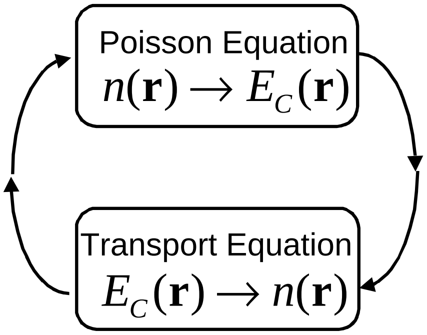
nanoMOS:

2D Simulation of Quantum Transport in Nanoscale, Double Gate MOSFETs

Mark Lundstrom

1) Ballistic quantum transport in 1D
2) Ballistic quantum transport in nanoMOS
3) A quick look at scattering
4) Quantum transport: The NEGF formalism

Device Simulation



Poisson Equation

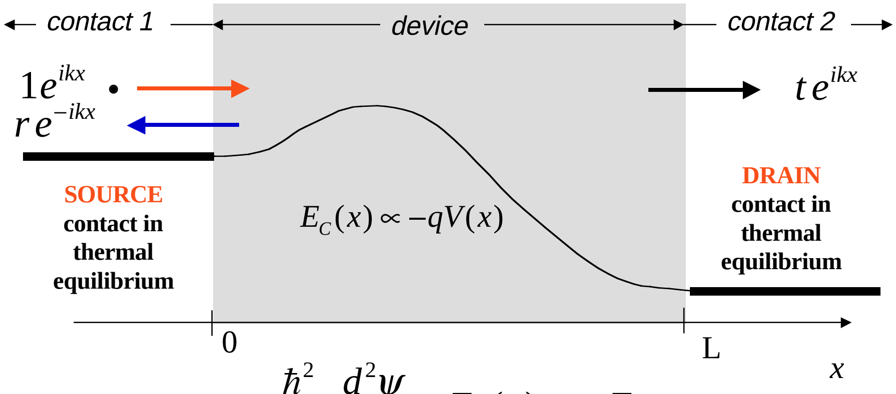
$$n(\mathbf{r}) \rightarrow E_C(\mathbf{r})$$

Transport Equation

$$E_C(\mathbf{r}) \rightarrow n(\mathbf{r})$$

drift-diffusion
energy transport
Boltzmann (ballistic)
quantum transport
-density gradient/effective potential
-NEGF approach

A 1D device



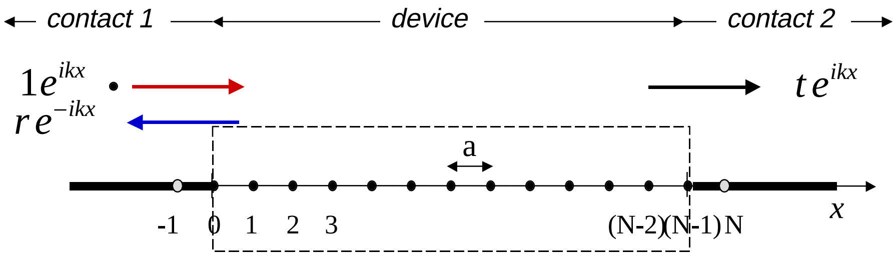
SOURCE
contact in
thermal
equilibrium

$E_C(x) \propto -qV(x)$

DRAIN
contact in
thermal
equilibrium

$$-\frac{\hbar^2}{2m^*}\frac{d^2\psi}{dx^2} + E_C(x)\psi = E\psi$$

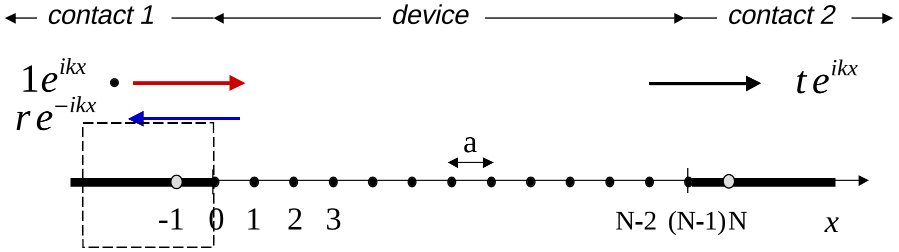
A 1D device



$$-t_0\psi_{i-1} + \left(2t_0 + E_{Ci} - E\right)\psi_i - t_0\psi_{i+1} = 0$$

$$t_0 \equiv \frac{\hbar^2}{2m^* a^2} \qquad i = 0,\ 1,\ 2, \ldots\ N-1$$ (N unknowns)

Open boundary conditions



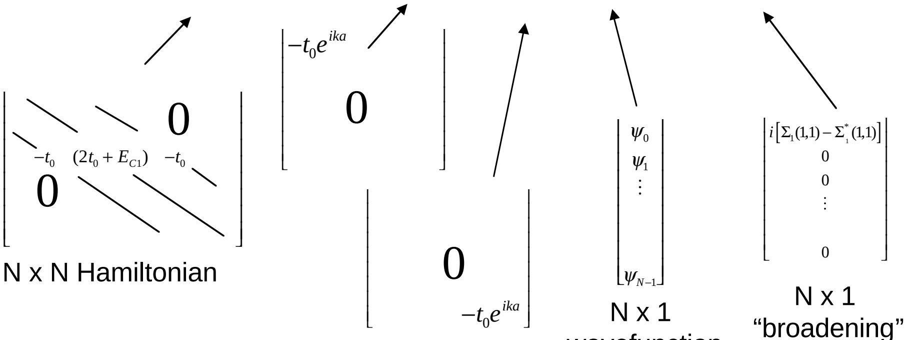
$$-t_0\psi_{-1} + \left(2t_0 + E_{Ci} - E\right)\psi_0 - t_0\psi_1 = 0$$

$$\psi(x) = 1e^{ikx} + re^{-ikx} \quad x \le 0$$

$$\psi_{-1} = \psi_0\, e^{ika} - \left(e^{ika} - e^{-ika}\right)$$

The discretized wave equation

$$\left[E\mathbf{I} - \mathbf{H} - \Sigma_S - \Sigma_D\right]\boldsymbol{\psi} = i\boldsymbol{\Gamma}$$



N x N Hamiltonian

N x N lead “self-energies”

N x 1
wavefunction

N x 1
“broadening”

The solution

$$[E\mathbf{I} - \mathbf{H} - \Sigma_S - \Sigma_D]\psi = i\Gamma$$

formal solution:

$$\boldsymbol{\psi} = i\mathbf{G}^R\boldsymbol{\Gamma}$$

$$\mathbf{G}^R = [E\mathbf{I} - \mathbf{H} - \Sigma_S - \Sigma_D]^{-1}$$

(N x N retarded Green's function)

