# Numerical Computations of Nanoelectronics Problems

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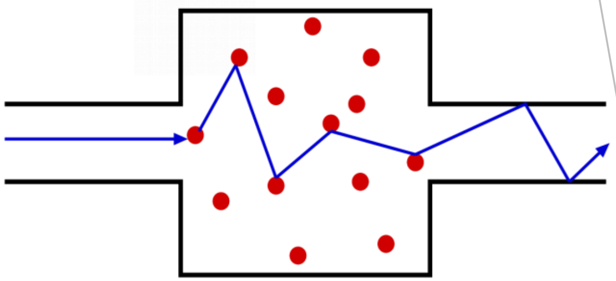
# Outline
# Three Lectures

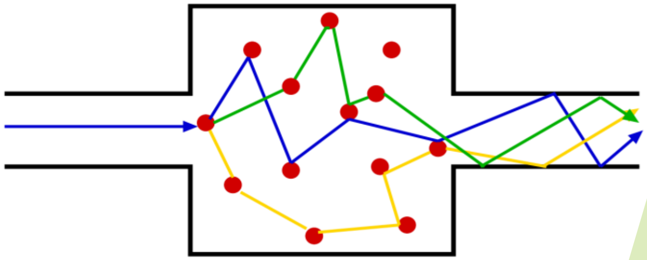
- Lecture on 5/14
  - Numerical Calculation of Schrödinger Equation
    - 1D ∞ Quantum Well
  - Numerical Newton Iteration
    - Transcendental Equation ( Capacitance of P-N Junction)
    - Poission's Equation (Band Diagram of P-N Junction)
- Lecture on 5/16
  - Numerical Calculation of Band Structures
    - 1D atom chain
    - Graphene Nanoribbon
    - Graphene
- Lecture today
  - Quantum Transport – Non-equilibrium Green's Function

# Transport (movement of electrons - current)

- Semiclassical Transport
  - Electron as Newtonian pinball



- Quantum Transport
  - Electron is in a pure state $|\Psi\rangle$
  - Recall Wave-partical duality



# Transport (current)

- Semiclassical Transport
  - Macroscopic solid
  - "Boltzman transport equation"

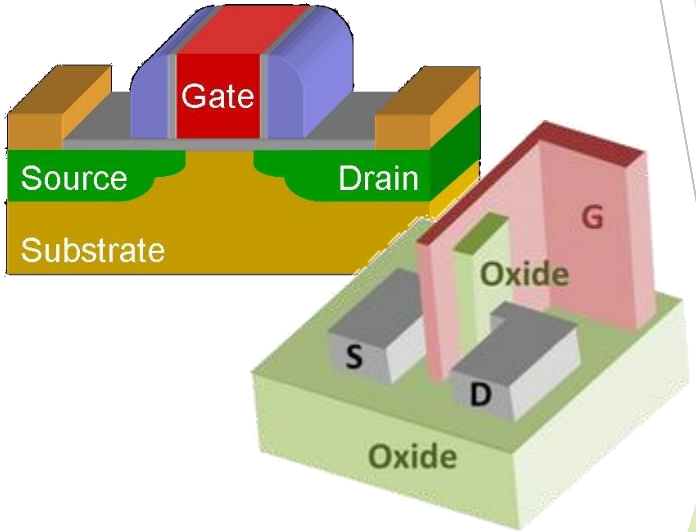
$$J_n = en\mu_n \mathcal{E}_x + eD_n \frac{dn}{dx}$$

- Quantum Transport
  - Applied in Nanoscale systems (mesoscopic/microscopic)
  - Where quantum mechanic effects cannot be ignored
  - "Non-equilibrium Green's Function"

