. 653-662.

P. Mazumder, J.P. Sun, S. Mohan and G.I. Haddad, "DC and Transient Simulation of Resonant Tunneling Devices in NDR-SPICE," ***Institute of Physics, No. 141,*** Sept. 1994, pp. 867-872.

J. P. Sun, W. Wang, N. Gu and P. Mazumder, "Gate Current and Capacitance Models of Nanoscale MOSFETs," ***IEEE Transactions on Electron Devices. vol. ED-53, no. 12,*** Dec.2006, pp. 2950-57.

W. Wang, N. Gu, J.P. Sun, and P. Mazumder, "Gate Current Modeling of High-*k* *S*tack Nanoscale MOSFETs," ***Solid-State Electronics,*** vol. 50, pp. 1489-94, Oct. 2006.

Outline

- The ITRS Look into Future
  (International Technology Roadmap for Semiconductors)
- Hierarchy of Mesoscopic Transport
- NanoMOS Device Modeling
  - **Gate Leakage Current**
  - **Engineering High-*k* stack Gate Dielectric**
  - **Other Leakage Components**

The ITRS Look into Future

- The goal is to push Moore's Law beyond the physical limits of current microchip technology
- The laws of physics will eventually limit the implementation of CMOS scaling technology
- Worldwide race for discovering new technologies that will sustain the pace of technology advancement occurred over the past 40 years
- The SIA (Semiconductor Industry Association) has launched Nanoelectronics Research Initiative for sub-10 nanometer technologies

The roadmap into the future 2018

Year	2003	2004	2005	2006	2007
Feature size (nm)	100	90	80	70	65
DRAM	4G	4G	8G	8G	16G
	2008	2009	2010	2015	2018
Feature size (nm)	57	50	45	25	18
DRAM	16G	16G	32G	64G	128G

Drift-Diffusion Models

Particle continuity equations

$$\frac{\partial n}{\partial t} = \frac{1}{q}\nabla \cdot J_n + G_n - R_n \quad (1)$$

$$\frac{\partial p}{\partial t} = -\frac{1}{q}\nabla \cdot J_p + G_p - R_p \quad (2)$$

Poisson's equation

$$\nabla \cdot E = \frac{q}{\varepsilon}(p - n + N_D - N_A) \quad (3)$$

Total current conservation (4)

$$\nabla \cdot (J_n + J_p + \varepsilon \frac{\partial E}{\partial t}) = 0$$

where (the drift-diffusion equations) (5) (6)

$$J_n = -qnV_n(E) + q\nabla(D_n(E)n)$$

$$J_p = qnV_p(E) - q\nabla(D_p(E)p)$$

2-Dimensional MOS Model

$$\varepsilon_S \Delta\psi = q\,(\,n - p - N_B\,)$$

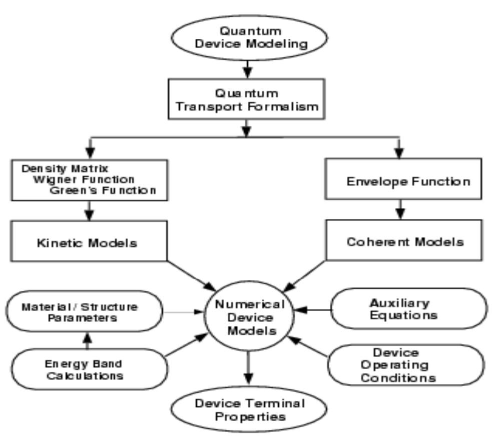
$$\frac{\partial n}{\partial t} = \nabla\cdot\left\{D\,e^{U}\,\nabla\left(e^{-U}\,n\right)\right\} - \frac{np - n_{i0}^{2}}{\tau_p\,(\,n + n_{i0}\,) + \tau_n\,(\,p + n_{i0}\,)} + \frac{1}{q}\left(\alpha_n\left|\boldsymbol{J}_n\right| + \alpha_p\left|\boldsymbol{J}_p\right|\right)$$

$$\frac{\partial p}{\partial t} = \nabla\cdot\left\{D\,e^{-U}\,\nabla\left(e^{U}\,p\right)\right\} - \frac{np - n_{i0}^{2}}{\tau_p\,(\,n + n_{i0}\,) + \tau_n\,(\,p + n_{i0}\,)} + \frac{1}{q}\left(\alpha_n\left|\boldsymbol{J}_n\right| + \alpha_p\left|\boldsymbol{J}_p\right|\right)$$

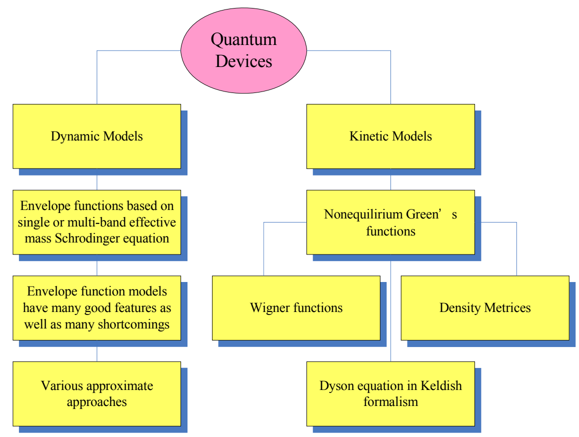
$$J_n = \;q\,D_n\,e^{U}\,\nabla\left(e^{-U}\,n\right)$$

$$J_p = \;-\,q\,D_p\,e^{-U}\,\nabla\left(e^{U}\,p\right)$$

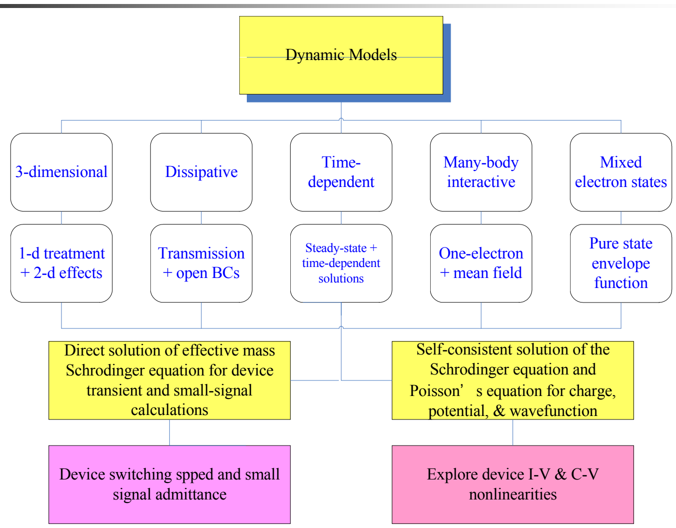
Elements of Device Modeling



Hierarchy of Mesoscopic Transport



Framework of Dynamic Models



Formulation of Nonequilibrium Green's Functions (NEGF)-1

$$G(E) = [EI - [h(x,z) + E_{k_j} I]]^{-1} = [E(k_x,k_z)I - h(x,z)]^{-1}$$

$$G[E(k_x,k_z)] = [E(k_x,k_z)I - h(x,z) - \Sigma_S - \Sigma_D]^{-1}$$

$$h(x,z) = \begin{bmatrix} \alpha_0 & \beta & 0 & \cdots & \cdots \\ \beta & \alpha_1 & \ddots & 0 & \cdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \cdots & 0 & \ddots & \alpha_{N_X} & \beta \\ \cdots & \cdots & 0 & \beta & \alpha_{N_{X+1}} \end{bmatrix}$$

$$\alpha[x] = \begin{bmatrix} 2t_x + 2t_z - qV_1(x) & -t_z & 0 & \cdots & \cdots \\ -t_z & 2t_x + 2t_z - qV_2(x) & \ddots & \cdots & \cdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \cdots & 0 & \ddots & 2t_x + 2t_z - qV_{N_Z-1}(x) & -t_z \\ \cdots & \cdots & 0 & -t_z & 2t_x + 2t_z - qV_{N_Z}(x) \end{bmatrix}$$

Formulation of Nonequilibrium Green's Functions (NEGF)-2

$$\beta = \begin{bmatrix} -t_x & 0 & \cdots & \cdots \\ 0 & -t_x & \cdots & \cdots \\ 0 & 0 & \ddots & \cdots \\ \cdots & \cdots & 0 & -t_x \end{bmatrix} \qquad t_x = \frac{\hbar^2}{2m_x^* a^2} \qquad t_z = \frac{\hbar^2}{2m_z^* b^2}$$

$$\Gamma \equiv i(\Sigma - \Sigma^+) \qquad A_S = G\Gamma_S G^+ \qquad A_D = G\Gamma_D G^+$$

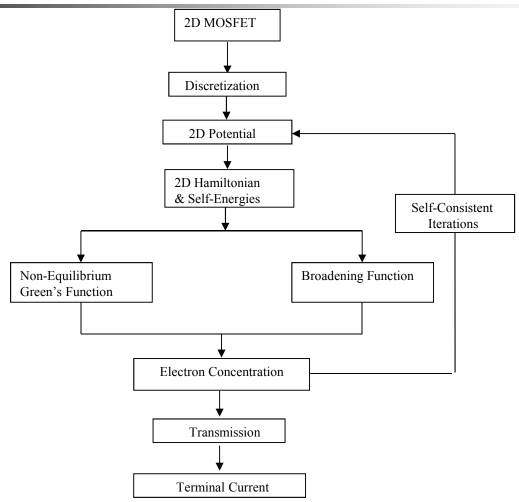
$$n[E(k_x,k_z)] = \frac{1}{2\pi ab}\int_0^{+\infty} D \cdot [f(\mu_S, E(k_x,k_z) + E_{k_j})A_S + f(\mu_D, E(k_x,k_z) + E_{k_j})A_D]dE_{k_j}$$

$$n[E(k_x,k_z)] = \frac{1}{ab}\sqrt{\frac{m_y^* k_B T}{2\pi^3\hbar^2}}[F_{-1/2}(\mu_S - E(k_x,k_z))A_S + F_{-1/2}(\mu_D - E(k_x,k_z))A_D]$$

$$T_{SD} = Trace[\Gamma_S G \Gamma_D G^+]$$

$$I[E(k_x,k_z)] = \frac{q}{\hbar^2}\sqrt{\frac{m_y^* k_B T}{2\pi^3}}[F_{-1/2}(\mu_S - E(k_x,k_z)) - F_{-1/2}(\mu_D - E(k_x,k_z))]T_{SD}[E(k_x,k_z)]$$

2-D Modeling of MOSFETs Using NEGF



Process of Quantum Transport in RTD

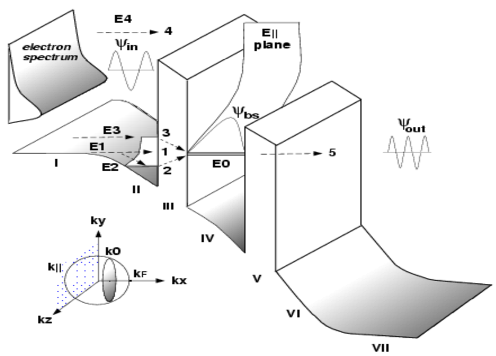


Figure 1: Processes in double-barrier tunneling

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Transmission

Transmission Calculation

(1) **The Schrödinger equation**

$$\frac{-\hbar^2}{2}\frac{\partial}{\partial x}\left[\frac{1}{m^*(x)}\frac{\partial\psi(x)}{\partial x}\right] - (E - V(x))\psi(x) = 0 \qquad (1)$$

is discretized as

$$\psi_{i+1} = \left(\frac{2m_i^*\Delta x^2(V_i - E)}{\hbar^2} + 1 + \frac{m_i^*}{m_{i-1}^*}\right)\psi_i - \frac{m_i^*}{m_{i-1}^*}\psi_{i-1}$$

$$\psi_{i-1} = \left(\frac{2m_{i-1}^*\Delta x^2(V_i - E)}{\hbar^2} + 1 + \frac{m_{i-1}^*}{m_i^*}\right)\psi_i - \frac{m_{i-1}^*}{m_i^*}\psi_{i+1}$$

with the open boudary conditions discussed previously.