Finding n(x_i) from $\psi(x_i)$

$$n_S(x_i) = \frac{1}{L}\sum_k \left|\psi_k(x_i)\right|^2 f(E_F - E_k)$$

computed assuming unit amplitude injected wave

sum over the distribution of injected k's from source contact

weight by Fermi function of the source

Finding n(x_i) from ψ(x_i)

$$n_S(x_i) = \int_0^{E_{CTop}} \underbrace{\left[\frac{1}{\pi}\frac{dk}{dE_k}\left|\psi_k(x_i)\right|^2\right]}_{\text{local DOS (source component)}} f(E_F - E_k)\, dE_k$$

$$\equiv 2\times\frac{A_S(E_k,x_i)}{2\pi}$$

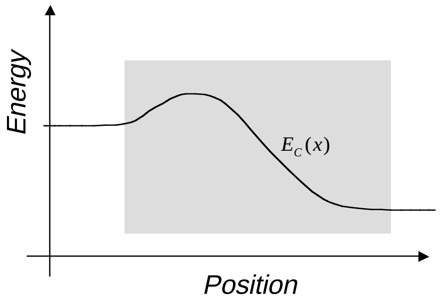
$$g_{1D}(E)=\frac{1}{\pi\hbar}\sqrt{\frac{m^*}{2E}}$$

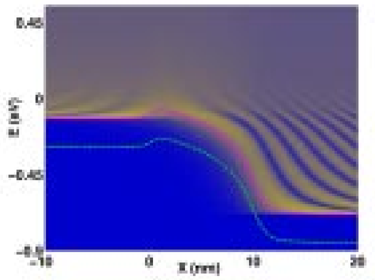
if

$$E_k=\frac{\hbar^2k^2}{2m^*} \qquad \psi(x)=e^{ikx}$$

Local DOS in a MOSFET

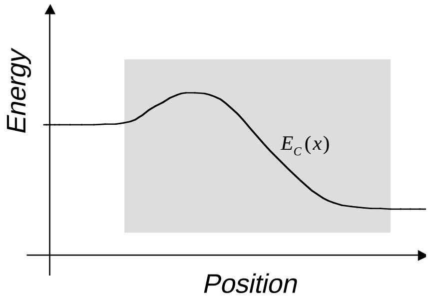
$$2\times\frac{A_S(E_k,x_i)}{2\pi}$$

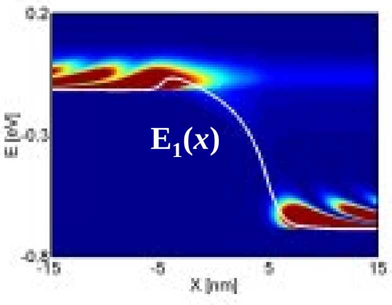




n(E) in a MOSFET

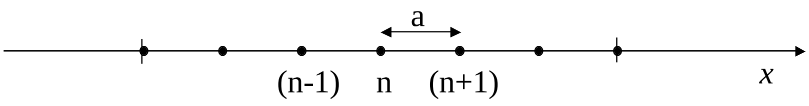
$$n(E) = 2 \times \frac{A_S(E_k, x_i)}{2\pi} f(E_F - E_k)$$





E_k in the leads

infinite lead



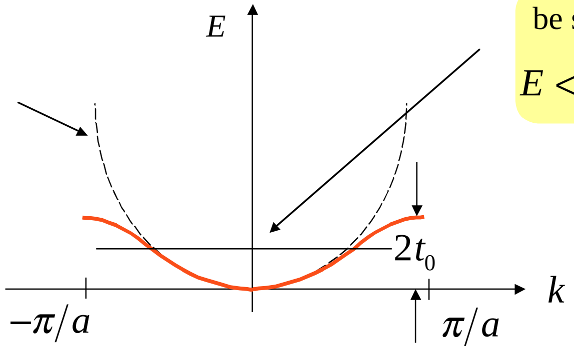
$$-\frac{\hbar^2}{2m^*}\frac{d^2\psi}{dx^2} = E\psi \rightarrow -\frac{\hbar^2}{2m^*}\left[\frac{\psi_{n+1} - 2\psi_n + \psi_{n-1}}{a^2}\right] = E\psi_n$$

$$\psi_n = e^{ikna} \rightarrow E_k = E_C + 2t_0(1 - \cos ka)$$

$$t_0 \equiv \frac{\hbar^2}{2m^* a^2}$$

E_k in the leads

$$E_k = \frac{\hbar^2 k^2}{2m^*}$$



be sure!

$E << 2t_0$

$$E_k = E_C + 2t_0\left(1 - \cos ka\right)$$

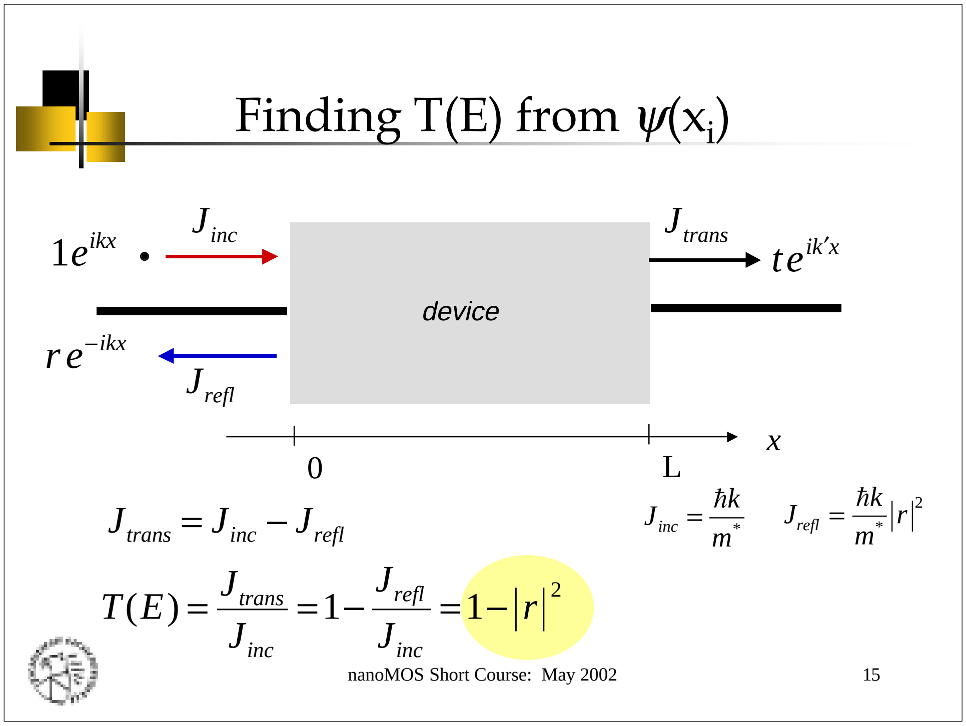
$$t_0 \equiv \frac{\hbar^2}{2m^* a^2}$$

Finding I_D from $\psi(\mathrm{x_i})$

$$I^{SD} = \frac{q}{L}\sum_k T_{SD}\left(E_k\right)\upsilon_k\, f\left(E_F - E_k\right)$$