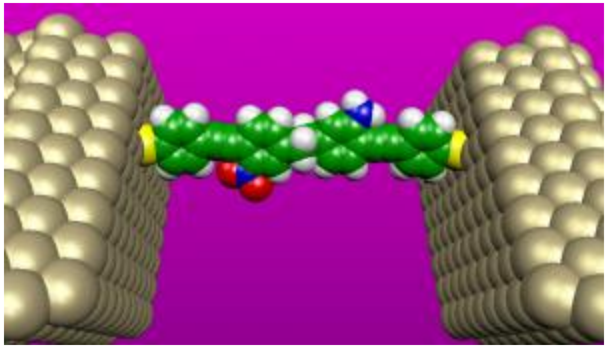
# Quantum Transport

- Applications

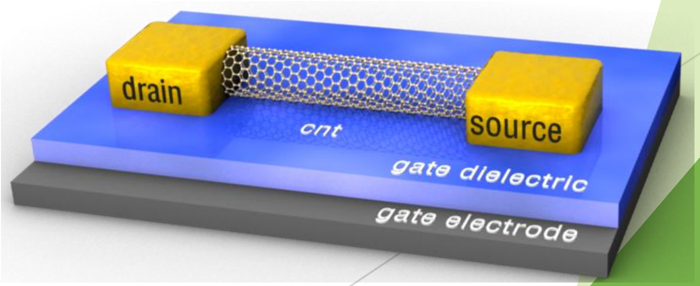
Conventional devices



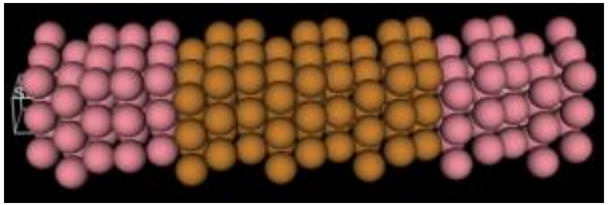

Molecular devices



Novel material devices

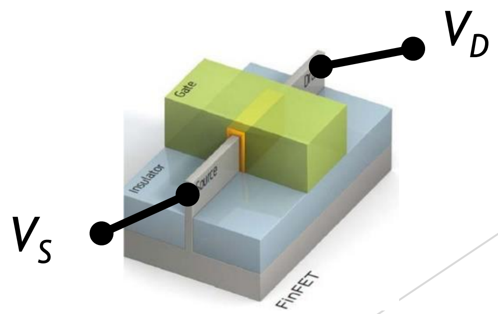



Spin electronic devices



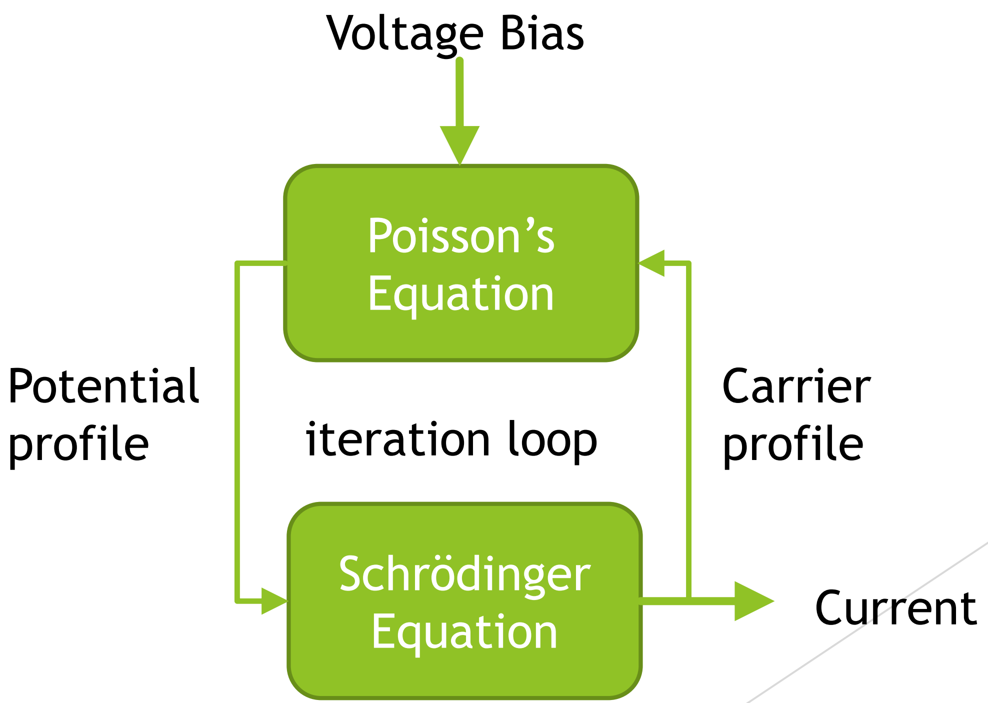
# Quantum Transport NEGF

- NEGF
  - “Non-equilibrium Green’s Function”
  - A method to solve quantum transport numerically
- Equilibrium
  - all chemical potential (Fermi level) gradients are zero
  - ie. $V_D=V_S$
- Non-equilibrium



# Numerical Quantum Transport

- Given $V_D$, $V_S$, $V_G$, etc.
- Solve for $I_{DS}$ , electron profile, potential profile
- How?