(2) **Transmission coefficient**

$$TT^* = \frac{|C|^2 k_r}{|A|^2 k_l}$$

(3) **Probability current density**

From the principle of particle continuity,

$$J(x) = -q\hbar\, Im\left[\psi^*(x)\frac{1}{m^*(x)}\frac{\partial\psi(x)}{\partial x}\right]$$

and discretized as

$$J_i = -q\hbar\, Im\left[\frac{\psi_i^*}{2}\left(\frac{1}{m_i^*}\frac{\psi_{i+1} - \psi_i}{\Delta x} + \frac{1}{m_{i-1}^*}\frac{\psi_i - \psi_{i-1}}{\Delta x}\right)\right]$$

Wigner Function 1

Wigner Function Models

(1) **Density matrix**

$$\rho(x, x'; t) = \sum_j A_j\psi_j(x; t)\psi_j^*(x'; t) \qquad (1)$$

Its time-evolution (Liouville-von Neumann equation)

$$i\hbar\frac{\partial\rho}{\partial t} = [H, \rho] = L\rho \qquad (2)$$

where L is the Liouville superoprator.

(2) **Wigner distribution function**

Taking the Fourier transform ⇒ the Wigner function

$$f(x, k, t) = \frac{1}{\pi}\int_{-\infty}^{\infty} dy\, \psi^*(x + y; t)\psi(x - y; t)e^{2iky} \qquad (3)$$

The time evolution of the Wigner function

$$\begin{aligned}\frac{\partial f(x,k)}{\partial t} &= \frac{-\hbar k}{m^*}\frac{\partial f(x,k)}{\partial x} + \left(\frac{\partial f(x,k)}{\partial t}\right)_C \\ &\quad -\frac{1}{2\pi\hbar}\int_{-\infty}^{\infty} dk'\left\{2\int_0^{\infty} dy\, Sin([k - k']y)\left[V\left(x + \frac{y}{2}\right) - V\left(x - \frac{y}{2}\right)\right]\right\} f(x, k') \\ &= \frac{-\hbar k}{m^*}\frac{\partial f}{\partial x} + \sum_{\lambda_{odd}}\frac{1}{\lambda!}\frac{\partial^\lambda v(x)}{\partial x^\lambda}\left(\frac{\hbar}{2i}\right)^{\lambda-1}\frac{\partial^\lambda f}{\partial p^\lambda} \qquad (4)\end{aligned}$$

in the classical limit ⇒

$$\begin{aligned}\frac{\partial f}{\partial t} &= \frac{-\hbar k}{m^*}\frac{\partial f}{\partial x} + \frac{\partial v}{\partial x}\frac{\partial f}{\partial p} \\ &= -v\frac{\partial f}{\partial x} - F\frac{\partial f}{\partial p} \qquad (5)\end{aligned}$$

The device is assumed to obey kinetic equation

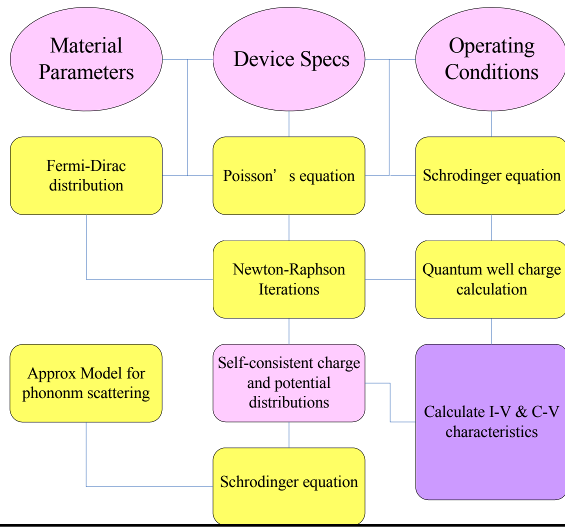
$$\frac{\partial f}{\partial t} = \frac{L}{i\hbar}f + Cf \qquad (6)$$

where C is the collision superoperator

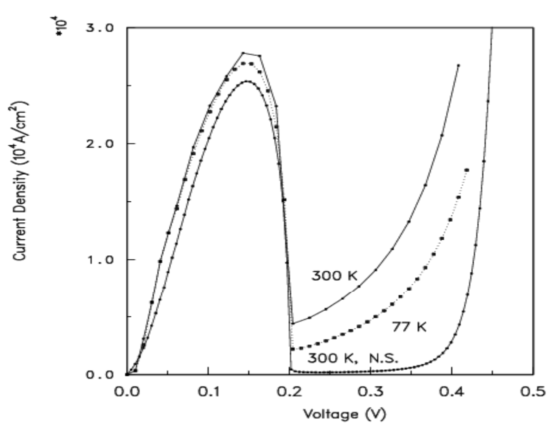
$$C\, f(x, k, t) = \int dk'\, [W_{kk'}f(x, k', t) - W_{k'k}f(x, k, t)] \qquad (7)$$

where $W_{kk'}$ is the transition rate from k' to k, etc.

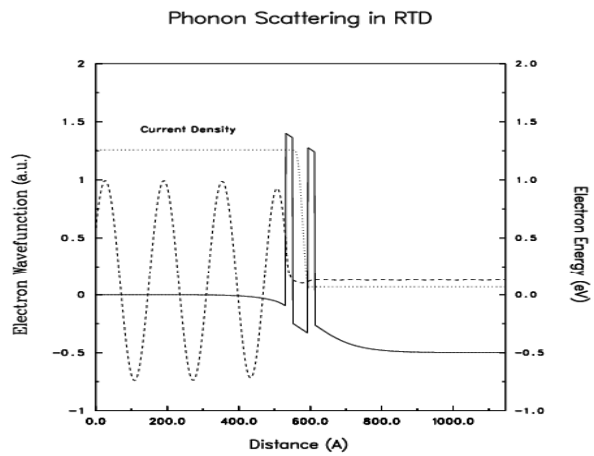
A Typical Envelope Function Model



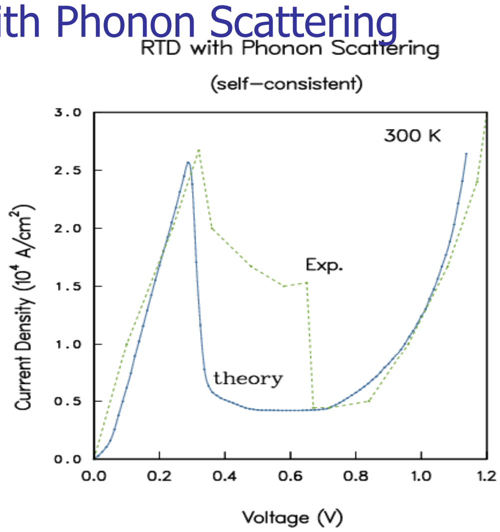
RTD w/o Phonon Scattering



Phonon Scattering in RTD



RTD with Phonon Scattering



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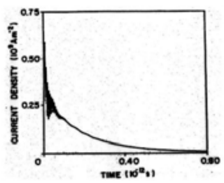
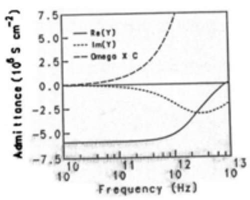
TIME-DEPENDENT MODELS

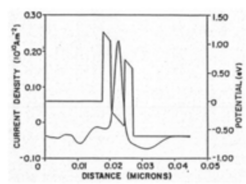
Time-dependent Model

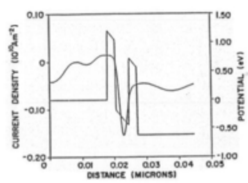
switching transients



small signal response







current density distribution

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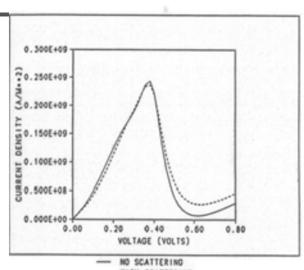
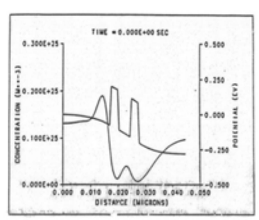
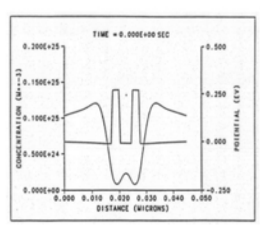
QUANTUM KINETIC MODELS
(Wigner Function Models)

Wigner Function 2



Static I-V curve at room temperature calculated for an $In_{0.53}Ga_{0.47}As$ -AlAs structure using the Wigner function, both with and without phonon scattering.





Var1

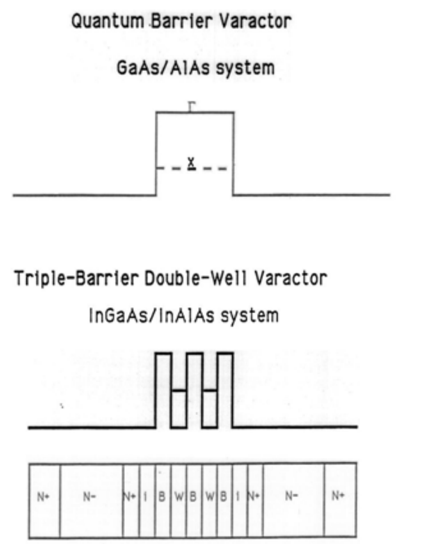


Figure : Conduction band profiles of the quantum barrier varactor and the TBDW varactor. Also shown is the layered structureof the TBDW varactor.

Var2

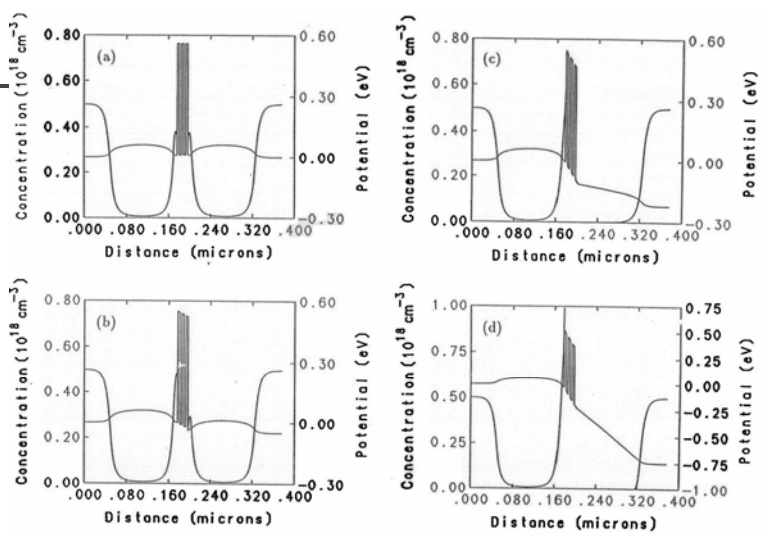


Figure : Charge and potential distributions of the TBDW varactor under (a) 0, (b) 0.05, (c) 0.2, and (d) 0.75 V bias voltages.