$$I^{SD} = \frac{2q}{h}\int_0^{E_{Top}} T\left(E_k\right) f\left(E_F - E_k\right) dE_k$$

need to find $T(E)$ from the wave function



Finding T(E) from $\psi(x_i)$

$$J_{inc} = \frac{\hbar k}{m^*} \qquad J_{refl} = \frac{\hbar k}{m^*}|r|^2$$

$$J_{trans} = J_{inc} - J_{refl}$$

$$T(E) = \frac{J_{trans}}{J_{inc}} = 1 - \frac{J_{refl}}{J_{inc}} = 1 - |r|^2$$

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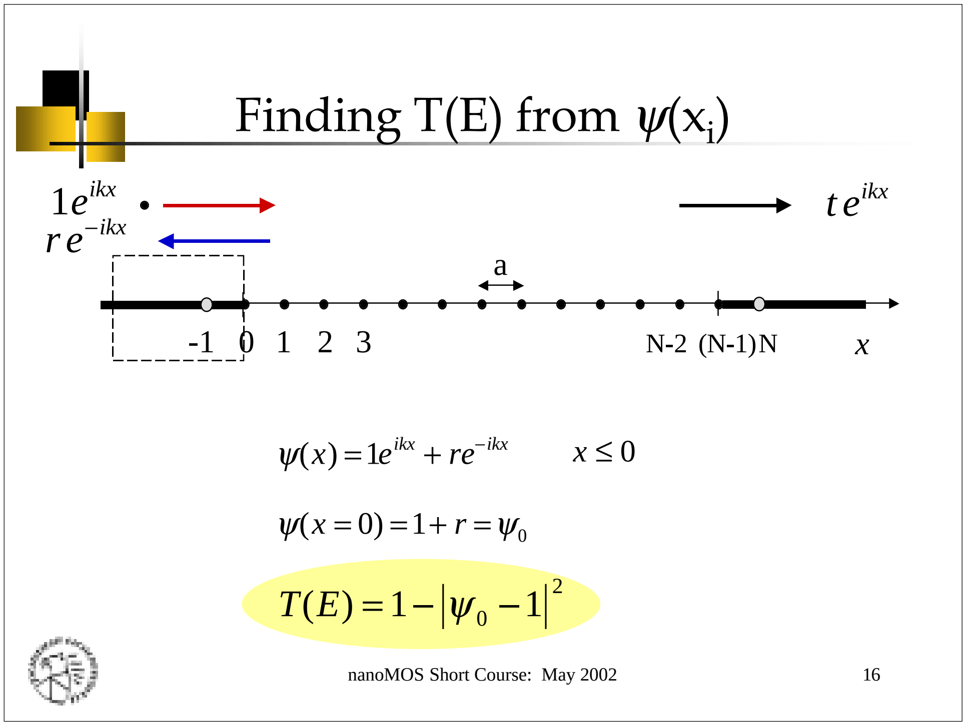

Finding T(E) from $\psi(x_i)$

$$\psi(x) = 1e^{ikx} + re^{-ikx} \qquad x \le 0$$

$$\psi(x=0) = 1 + r = \psi_0$$

$$T(E) = 1 - |\psi_0 - 1|^2$$

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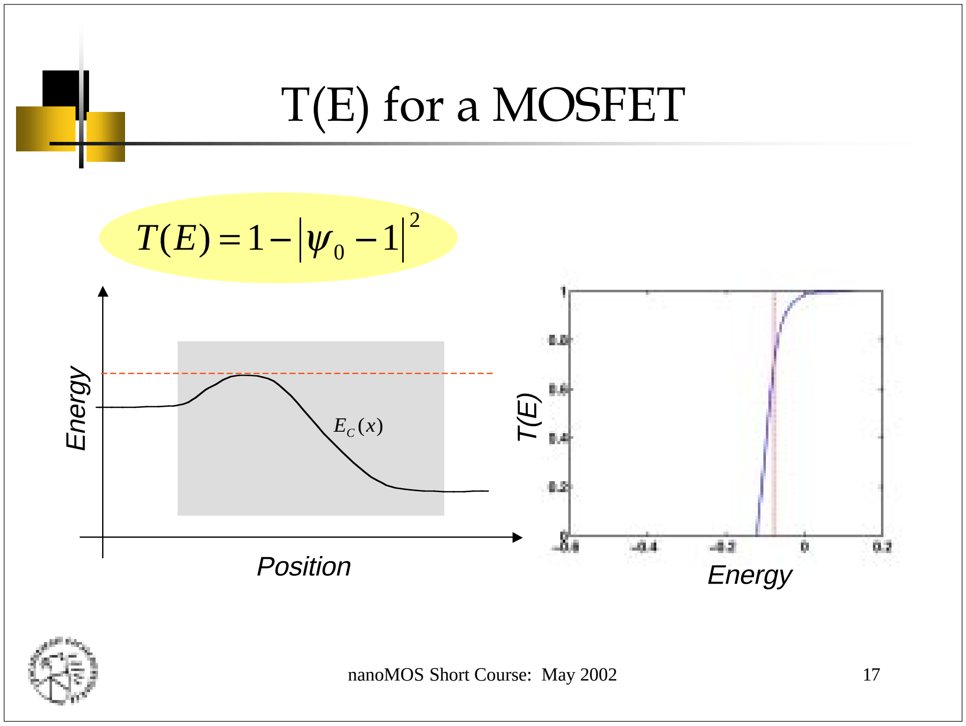
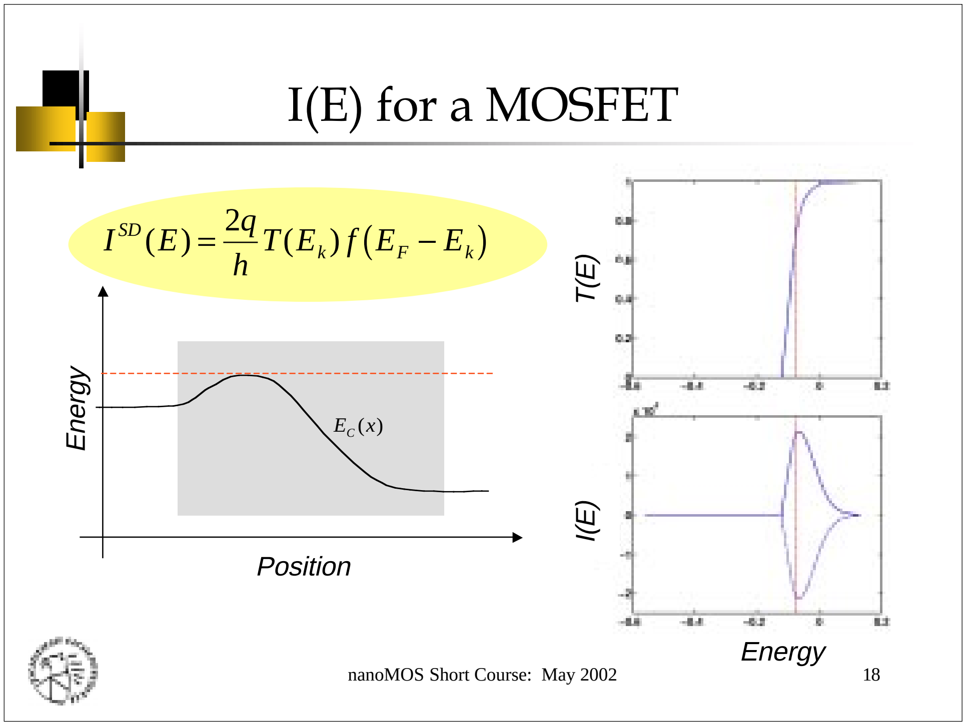