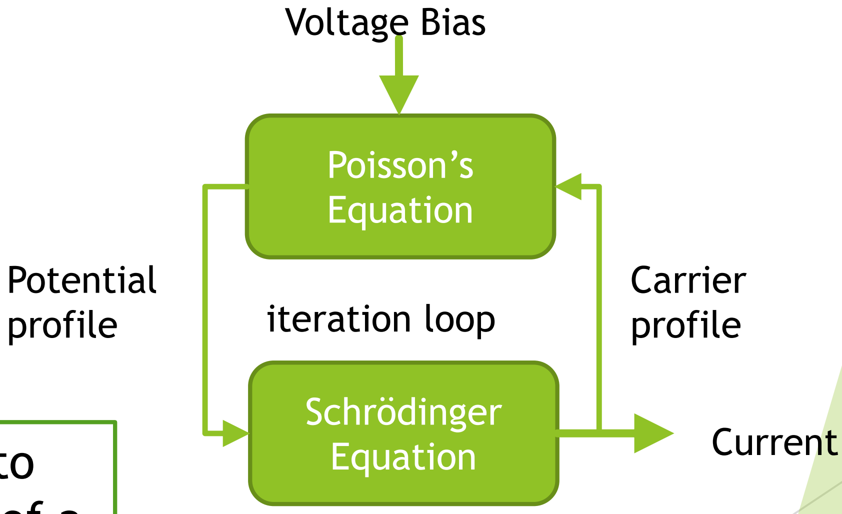


# Numerical Quantum Transport

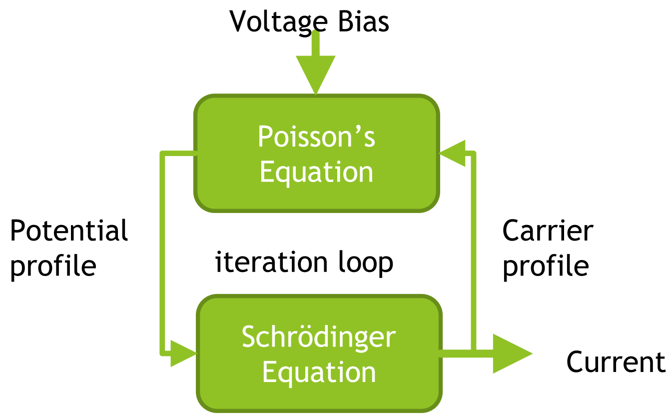
- Numerical Poisson's Equation

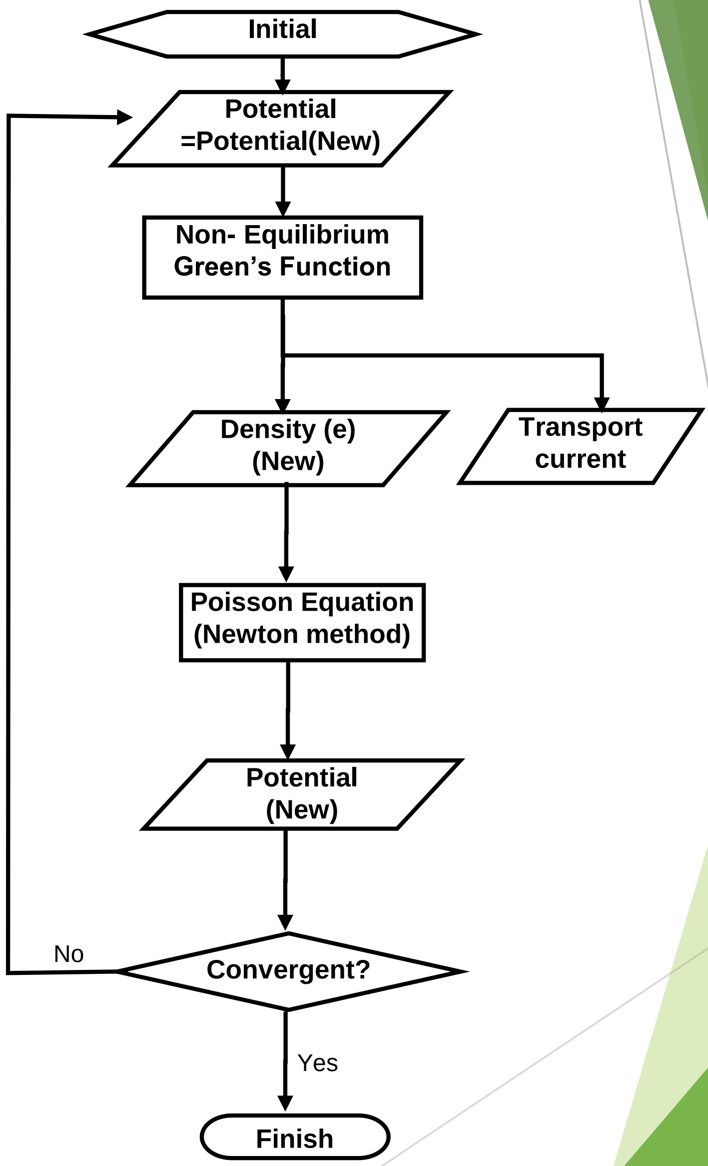
  $\nabla^2 U = Q/\epsilon$

  - Learnt on 5/16
  - Newton Iteration
- Schrodinger Equation
  - Solve using NEGF



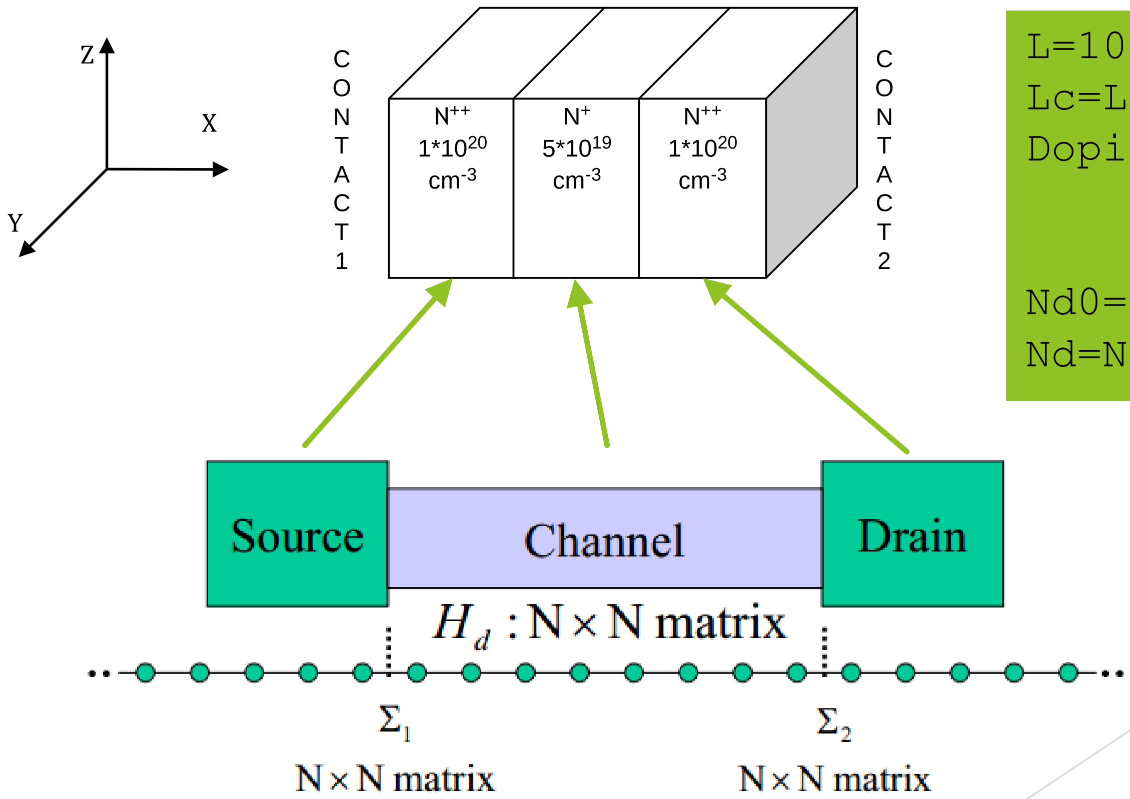

So, NEGF is a method to solve Schrodinger Eqn of a non-equilibrium system


Voltage Bias
Poisson's Equation
Potential profile
iteration loop
Carrier profile
Schrödinger Equation
Current


Initial
Potential =Potential(New)
Non- Equilibrium Green's Function
Density (e) (New)
Transport current
Poisson Equation (Newton method)
Potential (New)
Convergent?
No
Yes
Finish