Var3

STEADY-STATE MODELS

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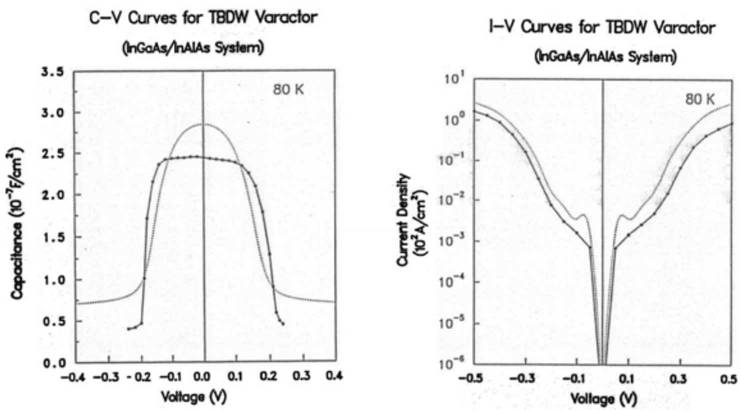
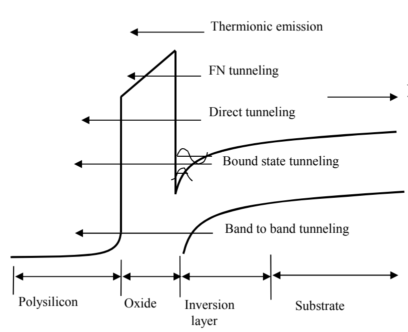
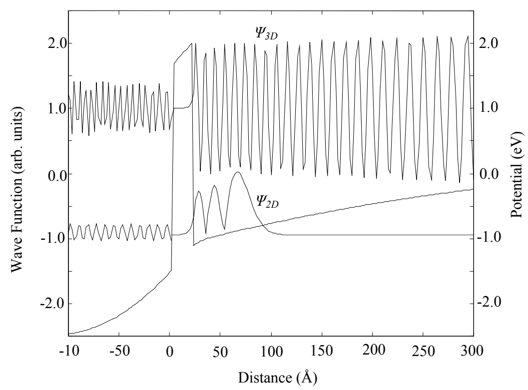


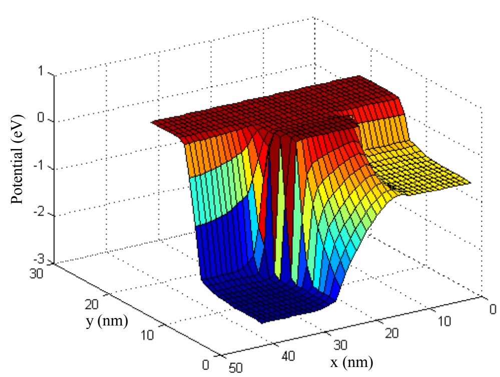
Application to Gate Leakage Model



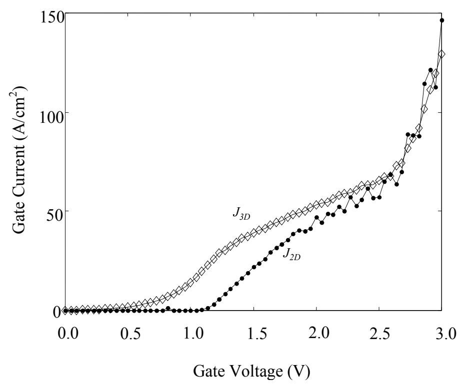
Electron Wave Function and Potential



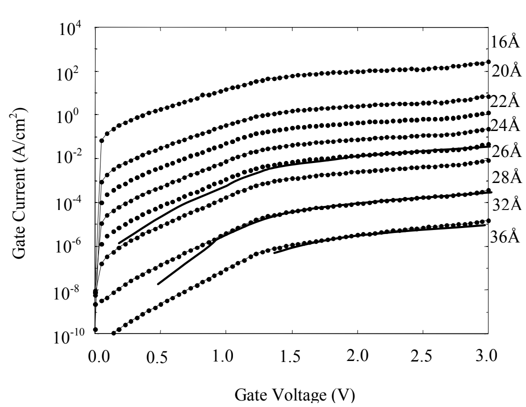
2-Dimensional Potential



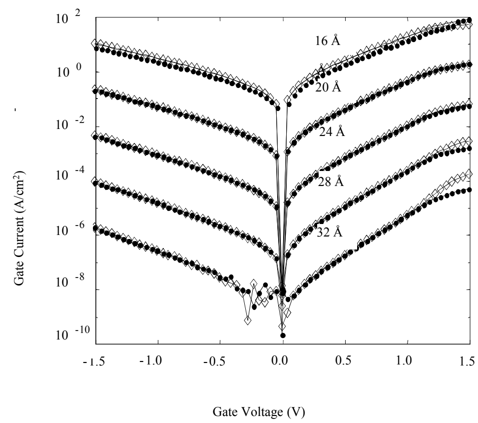
2-D and 3-D Gate Current Components



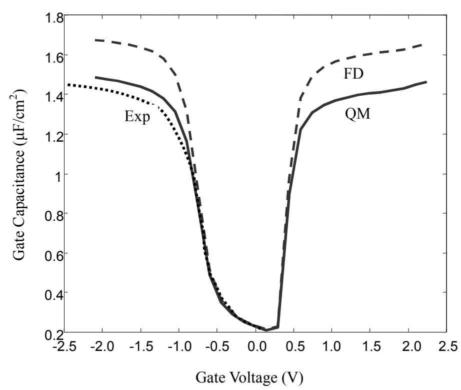
Gate Current for Different Oxide Thickness Agreeable with Experiment



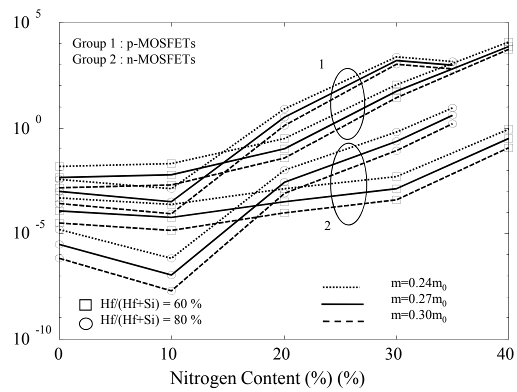
Models of Schrodinger-Poisson and WKB Approaches



NanoMos Gate Capacitance

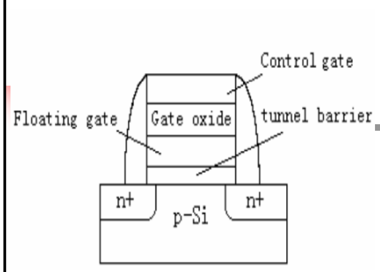


Engineering High-k Stack Gate Dielectric - Finding Optimum Nitrogen Incorporation

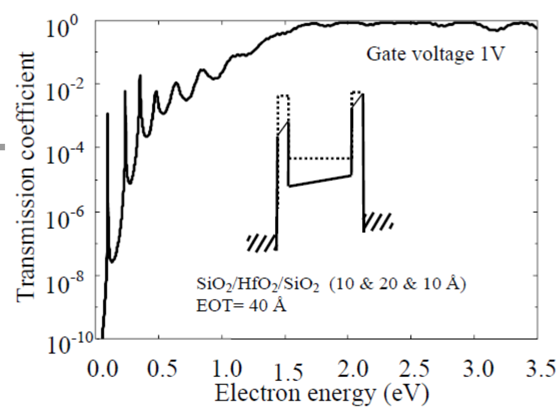


Modeling of High-k Gate Stack of Tunnel Barrier in Nonvolatile Memory MOS Structures

By Mazumder, Sun, Wang and Gu
IEEE Nano Conference, Dallas 2008



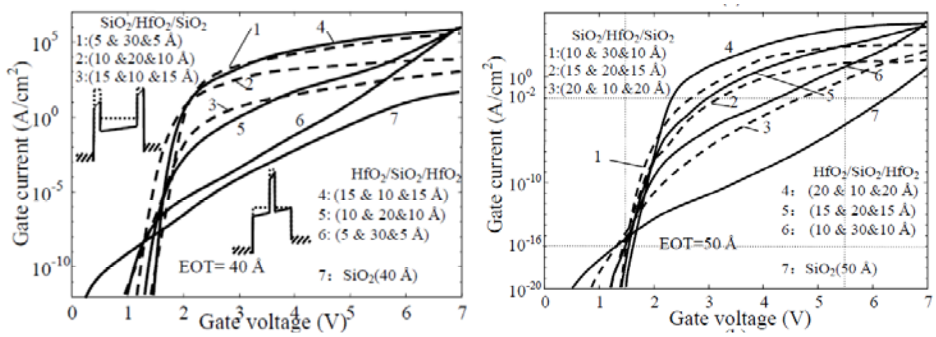
Cross section of a nonvolatile flash memory cell



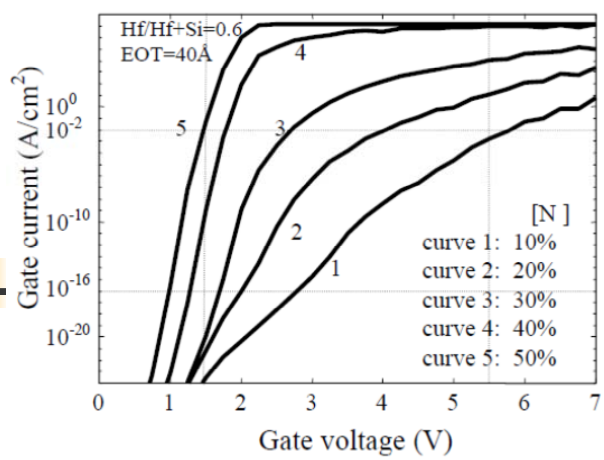
Transmission coefficients for SiO2/HfO2/SiO2 gate stack with the EOT of 4 nm, as function of energy.

Professor Pinaki Mazumder

EOT = 4 nm **EOT = 5 nm**



Calculated gate current vs. gate voltage with different physical thickness of the high-k dielectric with the same EOT (4 nm or 5 nm) for SiO2/HfO2/SiO2 or HfO2/SiO2/HfO2 gate stack structures. The electron barrier height, effective mass, and dielectric constant for HfO2 are 1.50 eV, 0.10 m0, and 25, respectively. The electron barrier height, effective mass, and dielectric constant for SiO2 are 3.15 eV, 0.50 m0, and 3.9.



Tunneling current through HfSiON dielectric films for different N contents with Hf/(Hf+Si) = 0.6.

The EOT is 4 nm for all the calculations and the electron effective mass is taken to be 0.27 m0.

Flash Memory Design Tradeoffs

Good engineering of the Nitrogen content can satisfy both the requirements for the program/erase current and the retention current.

The tunneling current satisfies the requirement of Retention Current, I_{ret} < 10E-16 A/cm^2 for the Nitrogen content of 10%, 20%, and 30%.

The tunneling current satisfies the requirement of Programming/Erase Current, I_{prog} > 0.1 A/cm^2 for the cases with the Nitrogen content of 20%, 30%, 40%, and 50%, respectively.