T(E) for a MOSFET

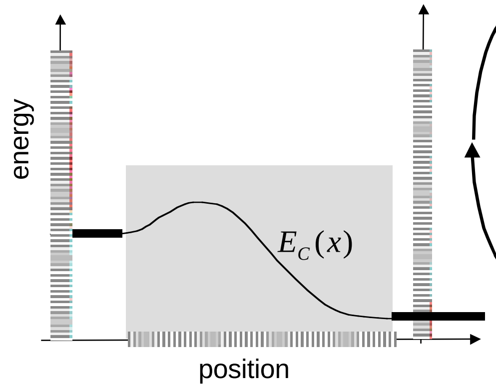
$$T(E) = 1 - \left|\psi_0 - 1\right|^2$$



I(E) for a MOSFET

$$I^{SD}(E) = \frac{2q}{h} T(E_k) f(E_F - E_k)$$

The wavefunction approach (1D)



1) Guess $E_C(x)$
2) For each energy:

$$[\mathbf{H} - E\mathbf{I} + \Sigma_S + \Sigma_D]\boldsymbol{\psi} = -i\boldsymbol{\Gamma}$$

3) Determine $n(x)$:

$$n(x_i) = n_S(x_i) + n_D(x_i)$$

4) solve Poisson for $E_C(x)$
5) go to 1

↓

6) Determine I_D

$$I_D = I^{SD} - I^{DS}$$

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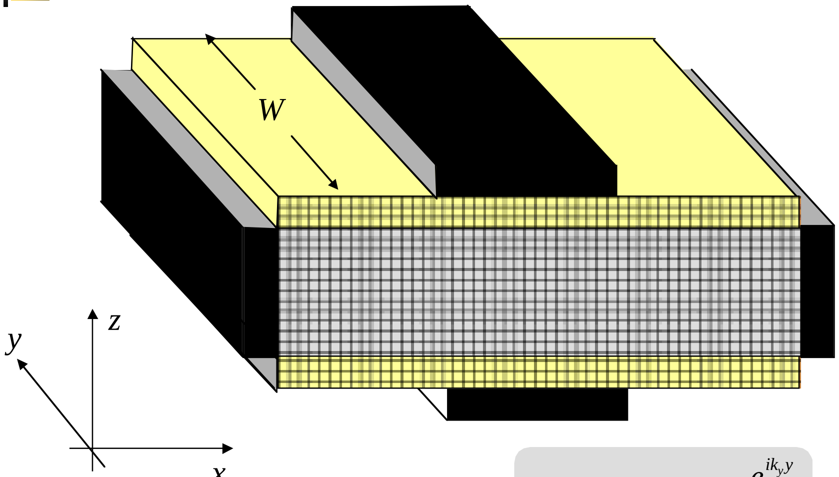
4) Quantum transport by the NEGF formalism

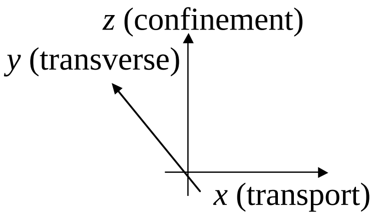
MOSFETs are 3D



$$\psi(x,y,z) = \Phi(x,z)\frac{e^{ik_y y}}{\sqrt{W}}$$

MOSFETs are 3D

$$-\frac{\hbar^2}{2m_x^*}\frac{\partial^2\Phi(x,z)}{\partial x^2} - \frac{\hbar^2}{2m_z^*}\frac{\partial^2\Phi(x,z)}{\partial z^2} - E_C(x,z)\Phi(x,z) = \left(E - E_{k_y}\right)\Phi(x,z)$$



z (confinement)

y (transverse)

x (transport)

$$\psi(x,y,z) = \Phi(x,z)\frac{e^{ik_y y}}{\sqrt{W}}$$

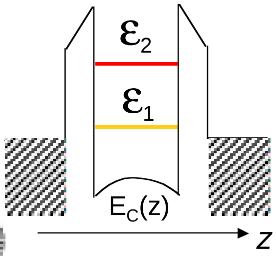
(N_x x N_z) unknowns

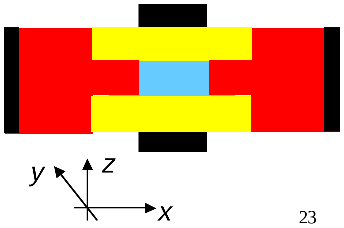
MOSFETs are 3D

$$-\frac{\hbar^2}{2m_x^*}\frac{\partial^2\Phi(x,z)}{\partial x^2}-\frac{\hbar^2}{2m_z^*}\frac{\partial^2\Phi(x,z)}{\partial z^2}-E_C(x,z)\Phi(x,z)=\left(E-E_{k_y}\right)\Phi(x,z)$$

$$\Phi(x,z)=\sum_{m=1}\delta(x-x')\Psi_m(x',z)$$

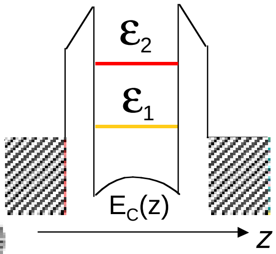
(N_x x M) unknowns

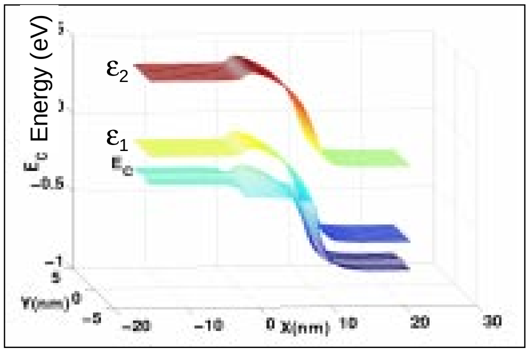




MOSFETs are 3D

$$-\frac{\hbar^2}{2m_z^*}\frac{\partial^2\Psi_m(x,z)}{\partial z^2}-E_C(x,z)\Psi_m(x,z)=E_m(x)\Psi_m(x,z)$$