# Numerical Quantum Transport Example 1: 1D silicon resistor

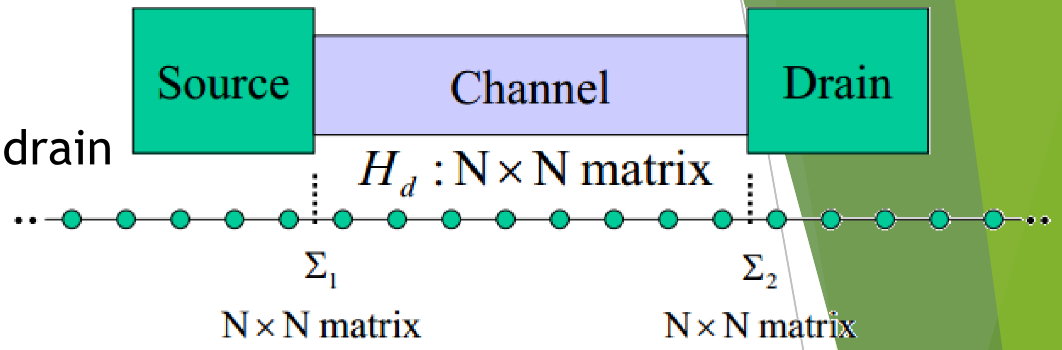
- 1D device with a large cross-section (effectively infinite in y-z)




```
L=100;  Ls=15/100*L;
Lc=L-2*Ls;    a=3e-10;
Doping=[ones(Ls,1);...
        1/2*ones(Lc,1);...
        ones(Ls,1)];
Nd0=1e26;
Nd=Nd0*Doping;
```

$H$: Hamiltonian of channel

$\Sigma_{1,2}$: Self energy of source/drain




NEGF Formulism:

$$G(E)_{N\times N} = \left[\left(E + i0^+\right)I - H - \Sigma_1(E) - \Sigma_2(E)\right]^{-1}$$ **Green's function**

$$\Gamma_{1,2}(E)_{N\times N} = i\left[\Sigma_{1,2}(E) - \Sigma_{1,2}(E)^+\right]$$

$$A_{1,2}(E)_{N\times N} = G(E)\Gamma_{1,2}(E)G(E)^+$$ **spectral function**

$$A(E)_{N\times N} = A_1(E) + A_2(E)$$ **DOS*2π**

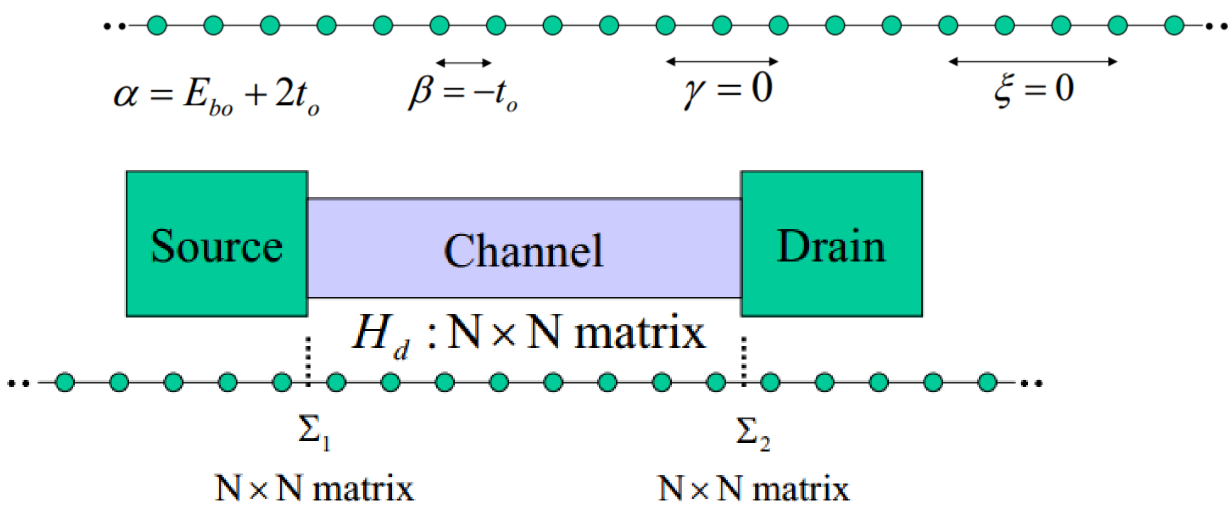
$$\left[\rho_k\right]_{N\times N} = \frac{1}{2\pi}\int_{-\infty}^{+\infty}\left[f_0(E+E_k-E_{F1})A_1(E) + f_0(E+E_k-E_{F1})A_2(E)\right]dE$$

$$\left[\rho\right]_{N\times N} = \sum_k \frac{1}{2\pi}\int_{-\infty}^{+\infty}\left[f_0(E+E_k-E_{F1})A_1(E) + f_0(E+E_k-E_{F1})A_2(E)\right]dE$$

$$= \frac{1}{2\pi}\int_{-\infty}^{+\infty}\left[F_0(E-E_{F1})A_1(E) + F_0(E-E_{F1})A_2(E)\right]dE$$ **Electron density**

$$I = (-q)Trace(\left[\rho\right]\left[J_{op}\right])$$ **current**

Recall tight binding model ...