**The tunneling current increases with increasing nitrogen content.
If the nitrogen content to fall into 20%-30% range, it will satisfy both the basic requirements for programming and data retention.**

The interplay of the barrier height and dielectric constant in the high-k dielectric due to N-incorporation and control may enable us to obtain favorable device parameters.

Professor Pinaki Mazumder

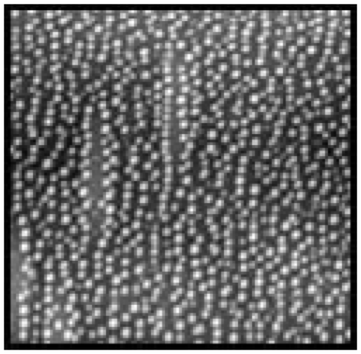
Modeling of I-V in 3-D Confined Quantum Structures

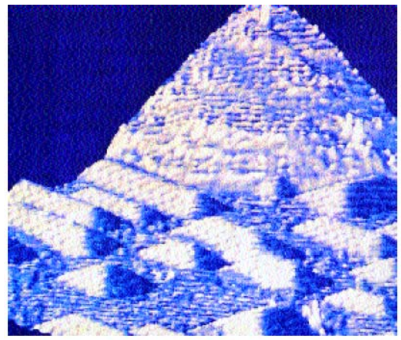
Prof. Pinaki Mazumder

GSRA: Dan Shi

Presented at: National Nanotechnology Initiative Workshop
And at Intl. Cellular Neural Networks Workshop

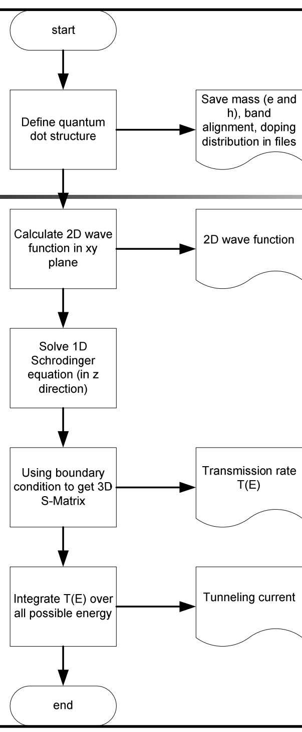
Formation of 3-D quantum structures





Stranski-Krastanov growth (Strained InGaAs on GaAs)

*Stephen Goodnick , Department of Electrical Engineering, Arizon State University



$$-\frac{\hbar^2}{2m^*}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}\right)\varphi_\gamma(x,y\,|\,z)+V_{LC}(x,y,z)\varphi_\gamma(x,y\,|\,z)=E_\gamma\varphi_\gamma(x,y\,|\,z)$$

$$-\frac{d^2}{dz^2}\chi_\gamma(z)+k_\gamma^2(z)\chi_\gamma(z)+\sum_{\gamma'}\left(2C_{\gamma,\gamma'}^{(0,1)}(z)\frac{d}{dz}\chi_{\gamma'}(z)+C_{\gamma,\gamma'}^{(0,1)}(z)\chi_{\gamma'}(z)\right)=0$$

$k_\gamma(z)$:complex wavenumber

$C_{\gamma,\gamma'}^{(0,1)}(z), C_{\gamma,\gamma'}^{(0,2)}(z$: mode mixing coefficients

$$\Psi(x,y,z)=\sum_\gamma \varphi_\gamma(x,y\,|\,z)\chi_\gamma(z)$$

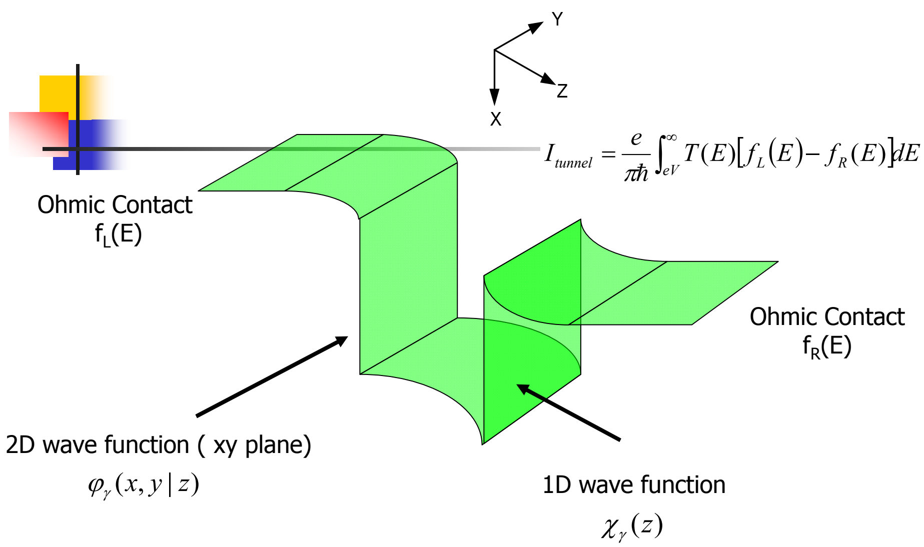
Transfer Matrix $T=T^{(N)}\cdot T^{(N-1)}\cdots T^{(2)}\cdot T^{(1)}$

⇩

Scattering Matrix S

⇩

$$I_{tunnel}=\frac{e}{\pi\hbar}\int_{eV}^{\infty}T(E)\left[f_L(E)-f_R(E)\right]dE$$



$$\Psi(x,y,z) = \sum_\gamma \varphi_\gamma(x,y \mid z)\chi_\gamma(z)$$

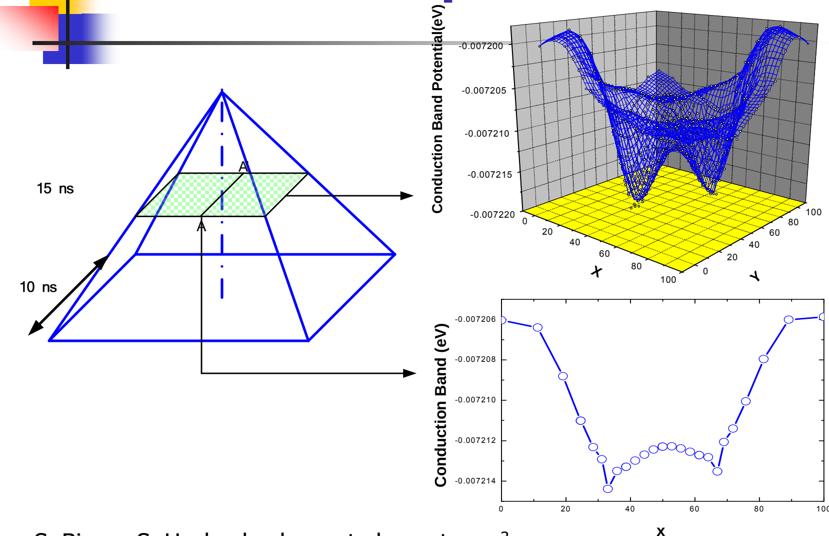
3-D to 2-D Schrodinger equation

$$-\frac{\hbar^2}{2m^*}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right)\Psi(x,y,z) + V(x,y,z)\Psi(x,y,z) = E\Psi(x,y,z)$$

$$\Psi(x,y,z) = \sum_\gamma \varphi_\gamma(x,y \mid z)\chi_\gamma(z)$$

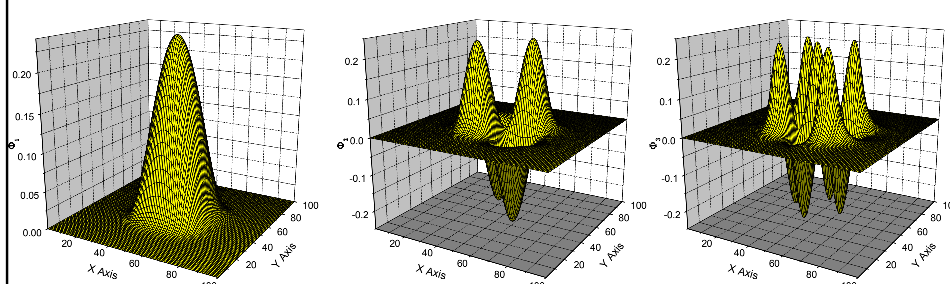
$$-\frac{\hbar^2}{2m^*}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right)\varphi_\gamma(x,y \mid z) + V_{confinement}(x,y,z)\varphi_\gamma(x,y \mid z) = \varepsilon_\gamma \varphi_\gamma(x,y \mid z)$$

Band structure of a 3-D confined quantum device



S. Birner, S. Hackenbuchner et al., nextnano[3]

2-D wave functions



Eigen energy

5.416×10^{-3}eV 2.151×10^{-2}eV 4.773×10^{-2}eV

1-D Schrodinger Equation

$$\frac{d^2}{dz^2}\chi_\gamma(z)+k_\gamma^{\,2}(z)\chi_\gamma(z)+\sum_{\gamma'}\left[2C^{(0,1)}_{\gamma,\gamma'}(z)\frac{d}{dz}\chi_{\gamma'}(z)+C^{(0,2)}_{\gamma,\gamma'}(z)\chi_{\gamma'}(z)-\frac{2m^*}{\hbar^2}V^{irregular}_{\gamma\gamma'}(z)\chi_{\gamma'}(z)\right]=0$$

$$k_\gamma(z)=\sqrt{2m^*\left[E-\varepsilon_\gamma(z)-V_{affinity}(x,y,z)\right]}/\hbar$$

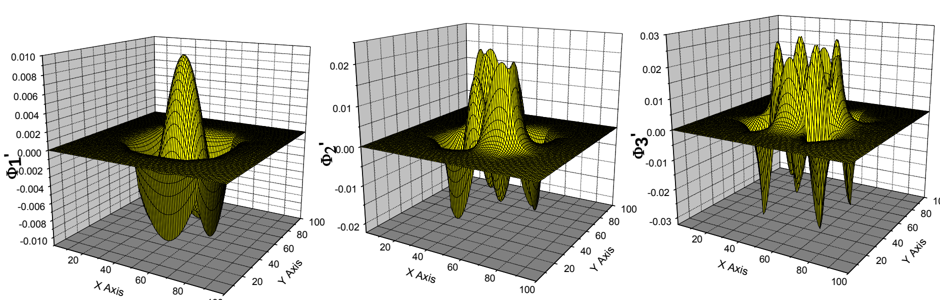
$$V^{irregular}_{\gamma\gamma'}(z)=\iint\varphi_\gamma^{\ *}(x,y\,|\,z)V_{irregular}(x,y,z)\varphi_{\gamma'}(x,y\,|\,z)dxdy$$