MOSFETs are 3D

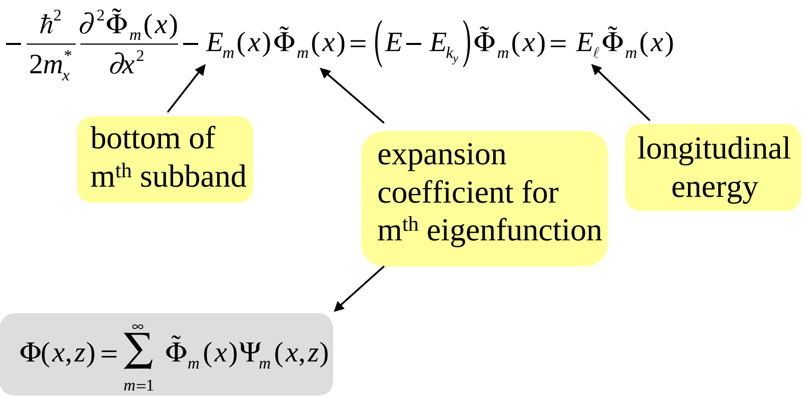
$$-\frac{\hbar^2}{2m_x^*}\frac{\partial^2\Phi(x,z)}{\partial x^2}-\frac{\hbar^2}{2m_z^*}\frac{\partial^2\Phi(x,z)}{\partial z^2}-E_C(x,z)\Phi(x,z)=\left(E-E_{k_y}\right)\Phi(x,z)$$

$$\Phi(x,z)=\sum_{m=1}\delta(x-x')\Psi_m(x',z)$$

(N_x x M unknowns)

if $\frac{\partial\Psi_m(x',z)}{\partial x}\approx 0$

MOSFETs are 3D



$$-\frac{\hbar^2}{2m_x^*}\frac{\partial^2\tilde{\Phi}_m(x)}{\partial x^2}-E_m(x)\tilde{\Phi}_m(x)=\left(E-E_{k_y}\right)\tilde{\Phi}_m(x)=E_\ell\tilde{\Phi}_m(x)$$

bottom of m^{th} subband

expansion coefficient for m^{th} eigenfunction

longitudinal energy

$$\Phi(x,z)=\sum_{m=1}^{\infty}\tilde{\Phi}_m(x)\Psi_m(x,z)$$

MOSFETs are 3D

1) transverse (y-direction) $\frac{e^{ik_y y}}{\sqrt{W}}$

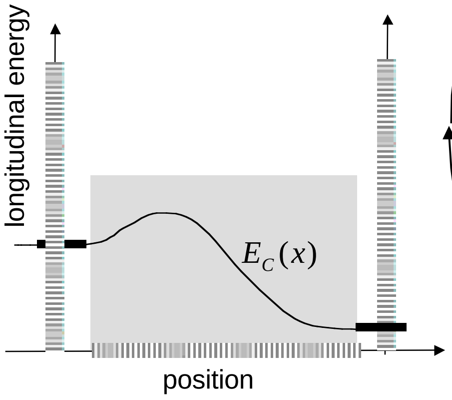
2) confinement (z-direction) $\Psi_m(x,z), E_m$

(N$_x$ 1D equations for N$_z$ unknowns)

3) transport (x-direction) $\tilde{\Phi}_m(x)$

(M 1D equations for N$_x$ unknowns)

The wavefunction approach (3D)



1) Guess $E_C(x,z)$
2) For each slice in x:

$$\mathbf{H}\tilde{\Psi}_m = E_m\tilde{\Psi}_m(x,z)$$

3) For each mode, *m*

$$[\mathbf{H} - E\mathbf{I} + \Sigma_S + \Sigma_D]\tilde{\Phi}_m = -i\Gamma$$

4) Determine $n_m(x)$
5) Repeat for each mode

6) Determine total $n(x)$
7) Solve Poisson for $E_C(x)$

8) go to 1

9) Determine I_D

Electron density

$$n_S^m(E_\ell, x_i) = \frac{1}{W}\sum_{k_y} f\left(E_F - E_\ell - E_{k_y}\right)\frac{A_S(E_\ell, x_i)}{2\pi}$$

$$n_S^m(E_\ell, x_i) = \int_0^\infty \left\{\frac{2}{\pi\hbar}\sqrt{\frac{m_y^*}{2E_{k_y}}}\right\} f\left(E_F - E_\ell - E_{k_y}\right)\frac{A_S}{2\pi}\, dE_{k_y}$$

$$n_S^m(E, x_i) = \frac{1}{\hbar a}\sqrt{\frac{m_y^* k_B T}{2\pi^3}}\mathcal{F}_{-1/2}(E_F - E_\ell)A_S = 2\times\left(\frac{A_S}{2\pi}\right)F(E_F - E_\ell)$$

$$n_S(E_\ell, x_i) = \sum_{m=1}^{M} n_S^m(E_\ell, x_i)$$

$$\left\{A_S(E_\ell, x_i) \equiv 2\pi\left[\frac{1}{\pi}\frac{dk}{dE_\ell}\left|\Phi_k^m(x_i)\right|^2\right]\right\}$$

Electron current

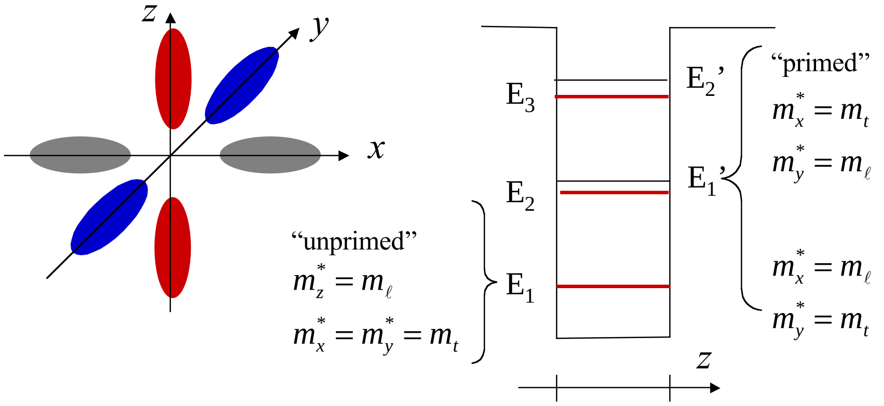
$$I_m^{SD}(E_\ell) = \frac{1}{W}\sum_{k_y}\left(\frac{2q}{h}\right)T(E_\ell)\, f\left(E_F - E_\ell - E_{k_y}\right)$$

$$I_m^{SD}(E_\ell) = \int_0^\infty \left\{\frac{2}{\pi\hbar}\sqrt{\frac{m_y^*}{2E_{k_y}}}\right\} T(E_\ell)\, f\left(E_F - E_\ell - E_{k_y}\right) dE_{k_y}$$

$$I_m^{SD}(E_\ell) = \frac{1}{\hbar^2}\sqrt{\frac{m_y^* k_B T_L}{2\pi^3}}\mathcal{F}_{-1/2}(E_F - E_\ell)T(E_\ell) = \frac{2q}{h}T(E_\ell)F(E_F - E_\ell)$$

total source-injected current by integrating over E_ℓ
and summing over *m*

Silicon conduction bands



"unprimed"