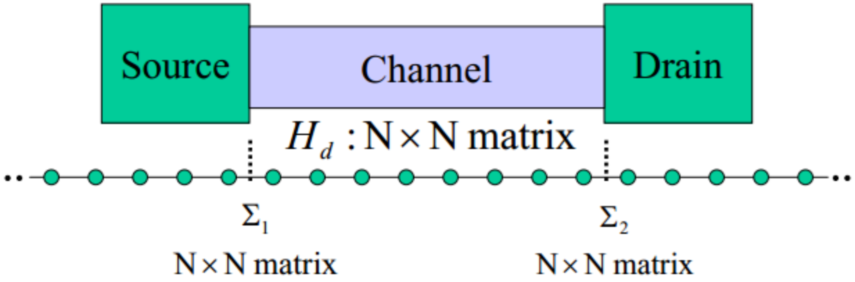

$$H = \begin{bmatrix} 2t_0 + U(x_1) & -t_0 & & \\ -t_0 & 2t_0 + U(x_2) & \ddots & \\ & \ddots & \ddots & -t_0 \\ & & -t_0 & 2t + U(x_n) \end{bmatrix}$$

where $t_0 = \dfrac{\hbar^2}{2m_n^*(dx)^2}$

$U(x) = E_c(x)$

(use conduction band as potential energy)

```
h_=1.06e-34; q=1.6e-19; m0=9.1e-31;
m=.25*m0; t=h_^2/(2*m*a^2)/q; L=100;
HL= diag(-t*ones(L-1,1), 1) ...
   +diag(2*t*ones(L,1))...
   +diag(-t*ones(L-1,1),-1)+diag(U);
```




$$\Sigma_1 = \begin{bmatrix} \frac{-e^{ik_1 dx}\hbar^2}{2m^*(dx)^2} & 0 & \cdots \\ 0 & 0 & \ddots \\ \vdots & \ddots & \ddots \end{bmatrix} = \begin{bmatrix} -t\exp(ik_1 dx) & 0 & \cdots \\ 0 & 0 & \ddots \\ \vdots & \ddots & \ddots \end{bmatrix}$$

$$\Sigma_2 = \begin{bmatrix} \ddots & \ddots & \vdots \\ \ddots & 0 & 0 \\ \cdots & 0 & -t\exp(ik_n dx) \end{bmatrix}$$

$$k_n dx = \arccos\left(1 - \frac{E - U_n}{2t}\right)$$

```
Sigma1=zeros(L);
k1a=acos(1-(E+i0-U(1))/(2*t));
Sigma1(1,1)=-t*exp(1i*k1a);
```

```
Sigma2=zeros(L);
kLa=acos(1-(E+i0-U(L))/(2*t));
Sigma2(L,L)=-t*exp(1i*kLa);
```

$$\Gamma_{1,2}(E)_{N\times N} = i\left[\Sigma_{1,2}(E) - \Sigma_{1,2}(E)^+\right]$$

```
Gamma1=1i*(Sigma1-Sigma1');
Gamma2=1i*(Sigma2-Sigma2');
```

$$G(E)_{N\times N} = \left[\left(E + i0^{+}\right)I - H - \Sigma_1(E) - \Sigma_2(E)\right]^{-1}$$

$$A_{1,2}(E)_{N\times N} = G(E)\Gamma_{1,2}(E)G(E)^{+}$$

$$A(E)_{N\times N} = A_1(E) + A_2(E)$$

```
G=inv((E+i0)*eye(L)-HL-Sigma1-Sigma2);
A1=G*Gamma1*G';
A2=G*Gamma2*G`;
A=A1+A2;
```

Fermi dirac func

Transport energy

Transverse energy

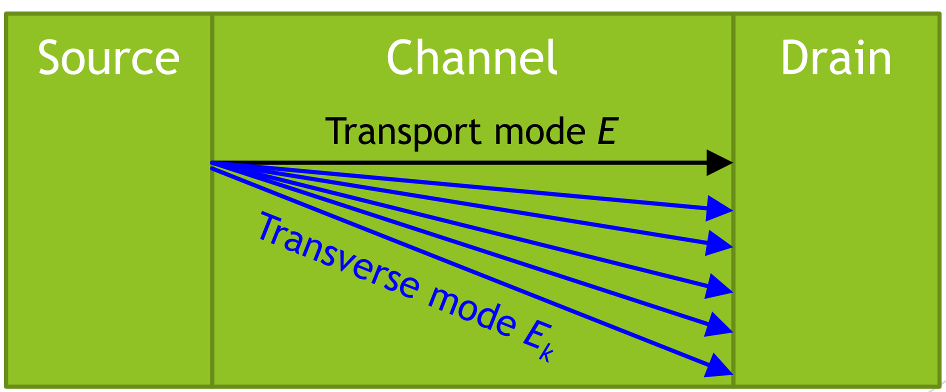
$$[\rho_k]_{N\times N} = \frac{1}{2\pi}\int_{-\infty}^{+\infty}[f_0(E+E_k-E_{F1})A_1(E)+f_0(E+E_k-E_{F1})A_2(E)]dE$$

$$[\rho]_{N\times N} = \sum_k \frac{1}{2\pi}\int_{-\infty}^{+\infty}[f_0(E+E_k-E_{F1})A_1(E)+f_0(E+E_k-E_{F1})A_2(E)]dE$$

$$= \frac{1}{2\pi}\int_{-\infty}^{+\infty}[F_0(E-E_{F1})A_1(E)+F_0(E-E_{F1})A_2(E)]dE$$

$$f_0(E-\mu) \equiv \left(1+\frac{1}{\nu}\exp[(E-\mu)/k_\mathrm{B}T]\right)^{-1}$$

$$F_0(E-\mu) = \sum_{\boldsymbol{k}} f_0(E+\varepsilon_{\boldsymbol{k}}-\mu) = S\frac{mk_\mathrm{B}T}{\pi\hbar^2}\ln\left(1+\exp\left(\frac{\mu-E}{k_\mathrm{B}T}\right)\right)$$



$$F_0(E-\mu) = \sum_{\boldsymbol{k}} f_0(E+\varepsilon_{\boldsymbol{k}}-\mu) = S\frac{mk_{\mathrm{B}}T}{\pi\hbar^2}\ln\left(1+\exp\left(\frac{\mu-E}{k_{\mathrm{B}}T}\right)\right)$$

```
function F=F0(E_miu)
    global m h_ kT S q
    F=S*m*kT*q/(pi*h_^2)*log(1+exp(-(E_miu)/kT));
end
```