Mode mixing coefficients

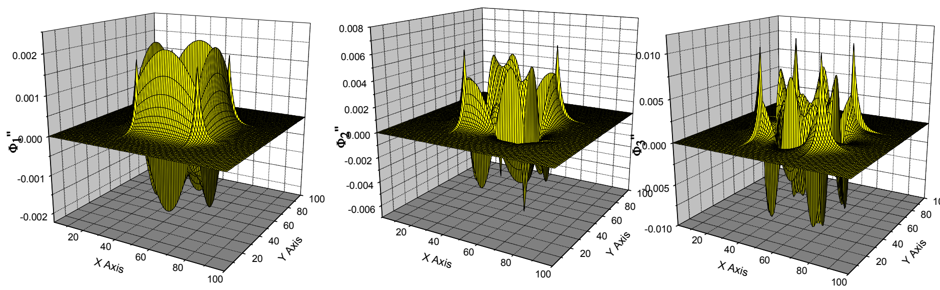
$$C^{(0,1)}_{\gamma,\gamma'}(z)=\iint\varphi_\gamma^{\ *}(x,y\,|\,z)\frac{\partial}{\partial z}\varphi_{\gamma'}(x,y\,|\,z)dxdy$$

$$C^{(0,2)}_{\gamma,\gamma'}(z)=\iint\varphi_\gamma^{\ *}(x,y\,|\,z)\frac{\partial^2}{\partial z^2}\varphi_{\gamma'}(x,y\,|\,z)dxdy$$

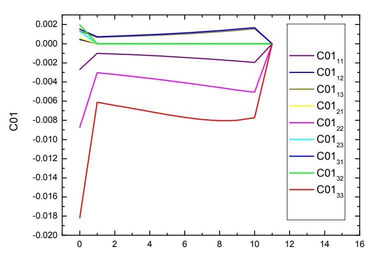
First order derivative of φ

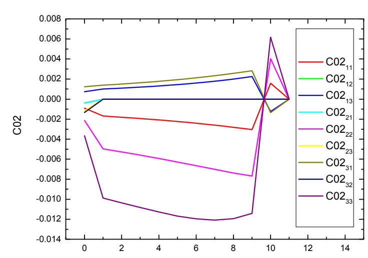


Second order derivative of φ



Mode mixing coefficients





Simplified 1-D Schrodinger Equation

$$\chi_\gamma = M_{\gamma,\gamma'}(z) f_{\gamma'}(z)$$

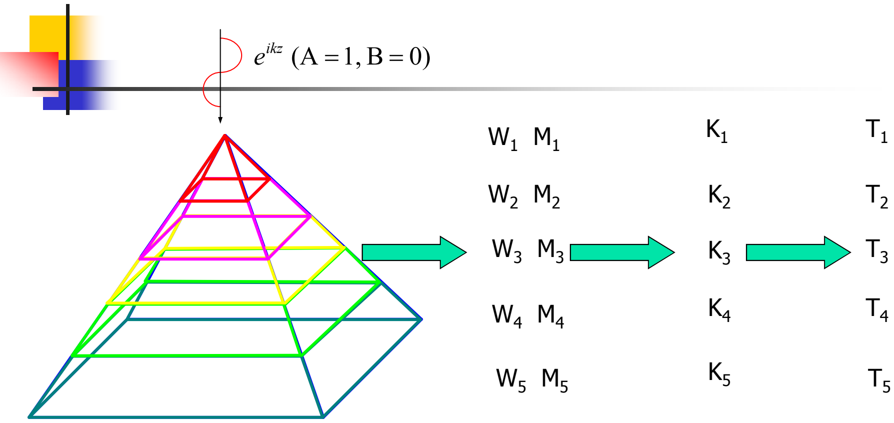
where $M_{\gamma,\gamma'}(z) = \exp\left[-\int_0^z C^{(0,2)}_{\gamma,\gamma'}(z')dz'\right]$

$$\frac{d^2 f_\gamma(z)}{dz^2} = -\sum_{\gamma'} \varpi_{\gamma,\gamma'}(z) f_{\gamma'}(z)$$

where

$$\varpi_{\gamma,\gamma'}(z) = \sum_{\gamma''}\sum_{\gamma'''} M_{\gamma,\gamma''}{}^{-1}(z) W_{\gamma'',\gamma'''}(z) M_{\gamma''',\gamma'}(z)$$

$$W_{\gamma'',\gamma'''}(z) = k_{\gamma''}{}^{2}\delta_{\gamma'',\gamma'''} - \left\{C^{(0,1)}(z)\right\}^2_{\gamma'',\gamma'''} - C^{(1,1)}_{\gamma'',\gamma'''}(z) - \frac{2m^*}{\hbar^2} V^{irregular}_{\gamma''\gamma'''}(z)$$



$$\chi(Z) = Ae^{iKz} + Be^{-ikz}$$

$$\begin{pmatrix} A^{i+1}_{\gamma} \\ B^{i+1}_{\gamma} \end{pmatrix} = T^{(i)}(\gamma,\gamma') \begin{pmatrix} A^{i}_{\gamma'} \\ B^{i}_{\gamma'} \end{pmatrix}$$

Boundary Condtions

$$\Psi^{(i)}(x,y,z_{i+1}) = \Psi^{(i+1)}(x,y,z_{i+1})$$

$$\frac{1}{m^*}\frac{\partial}{\partial z}\Psi^{(i)}(x,y,z)\,|_{z=z_{i+1}} = \frac{1}{m^*}\frac{\partial}{\partial z}\Psi^{(i+1)}(x,y,z)\,|_{z=z_{i+1}}$$

$$\begin{pmatrix} A_\gamma^{i+1} \\ B_\gamma^{i+1} \end{pmatrix} = T^{(i)}(\gamma,\gamma')\begin{pmatrix} A_{\gamma'}^{i} \\ B_{\gamma'}^{i} \end{pmatrix}$$

where $$T^{(i)}(\gamma,\gamma') = \begin{pmatrix} \alpha_+^{(i)}(\gamma,\gamma')e^{j(K_{\gamma'}^{(i)}-K_\gamma^{(i+1)})z_{i+1}} & \alpha_-^{(i)}(\gamma,\gamma')e^{-j(K_{\gamma'}^{(i)}+K_\gamma^{(i+1)})z_{i+1}} \\ \alpha_-^{(i)}(\gamma,\gamma')e^{j(K_{\gamma'}^{(i)}+K_\gamma^{(i+1)})z_{i+1}} & \alpha_+^{(i)}(\gamma,\gamma')e^{-j(K_{\gamma'}^{(i)}-K_\gamma^{(i+1)})z_{i+1}} \end{pmatrix} \cdot X_{\gamma,\gamma'}^{(i)}$$

$$\alpha_\pm^{(i)}(\gamma,\gamma') = \frac{1}{2}\left(1 \pm \frac{m_{i+1}^*}{m_i^*}\frac{K_{\gamma'}^{(i)}}{K_\gamma^{(i+1)}}\right)$$

$$X_{\gamma,\gamma'}^{(i)} = V_{\gamma_1,\gamma}^{(i+1)} M_{\gamma_2,\gamma_1}^{(i+1)} M_{\gamma_2,\gamma_3}^{(i)} V_{\gamma_3,\gamma'}^{(i)}$$

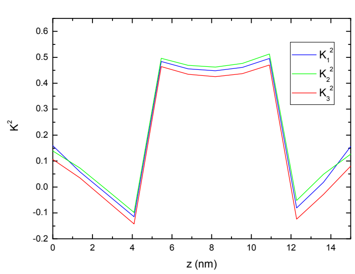
$$\chi_\gamma(z) = \sum_{\gamma'}\sum_{\gamma''} M_{\gamma,\gamma'}(z) V_{\gamma',\gamma''}(z)\left\{A_{\gamma''}(z)e^{jK_{\gamma''}(z)z} + B_{\gamma''}(z)e^{-jK_{\gamma''}(z)z}\right\}$$

$$M = \begin{pmatrix} 1.011 & 0.999 & 0.993 \\ 0.993 & 1.033 & 0.998 \\ 0.993 & 0.998 & 1.067 \end{pmatrix}$$

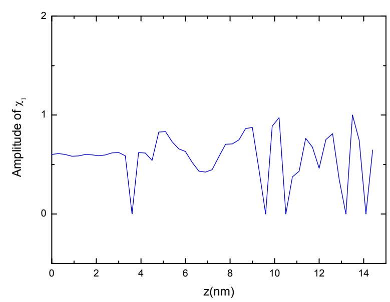
$$W = \begin{pmatrix} 0.462 & 0 & 0.002 \\ 0 & 0.448 & 0 \\ 0.002 & 0 & 0.426 \end{pmatrix}$$

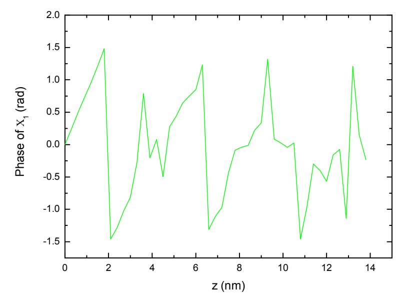
$$V = \begin{pmatrix} 0 & -0.999 & -0.047 \\ -1 & 0 & 0 \\ 0 & -0.047 & 0.999 \end{pmatrix}$$

($eigen$ vector of W)