$m_z^* = m_\ell$

$m_x^* = m_y^* = m_t$

"primed"

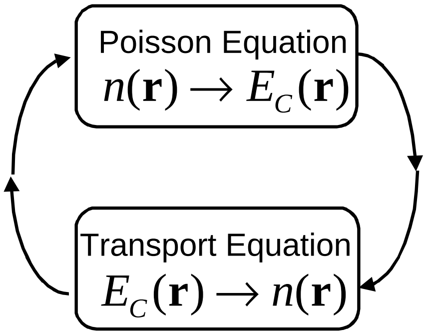
$m_x^* = m_t$

$m_y^* = m_\ell$

$m_x^* = m_\ell$

$m_y^* = m_t$

Poisson's equation



Poisson Equation

$n(\mathbf{r}) \rightarrow E_C(\mathbf{r})$

Transport Equation

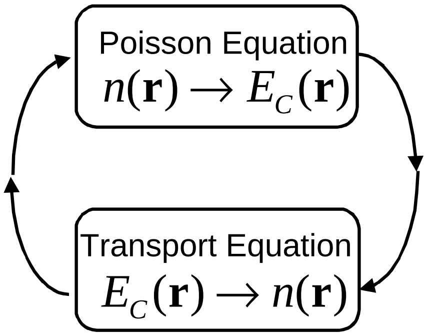
$E_C(\mathbf{r}) \rightarrow n(\mathbf{r})$

$$\nabla^2 V(x,z) = \frac{n(x,z) - (N_D - N_A)}{\varepsilon}$$

$$n(x,z) \equiv N_{2D} \mathcal{F}_0 [F_n(x,z) - qV(x,z)]$$

$$\nabla^2 V(x,z) = \frac{N_{2D} \mathcal{F}_0 [F_n(x,z) + qV(x,z)] - (N_D - N_A)}{\varepsilon}$$

Poisson's equation



Poisson Equation

$n(\mathbf{r}) \rightarrow E_C(\mathbf{r})$

Transport Equation

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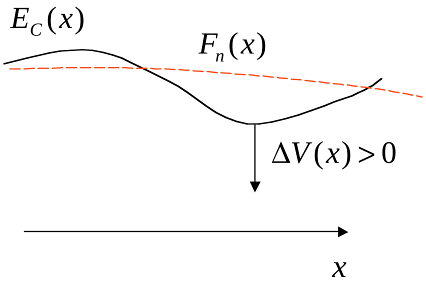
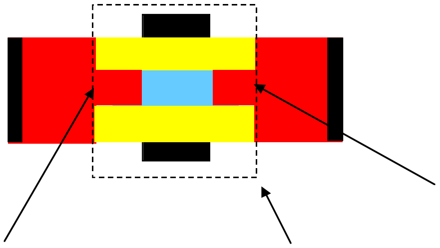


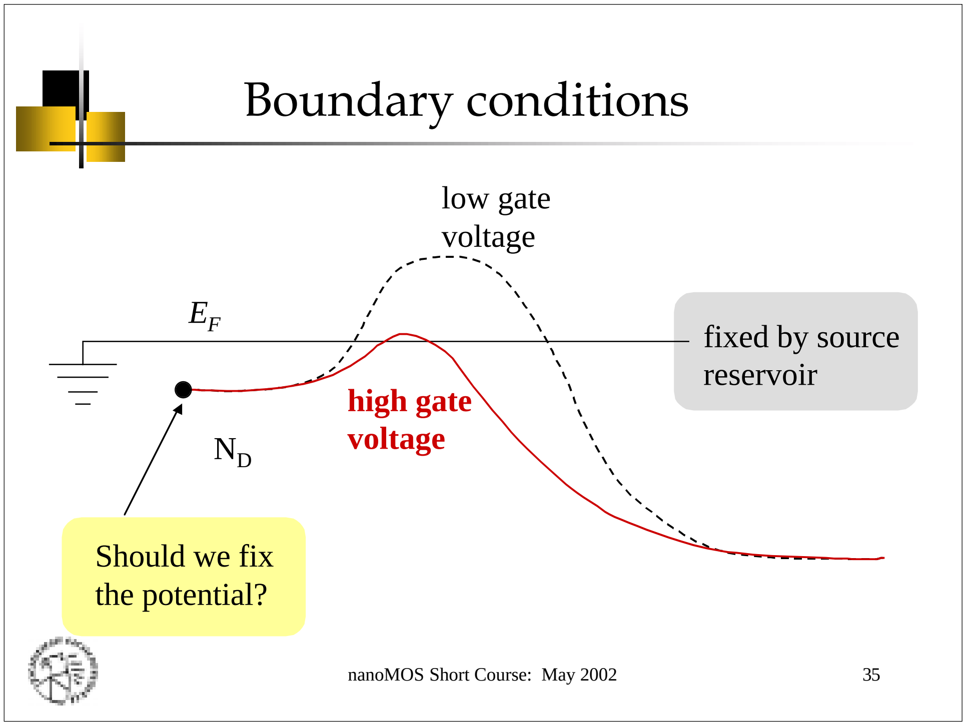
Boundary conditions



modes are coupled!

intrinsic device

what are the appropriate, ideal (upper limit) boundary conditions?