$$[\rho]_{N\times N} = \frac{1}{2\pi}\int_{-\infty}^{+\infty}\left[F_0(E-E_{F1})A_1(E)+F_0(E-E_{F1})A_2(E)\right]dE \quad = \int_{-\infty}^{+\infty} d\rho$$

$$d\rho = \frac{1}{2\pi}\left[F_0(E-E_{F1})A_1(E)+F_0(E-E_{F1})A_2(E)\right]$$

```
drho=1/(2*pi)*(F0(E-miu1)*A1+F0(E-miu2)*A2);
```

$$[\rho]_{N\times N} = \int_{-\infty}^{+\infty} d\rho$$

```
rho=quadv(@(E)NEGF(E,U,HL,miu1,miu2,Ec0,L),
                              E_Min,E_Max,Nd0*a/L);
```

$$d\rho = \frac{1}{2\pi}\left[F_0(E-E_{F1})A_1(E) + F_0(E-E_{F1})A_2(E)\right]$$

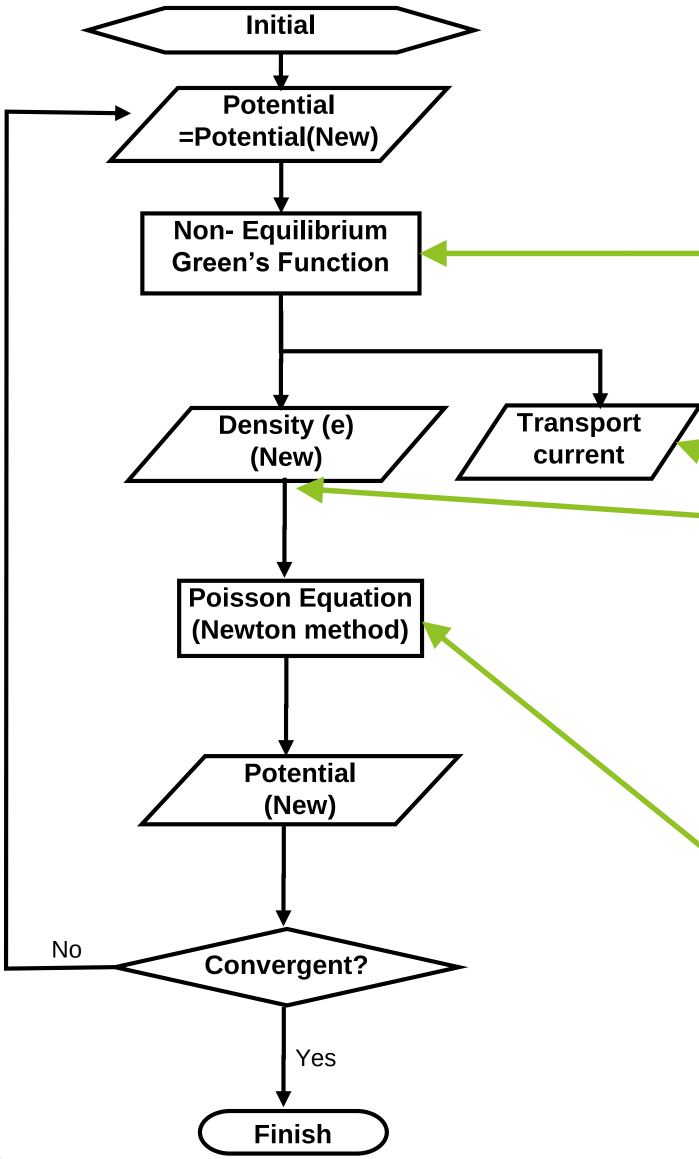
```
function drho=NEGF(E,U,HL,miu1,miu2,Ec0,L)
    global i0
    Sigma1=zeros(L); % Self-energy 1
    k1a=acos(1-(E+i0-Ec0-U(1))/(2*t));
    Sigma1(1,1)=-t*exp(1i*k1a);
    Gamma1=1i*(Sigma1-Sigma1');
    Sigma2=zeros(L); % Self-energy 2
    kLa=acos(1-(E+i0-Ec0-U(L))/(2*t));
    Sigma2(L,L)=-t*exp(1i*kLa);
    Gamma2=1i*(Sigma2-Sigma2');
    % Green's Function
    G=inv((E+i0)*eye(L)-HL-Sigma1-Sigma2
    A1=G*Gamma1*G';
    A2=G*Gamma2*G';
    A=A1+A2;
    drho=1/(2*pi)*(F0(E-miu1)*A1+F0(E-miu2)*A2);
end
```

$$\left[J_{op}\right] = \frac{\hbar}{2m^* dx^2}\begin{bmatrix} 0 & -i & & \\ i & \ddots & \ddots & \\ & \ddots & \ddots & -i \\ & & i & 0 \end{bmatrix}$$

```
Jop=-(t*q)/(h_*L)*
    (1i*diag(ones(L-1,1),-1)
    +(-1i)*diag(ones(L-1,1),1));
```

$$I = (-q) Trace(\left[\rho\right]\left[J_{op}\right])$$

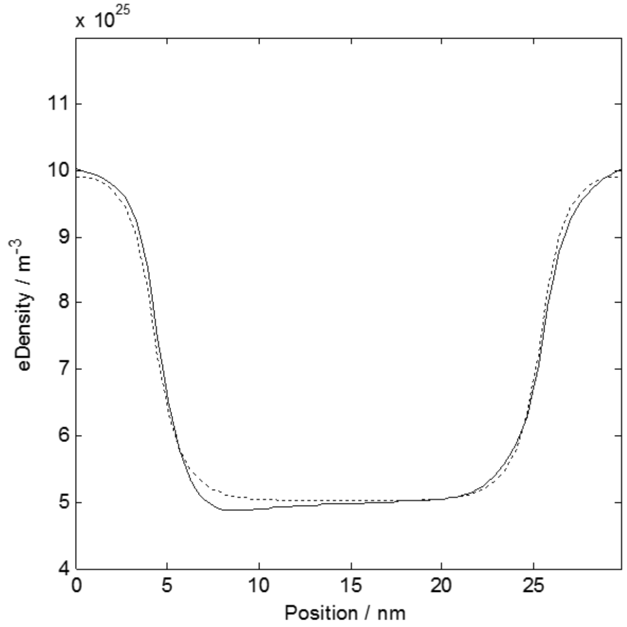
```
n_new=(1/a)*real(diag(rho));
I=real((-q)*trace(rho*Jop));
```