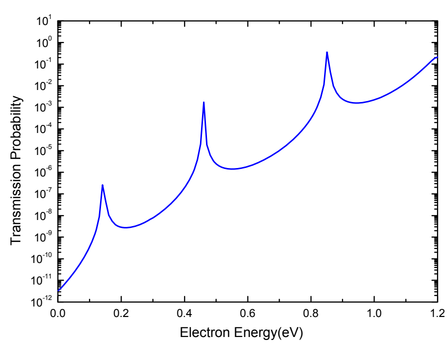


Wave function in z direction

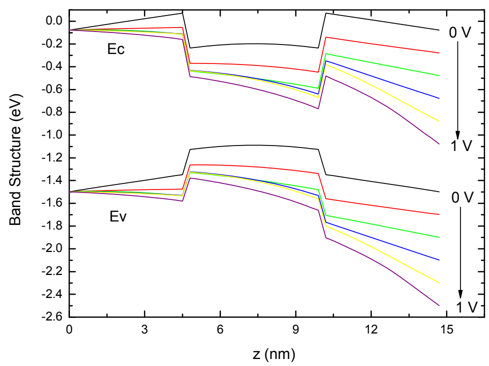




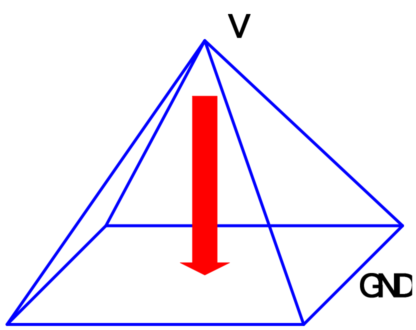
Transmission probability

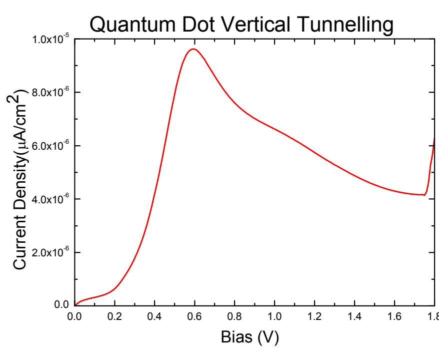


Band structure under different bias conditions

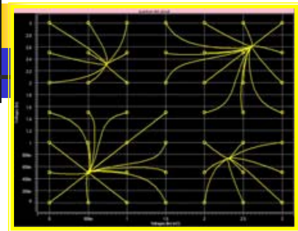


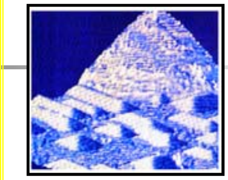
Tunneling current

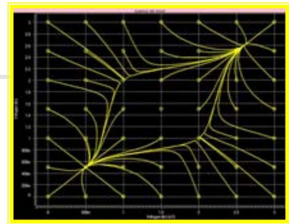




Simulation of Q-device pair

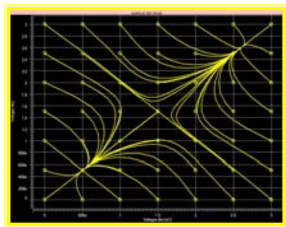


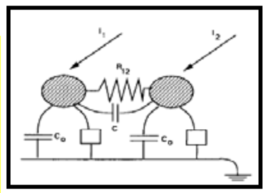


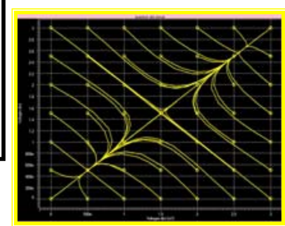


R12=5*R C12=C0

R12=2*R C12=C0







Phasor Diagram

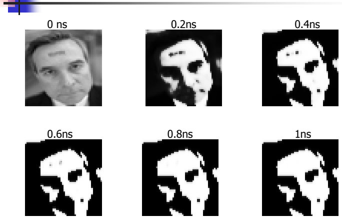
R12=R C12=C0

R12=0.5*R C12=C0

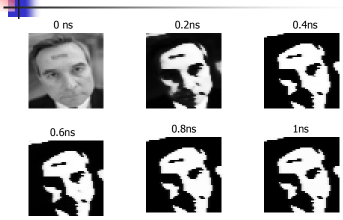
Image processing by 100 x 100 Q-device

Speculation for future quantum systems

Vertical Line Detection



Horizontal Line Detection

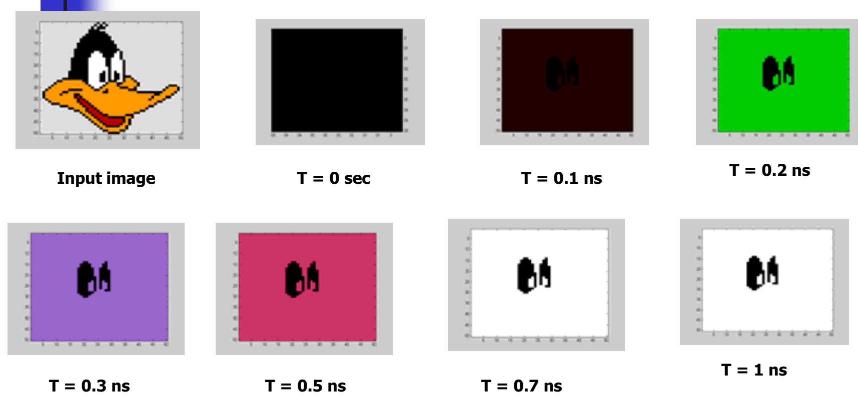


W.H. Lee and P. Mazumder, "Motion Detection by Quantum Dots Based Velocity-Tuned Filter", ***IEEE Transactions on Nanotechnology,*** Vol. 7, No. 3, May 2008, pp. 357-362.

http://web.eecs.umich.edu/~mazum/PAPERS-MAZUM/Nanoarchitectures.pdf

50X50 Q-device with multi quantum wells for color image processing

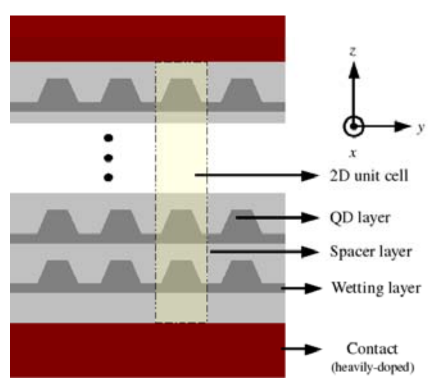
Speculation for future quantum systems



W. H. Lee and P. Mazumder, "Color Image Processing Using Multi-Peak RTD's", ***ACM Journal of Emerging Technologies.*** (to appear)

Theoretical Formulation: Device

- Voltage applied along growth direction does not affect lateral symmetry
- Effective 1D transport model possible
- All stacked layers must share same periodicity



Theoretical Formulation

Manoj Rajagopal and Pinaki Mazumder provided the theoretical Formulation of 3-D confined quantum tunneling in

A MODEL FOR STEADY-STATE, BALLISTIC CHARGE TRANSPORT THROUGH QUANTUM DOT LAYER SUPERLATTICES

MANOJ RAJAGOPALAN *AND PINAKI MAZUMDER*
http://web.eecs.umich.edu/~mazum/PAPERS-MAZUM/quantum%20dot%20modeling.pdf

Previous work (see Reference in above paper):

- **Ko and Inkson**
  - **S-matrix, multilayer aperiodic systems**
- **Xu**
  - **S-matrix, 1D antidot arrays in 2DEG**
- **Mizuta**
  - **S-matrix, isolated quantum dot with resonator structures**
  - **Vertical dot-slicing, mixing coefficients**

Theoretical Formulation: Assumptions and Approximations

- Single particle approximation
- Single-band, effective mass equation
- Abrupt changes in device properties between interior and exterior
- Identical dots in a layer with perfect Bravais lattice 2D layout

Theoretical Formulation: Model

- Contacts
- Spacers
- Quantum Dot Layers
- Inter-region coupling
- Current density per incident phase
- Integration over supplied phases
- Net current per carrier and sum over carriers

Theoretical Formulation: Contact Wave-functions

(incident)

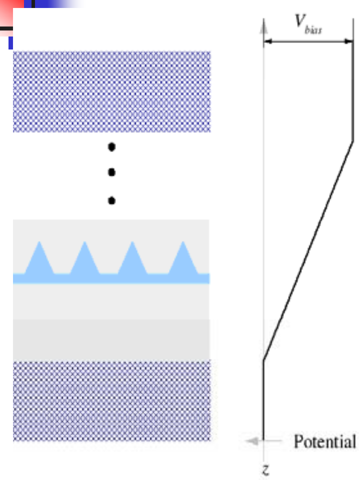
(reflected)

$$\Psi^{(inc)}(\mathbf{r}) = \frac{1}{\sqrt{N_{\parallel}\Omega_{\parallel}}}\left[a^{(inc)}(\mathbf{k}_0)\, e^{i\mathbf{k}_0 \bullet \mathbf{r}} + \iint_{\mathbb{K}_{\parallel}^{(inc)}\left(\frac{\hbar^2 k_{\parallel 0}^2}{2m}\right)} b^{(inc)}(\mathbf{k}_{\parallel};\mathbf{k}_0)\, e^{i\mathbf{k}_{\parallel}\bullet \mathbf{r}_{\parallel}} e^{-i\sqrt{k_0^2-k_{\parallel}^2}z}\, d^2k_{\parallel}\right]$$

Normalization factor for lateral nature

$$\Psi^{(trans)}(\mathbf{r}) = \frac{1}{\sqrt{N_{\parallel}\Omega_{\parallel}}}\iint_{\mathbb{K}_{\parallel}^{(trans)}\left(\frac{\hbar^2 k_{\parallel 0}^2}{2m}+\left(E_b^{(trans)}-E_b^{(recv)}\right)\right)} a^{(trans)}(\mathbf{k}_{\parallel})\, e^{i\sqrt{k_0^2-k_{\parallel}^2}z} e^{i\mathbf{k}_{\parallel}\bullet \mathbf{r}_{\parallel}}\, d^2k_{\parallel}$$

Spacers



- 1D PE variation

$$V(z) = V_0 + V'z$$

  - Airy function nature
- Laterally, PE constant
  - Solutions: planewaves
  - Preserves boundary conditions from contacts

Spacers: Analytical Solutions

TISE:

$$-\frac{\hbar^2}{2m}\frac{d^2}{dz^2}\psi(z) + (V_0 + V'z)\,\psi(z) = E_z\psi(z)$$

Solution: Airy functions

$$\psi(z) = a\,\mathrm{Ai}\left(\sqrt[3]{\frac{2mV'}{\hbar^2}}\left(z - \frac{(E_z - V_0)}{V'}\right)\right) + b\,\mathrm{Bi}\left(\sqrt[3]{\frac{2mV'}{\hbar^2}}\left(z - \frac{(E_z - V_0)}{V'}\right)\right)$$

Coefficients a and b, when determined from boundary conditions, complete the solution

Quantum Dot Layer

- Planar slices along growth direction
  - Thin: piecewise constant properties along z
- Solve 2D TISE
  - Periodic structure: Bloch form of wavefunctions
- Residual 1D effective vector ODE from 3D TISE
  - Mixing coefficients from tapering
- Inter-slice coupling
  - Transfer matrix

Intra-Slice 2D TISE

$$\mathbf{H}_{\|}\phi_{\gamma}\left(\mathbf{r}_{\|};z\right)=\varepsilon_{\gamma}\phi_{\gamma}\left(\mathbf{r}_{\|};z\right), \tag{1.14}$$

$$\mathbf{H}_{\|}=\left[-\frac{\hbar^2}{2}\nabla_{\|}\bullet\left\{\frac{1}{m\left(\mathbf{r}_{\|};z\right)}\nabla_{\|}\right\}+V_{struct}\left(\mathbf{r}_{\|};z\right)\right] \tag{1.15}$$

Material properties are periodic:

$$V_{struct}\left(\mathbf{r}_{\|}+l\mathbf{R}_{\|1}+n\mathbf{R}_{\|2};z\right)\equiv V_{struct}\left(\mathbf{r}_{\|};z\right), \tag{1.51}$$

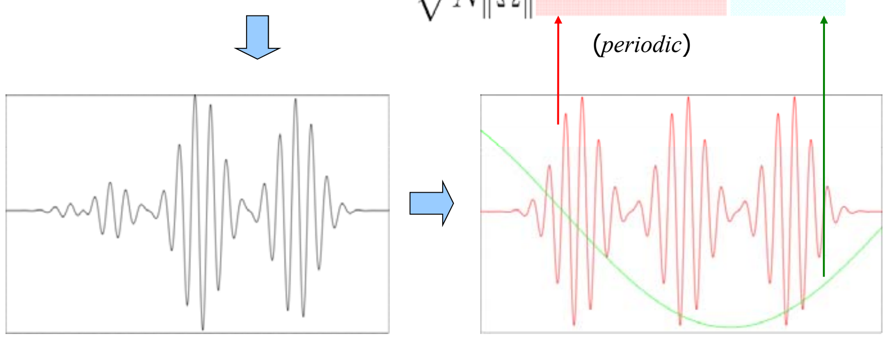
$$m\left(\mathbf{r}_{\|}+l\mathbf{R}_{\|1}+n\mathbf{R}_{\|2};z\right)\equiv m\left(\mathbf{r}_{\|};z\right). \tag{1.52}$$

$$l,n\in\mathbb{Z},\ 0\le z\le L_{N_z}$$

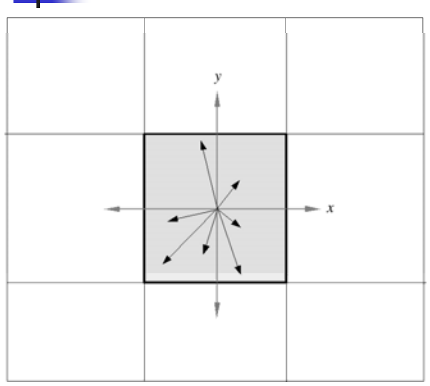
Bloch Form of Eigenfunctions

- Consequence of Bravais-lattice periodicity

$$(1.54)\quad \phi_{m\mathbf{k}_{||}}\left(\mathbf{r}_{||};z\right) = \frac{1}{\sqrt{N_{||}\Omega_{||}}} u_{m\mathbf{k}_{||}}\left(\mathbf{r}_{||};z\right) e^{i\mathbf{k}_{||}\bullet\mathbf{r}_{||}}$$