Boundary conditions

low gate voltage

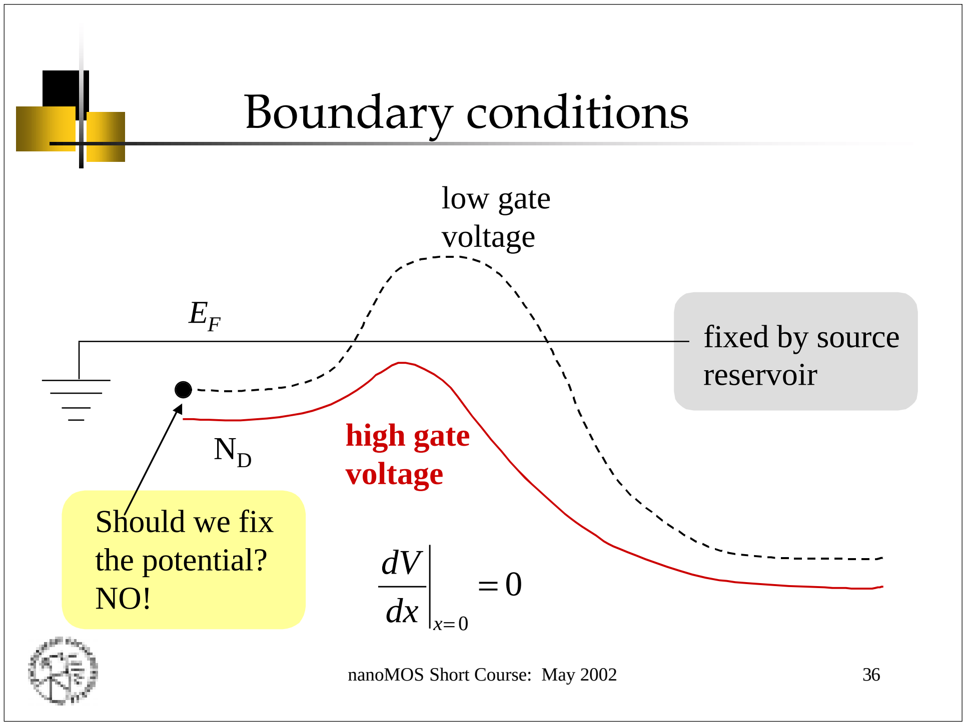
E_F

fixed by source reservoir

high gate voltage

N_D

Should we fix the potential?



Boundary conditions

low gate voltage

E_F

fixed by source reservoir

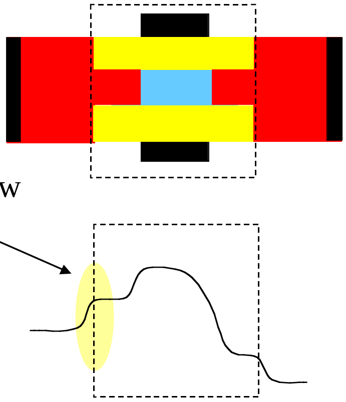
high gate voltage

N_D

Should we fix the potential?
NO!

$$\left.\frac{dV}{dx}\right|_{x=0} = 0$$

Boundary conditions



bandbending
across wide/narrow
source

$$\left.\frac{dV}{dx}\right|_{x=0} = 0$$

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Analogy to the RTA

Boltzmann Transport Equation:

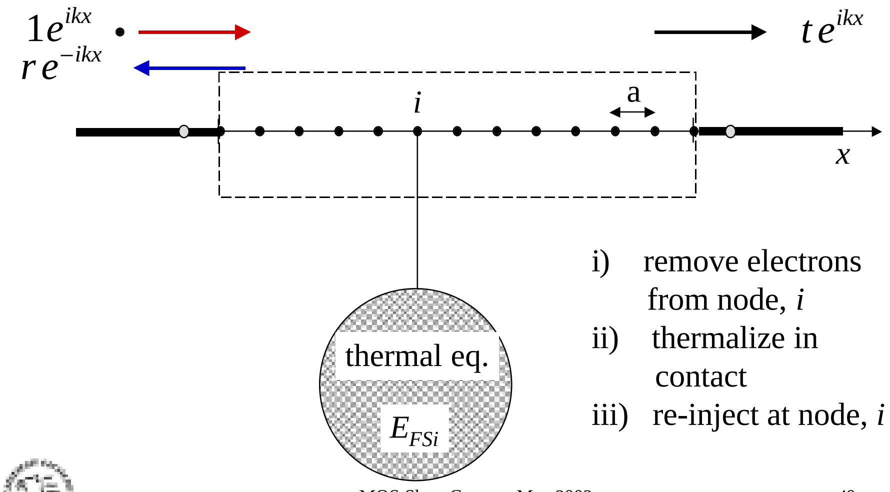
$$\frac{\partial f}{\partial t} = \upsilon_x \frac{\partial f}{\partial x} - q\mathcal{E}_x \frac{\partial f}{\partial p_x} = \hat{C} f$$

Relaxation Time Approximation:

$$\hat{C}f = -\frac{(f - f_0)}{\tau} = -\frac{f}{\tau} + \frac{f_0}{\tau}$$

out-scattering **in-scattering**

Scattering by “Büttiker probes”



i) remove electrons from node, *i*

ii) thermalize in contact

iii) re-inject at node, *i*

Out-scattering

$$G(E)=\left[\mathbf{EI}-\mathbf{H}-\Sigma_S-\Sigma_D-\Sigma_{Scatt}\right]^{-1}$$

$$\Sigma_S=\begin{bmatrix}-t_0e^{ik_1a} & 0 & \ldots\\ 0 & 0 & \ldots\\ \ldots & \ldots & \ldots\end{bmatrix}_{N\times N}$$

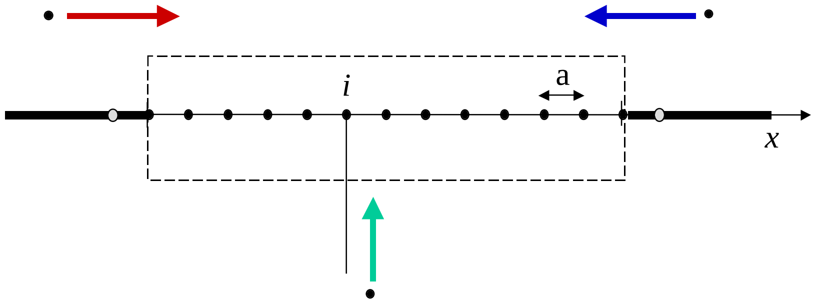
$$\Sigma_{Scatt}=\begin{bmatrix}0 & 0 & \ldots\\ 0 & t_Se^{ika} & 0\\ \ldots & 0 & 0\end{bmatrix}_{N\times N}$$

$$\Sigma_D=\begin{bmatrix}\ldots & \ldots & \ldots\\ \ldots & 0 & 0\\ \ldots & 0 & -t_0e^{ik_Na}\end{bmatrix}_{N\times N}$$

or: $i\eta$

- t_S (η) is related to the out-scattering time, τ $\left(\tau=\hbar/2\eta\right)$
- the out-scattering time is related to the local mobility ($\mu = q\tau/m^*$)

In-scattering



$$n(E,x_i)=f\left(E_F-E\right)\frac{A_S}{2\pi}+f\left(E_F-qV_D-E\right)\frac{A_D}{2\pi}+f\left(E_{Fscatt}-E\right)\frac{A_{scatt}}{2\pi}$$

$$A_S(E_\ell,x_i)\equiv 2\pi\left[\frac{1}{\pi}\frac{dk}{dE_\ell}\left|\psi_k(x_i)\right|^2\right]$$

adjust E_{Fscatt} for current continuity

nanoMOS:

2D Simulation of Quantum Transport in Nanoscale, Double Gate MOSFETs

Mark Lundstrom

1) Ballistic quantum transport in 1D

2) Ballistic quantum transport in nanoMOS

3) A Quick look at scattering

4) Quantum transport: The NEGF formalism

Key Results (1D wave functions)

$$[E\mathbf{I}-\mathbf{H}-\Sigma_S-\Sigma_D]_{\mathrm{NxN}}\Psi_{\mathrm{Nx1}}=i\Gamma_{\mathrm{Nx1}}$$

$$n_S(x_i)=\int_0^{E_{Top}}2\times\frac{A_S(E_k,x_i)}{2\pi}f(E_F-E_k)\,dE_k$$

$$A_S(E,x_i)=2\pi\left(\frac{1}{\pi}\frac{dk}{dE}\left|\psi_k(x_i)\right|^2\right)$$

$$I^{S-D}=\frac{2q}{h}\int_0^{E_{Top}}T(E)f(E_k)\,dE_k$$

$$T(E)=1-\left|\psi_0-1\right|^2$$

$$\Psi_{\mathbf{Nx1}}=i\mathbf{G}_{\mathrm{NxN}}\Gamma_{\mathrm{Nx1}}$$

$$\mathbf{G}_{\mathrm{NxN}}=[E\mathbf{I}-\mathbf{H}-\Sigma_{\mathbf{1}}-\Sigma_{\mathbf{2}}]^{-1}_{\mathrm{NxN}}$$

Can we do everything with the Green's function?

The density matrix

We need $\psi^*\psi$ at each node. $\boldsymbol{\psi}\boldsymbol{\psi}^H = \mathbf{G}\boldsymbol{\Gamma}_S\boldsymbol{\Gamma}_S^{\mathbf{H}}\mathbf{G}^{\mathbf{H}}$

We have:

$$\boldsymbol{\psi} = \begin{bmatrix} \psi_0 \\ \psi_1 \\ \\ \\ \\ \psi_{N-1} \end{bmatrix} \qquad \begin{pmatrix} \psi_0^*\psi_0 & \psi_0^*\psi_1 & \psi_0^*\psi_2 & \cdots & \\ \psi_1^*\psi_0 & \psi_1^*\psi_1 & & & \\ \psi_2^*\psi_0 & & \psi_2^*\psi_2 & & \\ \vdots & & & \ddots & \\ & & & & \psi_{N-1}^*\psi_{N-1} \end{pmatrix}$$

nanoMOS Short Course: May 2002 45

The density matrix

(N x 1) $$n_S(x_i) = \int_0^{E_{Top}} \frac{2}{\pi}\frac{dk}{dE_k}\left|\psi_k(x_i)\right|^2 f(E_k)\,dE$$

(N x N) $$\boldsymbol{\rho}_S = \int_0^{E_{Top}} \frac{1}{\pi}\frac{dk}{dE_k}\left\{\mathbf{G}\boldsymbol{\Gamma}_S\boldsymbol{\Gamma}_S^{\mathbf{H}}\mathbf{G}^{\mathbf{H}}\right\} f(E)\,dE$$

$$\Gamma_S = \begin{bmatrix} i\left[\Sigma_S(1,1) - \Sigma_s^*(1,1)\right] \\ \vdots \\ \\ 0 \end{bmatrix} = \begin{bmatrix} 2t_0\sin ka \\ \vdots \\ \\ 0 \end{bmatrix} \qquad \Gamma_S\Gamma_S^H = \begin{bmatrix} 4t_0^2\sin^2 ka & \dots & 0 \\ \vdots & \ddots & \\ & & \\ 0 & & 0 \end{bmatrix}$$

nanoMOS Short Course: May 2002 46

The density matrix

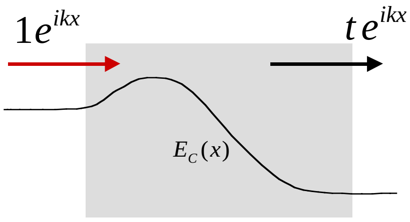
$$E(k) = 2t_0(1-\cos ka) \qquad \frac{dk}{dE} = \frac{1}{2at_0 \sin ka}$$

$$\boldsymbol{\rho}_S\Big|_{\mathrm{NxN}} = 2\times\int \frac{dE}{2\pi}\mathbf{A}_S\Big|_{\mathrm{NxN}} f(E_F - E)\,dE$$

$$\mathbf{A}_S = \mathbf{G}\Gamma_S\mathbf{G}^{\mathbf{H}}$$

$$\Gamma_S = \begin{bmatrix} 2t_0 \sin ka & \cdots & 0 \\ \vdots & \ddots & \\ & & \\ 0 & & 0 \end{bmatrix} = i\left(\Sigma_S - \Sigma_S^H\right)$$

Transmission



$$J_{inc} = 1\upsilon_0$$

$$J_{trans} = |t|^2\upsilon_N$$

$$T = |t|^2\left(\frac{\upsilon_N}{\upsilon_1}\right)$$

$$\upsilon_0 = \frac{2at_0}{\hbar}\sin k_0 a = \left(\frac{a}{\hbar}\right)\Gamma_S(1{,}1)$$

$$\upsilon_N = \frac{2at_0}{\hbar}\sin k_N a = \left(\frac{a}{\hbar}\right)\Gamma_D(N,N)$$

Transmission

$$T(E)=\left|t\right|^2\frac{\upsilon_1}{\upsilon_N}=\left|\psi_N\right|^2\frac{\Gamma_{NN}}{\Gamma_{11}} \qquad \psi_N=G_{N1}\Gamma_{11}$$

$$T(E)=G_{N1}^2\,\Gamma_S(1,1)\Gamma_D(N,N)$$

more generally, for transmission from contact S to D:

$$T(E)=\mathrm{trace}\left[\Gamma_S\mathbf{G}\Gamma_D\mathbf{G}^{\mathrm{H}}\right]$$

Key results (NEGF)

$$\mathbf{G}=[\mathbf{H}-E\mathbf{I}+\Sigma_S+\Sigma_D]^{-1}$$

$$\rho_S=\int\frac{dE}{2\pi}\mathbf{A}_S(E)f(E_F-E)$$

$$\mathbf{A}_S(E)=\mathbf{G}\Gamma_S\mathbf{G}^H$$

$$I^{SD}=\frac{2q}{h}\int T^{SD}(E)f(E_F-E_k)\,dE$$

$$T^{SD}(E)=\mathrm{trace}\left[\Gamma_S\mathbf{G}\Gamma_D\mathbf{G}^{\mathrm{H}}\right]$$

$$\Sigma_S=\begin{bmatrix}-t_0e^{ik_1a} & 0 & \ldots\\ 0 & 0 & \ldots\\ \ldots & \ldots & \ldots\end{bmatrix}$$

$$\Sigma_D=\begin{bmatrix}\ldots & \ldots & \ldots\\ \ldots & 0 & 0\\ \ldots & 0 & -t_0e^{ik_Na}\end{bmatrix}$$

$$\Gamma_S=\Sigma_S-\Sigma_S^H$$

$$\Gamma_D=\Sigma_D-\Sigma_D^H$$