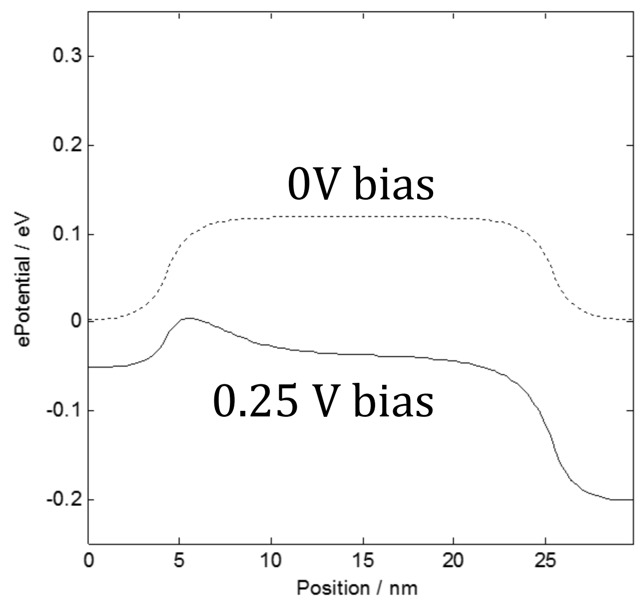

```
HL= diag(-t*ones(L-1,1), 1)
   +diag(2*t*ones(L,1))...
   +diag(-t*ones(L-1,1),-1)+diag(U);
rho=quadv(@(E)NEGF())
function drho=NEGF()
```

```
n=(1/a)*real(diag(rho));
I=real((-q)*trace(rho*Jop));
```

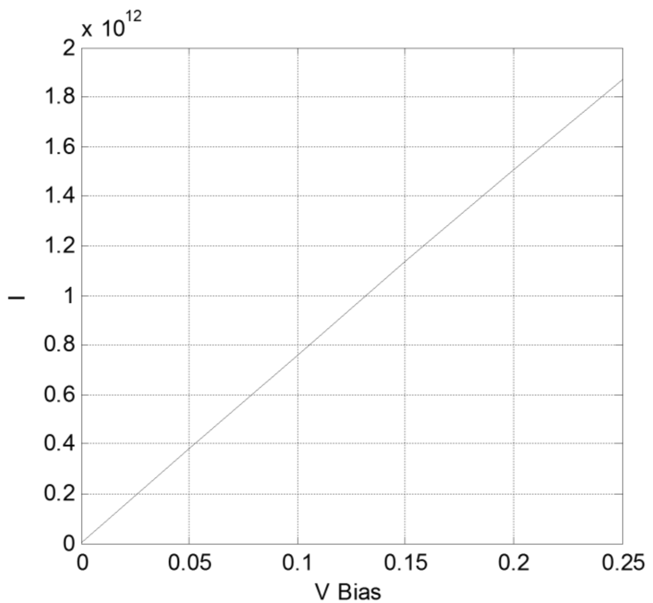
```
while norm(dU)>0.01*norm(U1)
  F_U1=epsilon*d2*U1+q*(n.*exp((U0-U1)/kT)-Nd);
  dF_U1=epsilon*d2+...
        diag((-1/kT)*q*n.*exp((U0-U1)/kT));
  dU=dF_U1\F_U1;
  U2=U1-dU;
  U1=U2;
end
```



x 10^25
11
10
9
8
7
6
5
4
eDensity / m^-3
0
5
10
15
20
25
Position / nm

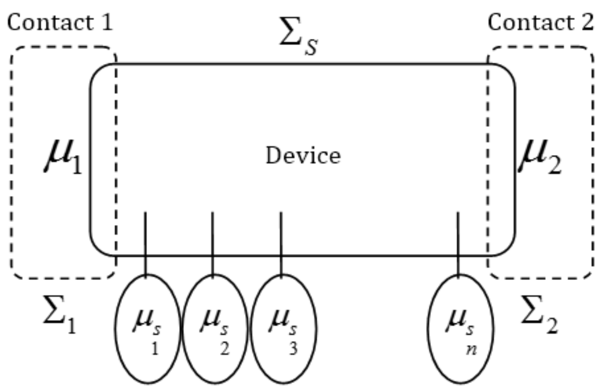



0.3
0.2
0.1
0
-0.1
-0.2
ePotential / eV
0V bias
0.25 V bias
0
5
10
15
20
25
Position / nm