$k_{||}$ - Space Partitioning



- Lateral wavefunctions are also periodic in $k_{||}$
  - Can only be selected from fundamental unit-cell or **Brillouin Zone**
- For each $k_{||}$ bands of solutions exist, indexed by m
  - 1-1 mapping between bands and tiles

Lateral Wavefunction Properties

- Orthonormality

(1.57)

$$\frac{1}{\Omega_{\|}} \iint_{\Omega_{\|}} u^{*}_{m_1 \mathbf{k}_{\|1}} \left(\mathbf{r}_{\|}; z\right) u_{m_2 \mathbf{k}_{\|2}} \left(\mathbf{r}_{\|}; z\right) d^2 r_{\|} = \delta_{m_1 m_2} \delta \left(\mathbf{k}_{\|1} - \mathbf{k}_{\|2}\right)$$

$$(1.55) \qquad \iint_{\mathbb{R}^2} \left\| \phi_{m\mathbf{k}_{\|}} \left(\mathbf{r}_{\|}; z\right) \right\|^2 d^2 r_{\|} = 1,$$

$$(1.56) \qquad \Rightarrow \frac{1}{\Omega_{\|}} \iint_{\Omega_{\|}} \left\| u_{m\mathbf{k}_{\|}} \left(\mathbf{r}_{\|}; z\right) \right\|^2 d^2 r_{\|} = 1.$$

Lateral Wavefunction Properties

- Completeness
  - Any well-behaved 2D function expressible as a linear combination of these basis functions
  - Also true 3D wavefunction section within slice

$$(1.61) \qquad \Psi\left(\mathbf{r}_{||}; z, E\right) = \sum_{m \in \mathbb{N}} \iint_{\mho_{||}} c_{m\mathbf{k}_{||}} (z; E)\, \phi_{m\mathbf{k}_{||}} \left(\mathbf{r}_{||}; z\right)\, d^2 k_{||}$$

Coefficients that determine solution

Effective 1D Transport

- 3D wavefunction: change of $c_{m\mathbf{k}_{\|}}(\mathbf{r}_{\|};z)$ with z
- Substitute into 3D TISE

$$(1.62)\quad \frac{d}{dz}\frac{1}{m(\mathbf{r}_{\|};z)}\frac{d}{dz}\sum_{m\mathbf{k}_{\|}} c_{m\mathbf{k}_{\|}}(z;E)\,\phi_{m\mathbf{k}_{\|}}(\mathbf{r}_{\|};z) + \frac{2m_e}{\hbar^2}\sum_{m\mathbf{k}_{\|}}\left(E - V_{bias}(z) - \varepsilon_{m\mathbf{k}_{\|}}(z)\right) c_{m\mathbf{k}_{\|}}(z;E)\,\phi_{m\mathbf{k}_{\|}}(\mathbf{r}_{\|};z) = 0.$$

- Distribute d/dz, project onto each basis state

$$(1.64)\quad \frac{d^2}{dz^2}\mathbf{c}(z;E) + \left[\mathbf{P}(z) + 2\boldsymbol{\Upsilon}^{(0,1)}(z)\right]\frac{d}{dz}\mathbf{c}(z;E) + \left[\mathbf{Q}(z) + \boldsymbol{\Upsilon}^{(0,2)}(z) + \boldsymbol{\Gamma}\mathbf{K}_z^2\right]\mathbf{c}(z;E) = \mathbf{0}$$

1D Transport Vector ODE

Mixing Coefficients: (identical)

$$P_{m_1\mathbf{k}_{\|},m_2\mathbf{k}_{\|}}(z) = \frac{1}{\Omega_{\|}}\iint_{\Omega_{\|}} u^*_{m\mathbf{k}_{\|}}(\mathbf{r}_{\|};z)\left\{m(\mathbf{r}_{\|};z)\frac{\partial}{\partial z}\frac{1}{m(\mathbf{r}_{\|};z)}\right\} u_{m\mathbf{k}_{\|}}(\mathbf{r}_{\|};z)\,d^2r_{\|}$$

$$Q_{m_1\mathbf{k}_{\|},m_2\mathbf{k}_{\|}}(z) = \frac{1}{\Omega_{\|}}\iint_{\Omega_{\|}} u^*_{m_1\mathbf{k}_{\|}}(\mathbf{r}_{\|};z)\left\{m(\mathbf{r}_{\|};z)\frac{\partial}{\partial z}\frac{1}{m(\mathbf{r}_{\|};z)}\right\}\frac{\partial}{\partial z}u_{m_2\mathbf{k}_{\|}}(\mathbf{r}_{\|};z)\,d^2r_{\|}$$

$$\Upsilon^{(l,n)}_{m_1\mathbf{k}_{\|},m_2\mathbf{k}_{\|}}(z) = \frac{1}{\Omega_{\|}}\iint_{\Omega_{\|}}\left\{\frac{\partial^l}{\partial z^l}u^*_{m_1\mathbf{k}_{\|}}(\mathbf{r}_{\|};z)\right\}\left\{\frac{\partial^k}{\partial z^k}u_{m_2\mathbf{k}_{\|}}(\mathbf{r}_{\|};z)\right\}d^2r_{\|}$$

$$R_{m_1\mathbf{k}_{\|},m_2\mathbf{k}_{\|}}(z) = \frac{1}{\Omega_{\|}}\iint_{\Omega_{\|}} u^*_{m_1\mathbf{k}_{\|}}(\mathbf{r}_{\|};z)\left[\frac{\partial}{\partial z}m(\mathbf{r}_{\|};z)\frac{\partial}{\partial z}\frac{1}{m(\mathbf{r}_{\|};z)} + m(\mathbf{r}_{\|};z)\frac{\partial^2}{\partial z^2}\frac{1}{m(\mathbf{r}_{\|};z)}\right]u_{m_2\mathbf{k}_{\|}}(\mathbf{r}_{\|};z)\,d^2r_{\|}$$

Block-Diagonal Nature

All matrices in 1D effective vector ODE are of the form:

$$A_{m_1\mathbf{k}_{\|1},m_2\mathbf{k}_{\|2}}(z) = \iint_{\mathbb{R}^2} \phi^*_{m_1\mathbf{k}_{\|1}}\left(\mathbf{r}_{\|};z\right) a\left(\mathbf{r}_{\|};z\right) \phi_{m_2\mathbf{k}_{\|2}}\left(\mathbf{r}_{\|};z\right) d^2 r_{\|}$$

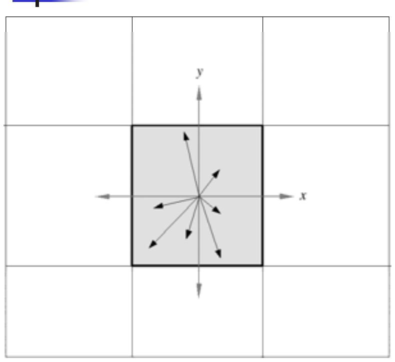
(Bloch) (periodic) (Bloch)

$$A_{m_1\mathbf{k}_{\|1},m_2\mathbf{k}_{\|2}}(z) = \iint_{\mathbb{R}^2} e^{-i\left(\mathbf{k}_{\|1}-\mathbf{k}_{\|2}\right)} b\left(\mathbf{r}_{\|};z\right) d^2 r_{\|}$$

$$\sum_{(i,j)\in\mathbb{Z}^2} \hat{b}_{ij}(z)\, e^{i\mathbf{G}_{\|ij}\bullet\mathbf{r}_{\|}}$$

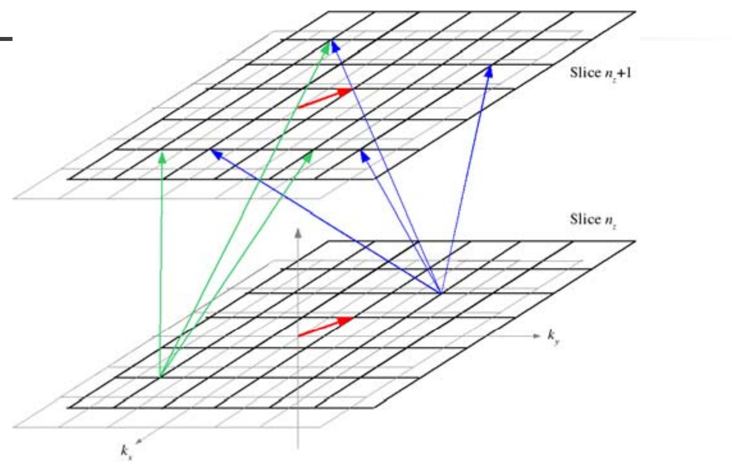
≠ 0 only when $(\mathbf{k}_{\|1} - \mathbf{k}_{\|2}) = \mathbf{G}_{\|ij}$ for some i,j

Block Diagonal Nature



- $\mathbf{k}_{\|1}$, $\mathbf{k}_{\|2}$ are both within Brillouin zone
- $(\mathbf{k}_{\|1}-\mathbf{k}_{\|2})=\mathbf{G}_{\|,ij}$ iff $\mathbf{k}_{\|1}=\mathbf{k}_{\|2}$ $= \mathbf{G}_{\|,00} \equiv \mathbf{0}$
- QED

Block Diagonal

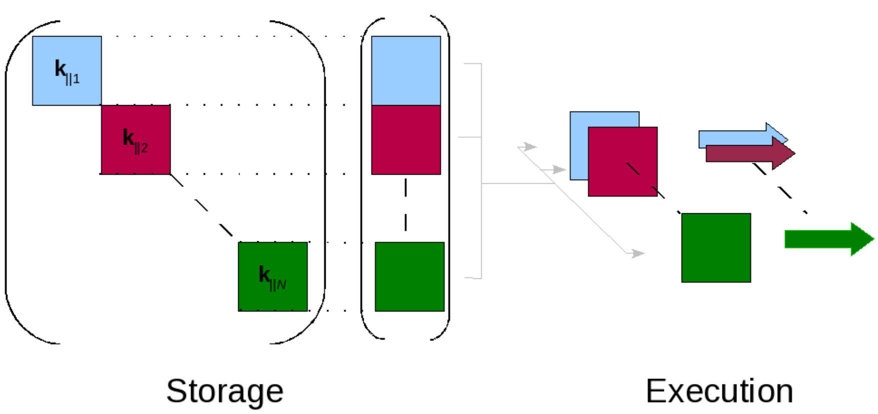


For each $\mathbf{k}_{||}$ in the first Brillouin zone, all points at lattice displacements form a subspace. Coupling across slices occurs only between elements in the same subspace.

Block Diagonality: Memory Implications

Basis-set ordering:

$$\left|1, \mathbf{k}_{||1}\right\rangle, \left|2, \mathbf{k}_{||1}\right\rangle, \ldots, \left|M, \mathbf{k}_{||1}\right\rangle, \left|1, \mathbf{k}_{||2}\right\rangle, \left|2, \mathbf{k}_{||2}\right\rangle, \ldots, \left|M, \mathbf{k}_{||2}\right\rangle$$



1D Transport Vector ODE

$$(1.64)\quad \frac{d^2}{dz^2}\mathbf{c}(z;E) + \left[\mathbf{P}(z) + 2\boldsymbol{\Upsilon}^{(0,1)}(z)\right]\frac{d}{dz}\mathbf{c}(z;E) + \left[\mathbf{Q}(z) + \boldsymbol{\Upsilon}^{(0,2)}(z) + \boldsymbol{\Gamma}\mathbf{K}_z^2\right]\mathbf{c}(z;E) = \mathbf{0}$$

Effective-mass averaging:

$$\Gamma_{m_1\mathbf{k}_{||},m_2\mathbf{k}_{||}}(z) = \frac{1}{\Omega_{||}}\iint_{\Omega_{||}} u^*_{m_1\mathbf{k}_{||}}(\mathbf{r}_{||};z)\, m(\mathbf{r}_{||};z)\, u_{m_2\mathbf{k}_{||}}(\mathbf{r}_{||};z)\, d^2r_{||}$$

Effective longitudinal "free-space" wavevector:

$$K^2_{z,m\mathbf{k}_{||},m\mathbf{k}_{||}}(z;E) = \frac{2m_e}{\hbar^2}\left(E - \varepsilon_{m\mathbf{k}_{||}}(z) - V_{bias}(z)\right)$$

(diagonal)

Diagonalization

To eliminate first-derivative term:

$$(1.27)\quad \mathbf{c}(z;E) = \mathbf{M}(z)\mathbf{f}(z;E)$$

$$\left[\frac{d^2}{dz^2}\mathbf{M}(z)\right]\mathbf{f}(z;E) + 2\left[\frac{d}{dz}\mathbf{M}(z)\right]\left[\frac{d}{dz}\mathbf{f}(z;E)\right] + \mathbf{M}(z)\left[\frac{d^2}{dz^2}\mathbf{f}(z;E)\right]$$
$$+ \left[\mathbf{P}(z) + 2\boldsymbol{\Upsilon}^{(0,1)}(z)\right]\left[\left(\frac{d}{dz}\mathbf{M}(z)\right)\mathbf{f}(z;E) + \mathbf{M}(z)\left(\frac{d}{dz}\mathbf{f}(z;E)\right)\right]$$
$$+ \left[\mathbf{Q}(z) + \boldsymbol{\Upsilon}^{(0,2)}(z) + \boldsymbol{\Gamma}(z)\mathbf{K}_z^2(z,E)\right]\mathbf{M}(z)\mathbf{f}(z;E) = \mathbf{0}$$

$$(1.29)\quad \frac{d}{dz}\mathbf{M}(z) = -\frac{1}{2}\left[\mathbf{P}(z) + 2\boldsymbol{\Upsilon}^{(0,1)}(z)\right]\mathbf{M}(z)$$

Diagonalized 1D Vector ODE

$$\frac{d^2}{dz^2}\mathbf{f}(z;E)+\mathbf{W}(z;E)\,\mathbf{f}(z;E)=\mathbf{0} \tag{1.30}$$

Vector Harmonic Oscillator

$$\mathbf{W}(z;E)=\mathbf{M}^{-1}(z)\,\mathbf{G}(z;E)\,\mathbf{M}(z) \tag{1.31}$$

Symbolic use only

$$\begin{aligned}\mathbf{G}(z;E) &= \frac{1}{2}\left(\mathbf{Q}(z)-\mathbf{Q}^{H}(z)-\mathbf{R}(z)\right)-\boldsymbol{\Upsilon}^{(1,1)}(z)\\ &\quad -\frac{1}{4}\left\{\mathbf{P}(z)+2\boldsymbol{\Upsilon}^{(0,1)}(z)\right\}^{2}+\boldsymbol{\Gamma}(z)\mathbf{K}_z^2(z;E)\end{aligned} \tag{1.32}$$

Piecewise Constant Approximation

- Assume slice is so thin that $\mathbf{W}(z;E)$ and $\mathbf{M}(z;E)$ are constant
  - Set of independent (damped) harmonic oscillators

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$$\mathbf{W}(z;E)\,\boldsymbol{\Theta}_1(z;E)=\boldsymbol{\Theta}_1(z;E)\,\boldsymbol{\Xi}^2(z;E) \tag{1.34}$$

$$\mathbf{f}(z;E)=\boldsymbol{\Theta}_1(z;E)\left[\exp\left(i\boldsymbol{\Xi}(z;E)\,z\right)\mathbf{a}(E)+\exp\left(-i\boldsymbol{\Xi}(z;E)\,z\right)\mathbf{b}(E)\right] \tag{1.35}$$

Diagonal matrix

Unknown coefficients
(*from boundary conditions*)

Simplification

Recall:

$$\mathbf{W}(z;E) = \mathbf{M}^{-1}(z)\,\mathbf{G}(z;E)\,\mathbf{M}(z)$$

$$\frac{d}{dz}\mathbf{M}(z) = -\frac{1}{2}\left[\mathbf{P}(z) + 2\boldsymbol{\Upsilon}^{(0,1)}(z)\right]\mathbf{M}(z)$$

Slice is thin – assume $\mathbf{M}(z)$ constant

- Eigenproblem of $\mathbf{W}(z;E)$ and $\mathbf{G}(z;E)$ related
  - Eigenvalues equal
  - Eigenfunctions: $\boldsymbol{\Theta}(z;E) = \mathbf{M}(z)\boldsymbol{\Theta}_1(z;E)$

Transfer Matrix (T-matrix)

$$\begin{bmatrix} \mathbf{a}_{[n_z+1]}(E) \\ \mathbf{b}_{[n_z+1]}(E) \end{bmatrix} = \mathbf{T}_{[n_z+1,n_z]}(E) \begin{bmatrix} \mathbf{a}_{[n_z]}(E) \\ \mathbf{b}_{[n_z]}(E) \end{bmatrix} \quad (1.48)$$

$$\begin{aligned} \mathbf{T}_{[n_z+1,n_z]}(E) = & \begin{bmatrix} \exp\left(-iL_{n_z}\boldsymbol{\Xi}_{[n_z+1]}(E)\right) & \mathbf{0} \\ \mathbf{0} & -\exp\left(iL_{n_z}\boldsymbol{\Xi}_{[n_z+1]}(E)\right) \end{bmatrix} \\ & \times\frac{1}{2}\begin{bmatrix} \mathbf{I} & \mathbf{I} \\ \mathbf{I} & -\mathbf{I} \end{bmatrix}\begin{bmatrix} \mathbf{I} & \mathbf{0} \\ \mathbf{0} & \boldsymbol{\Xi}^{-1}_{[n_z+1]}(E) \end{bmatrix} \\ & \times\left(\mathbf{I}_2\otimes\boldsymbol{\Theta}^{-1}_{[n_z+1]}(E)\right)\begin{bmatrix} \mathbf{S}_{[n_z+1,n_z]} & \mathbf{0} \\ \mathbf{0} & \mathbf{X}_{[n_z+1,n_z]} \end{bmatrix}\left(\mathbf{I}_2\otimes\boldsymbol{\Theta}_{[n_z]}(E)\right) \\ & \times\begin{bmatrix} \mathbf{I} & \mathbf{0} \\ \mathbf{0} & \boldsymbol{\Xi}_{[n_z]}(E) \end{bmatrix}\begin{bmatrix} \mathbf{I} & \mathbf{I} \\ \mathbf{I} & -\mathbf{I} \end{bmatrix} \\ & \begin{bmatrix} \exp\left(in_z\Delta z\,\boldsymbol{\Xi}_{[n_z]}(E)\right) & \mathbf{0} \\ \mathbf{0} & -\exp\left(-in_z\Delta z\,\boldsymbol{\Xi}_{[n_z]}(E)\right) \end{bmatrix}. \end{aligned} \quad (1.49)$$

Full Device 3D Wavefunction

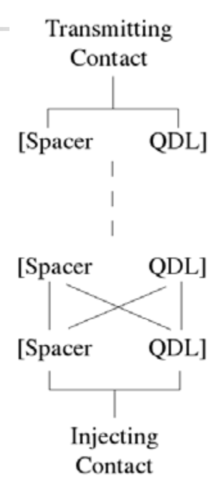
- Stitch wavefunction sections within slices across whole device
  - Device T-matrix is product of slice T-matrices

$$\mathbf{T}_{[N_z,1]}(E) = \mathbf{T}_{[N_z,N_z-1]}(E)\ldots\mathbf{T}_{[3,2]}(E)\,\mathbf{T}_{[2,1]}(E)$$

  - Relates incident wave coefficients to transmitted wave coefficients
  - Need boundary conditions to specify these two waves and complete solution

Inter-Region Coupling

- 8 combinations
  - Contact | Spacer
  - Contact | QDL
  - Spacer | QDL
  - QDL | Spacer
  - Spacer | Spacer
  - QDL | QDL
  - QDL | Contact
  - Spacer | Contact



Current Calculation

$$\text{(1.97)} \quad \begin{bmatrix} \mathbf{a}^{(trans)}(\mathbf{g}_{\parallel}, E) \\ \mathbf{b}^{(trans)}(\mathbf{g}_{\parallel}, E) \end{bmatrix} = \begin{bmatrix} \mathbf{T}_{11} & \mathbf{T}_{12} \\ \mathbf{T}_{21} & \mathbf{T}_{22} \end{bmatrix} \begin{bmatrix} \mathbf{a}^{(inc)}(\mathbf{g}_{\parallel}, E) \\ \mathbf{b}^{(inc)}(\mathbf{g}_{\parallel}, E) \end{bmatrix}$$

Reflectionl-ess contacts: $\mathbf{b}^{(trans)}$ ♋ 0

$$\text{(1.99)} \quad \mathbf{a}^{(trans)}(\mathbf{g}_{\parallel}, E) = \left[\mathbf{T}_{11} - \mathbf{T}_{12}\mathbf{T}_{22}^{-1}\mathbf{T}_{21}\right]\mathbf{a}^{(inc)}(\mathbf{g}_{\parallel}, E)$$

Per-incident-phase current:

$$J_z(\mathbf{k}_0) = \frac{q\hbar}{m}\sum_{ln}\left|a_{ln}\left(\mathbf{g}_{\parallel}; E(\mathbf{k}_0)\right)\right|^2 k_{z,ln}$$

$$\frac{1}{N_{\parallel}} I_{12,e} = \frac{\Omega_{\parallel}}{(2\pi)^3}\left(\frac{q\hbar}{m}\right)\iint_{\mathbb{R}^2}\int_0^{\infty} f_i\left(\frac{\hbar^2 k^2}{2m_1 m_e}; V_{bias,i}\right) J_{z,ij,c}(\mathbf{k}_0)\, dk_z\, d^2k_{\parallel}$$

Model Virtues

- Multiscale nature
- Any combination of spacers and QDL
- End-to-end I-V characteristics
- Best wavefunction forms for each layer
- Identification+proof for subspace partitioning
- One-time structure calculation results reused for all voltage sample calculations
- Efficient Monte Carlo integration by grouping same-lateral-subspace iso-energy wavevectors

Model Virtues

- Implementation based on external storage
  - High computation-to-disk access ratio
  - Small RAM footprint
- Design and provisions for numerical stability
- Model description extensible to systems with other types of symmetry
  - Lateral eigenfunction selection
- Describes large family of device constructions
- Extensible to anisotropic systems with diagonal effective mass tensors

Model Limitations

- Overly simplistic
  - Envelope function is not the best approach
- Neglects space-charge effects
- Neglects strain
- Current implementation not numerical stable
- Feature-limited current implementation
- Long run-times