x 10^12
2
1.8
1.6
1.4
1.2
1
0.8
0.6
0.4
0.2
0
I
0
0.05
0.1
0.15
0.2
0.25
V Bias

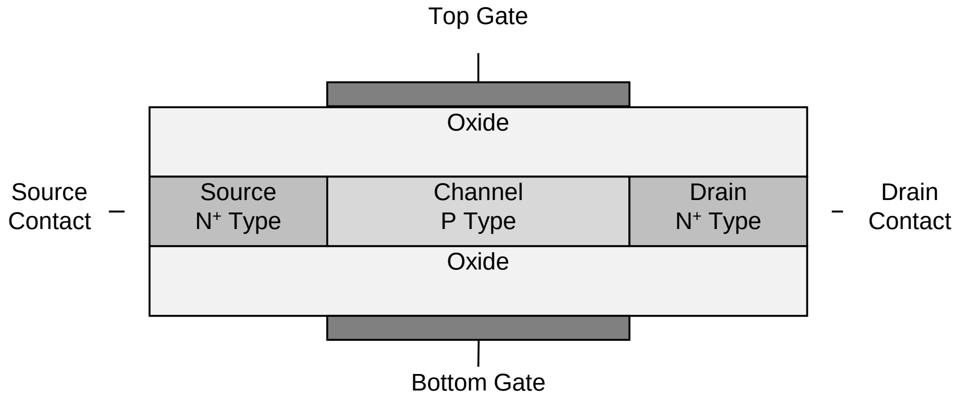
# Extension – NEGF with Scattering

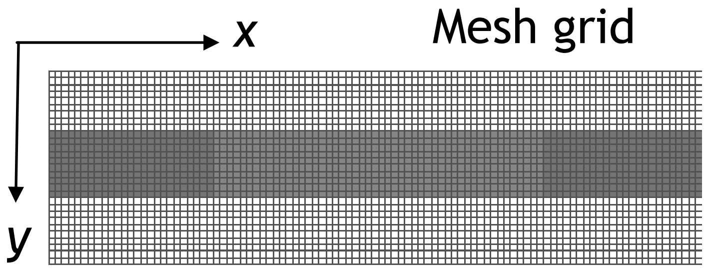



$$G = \left[ EI - H - \Sigma_1 - \Sigma_2 - \Sigma_S \right]^{-1}$$

$$\Sigma_S = -i \begin{bmatrix} \eta_1 & & & \\ & \eta_2 & & \\ & & \eta_3 & \\ & & & \ddots \end{bmatrix}$$

# Numerical Quantum Transport Example 2: 2D Double gate MOSFET



$$\left[-\frac{\hbar^2}{2m_x^*}\frac{\partial}{\partial x^2}-\frac{\hbar^2}{2m_y^*}\frac{\partial}{\partial y^2}+U(x,y)\right]\psi(x,y)=E\psi(x,y)$$

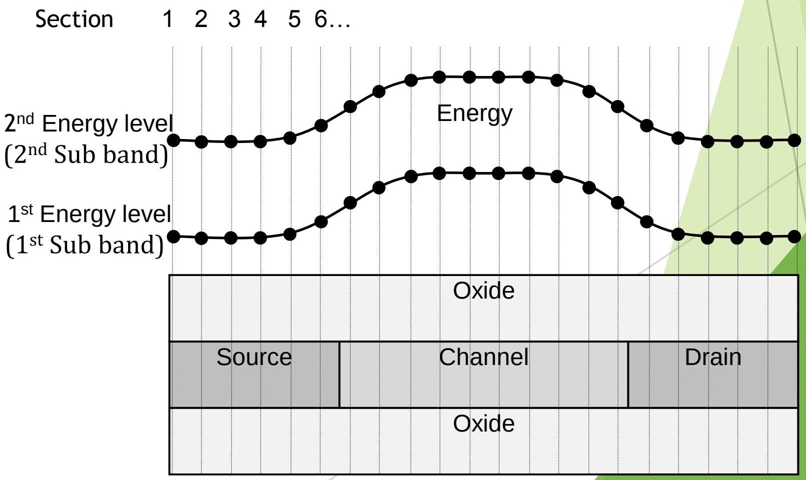
$$m_x^*=0.97m_e \qquad m_y^*=0.19m_e$$

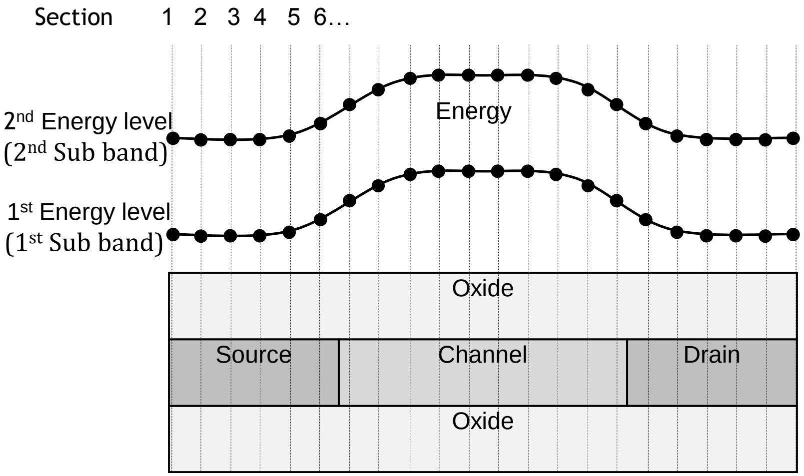
$$\psi(x,y)=X(x)\psi(y)=A(x)e^{ik(x)x}\psi(y)$$

1D Schrödinger Equation on transverse dimension

$$\left[-\frac{\hbar^2}{2m_y^*}\frac{\partial}{\partial y^2}+U_x(y)\right]\psi_x(y)=E_{x,t}\psi_x(y)$$

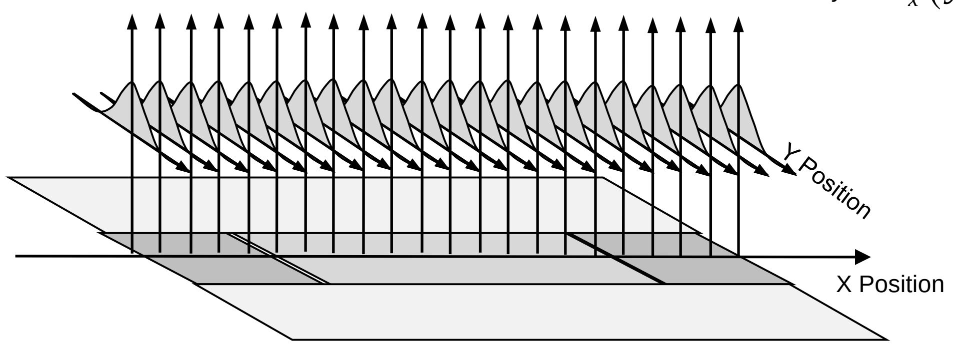
$$E_{x,t}=E-\hbar^2k_x^2/2m_x^*$$

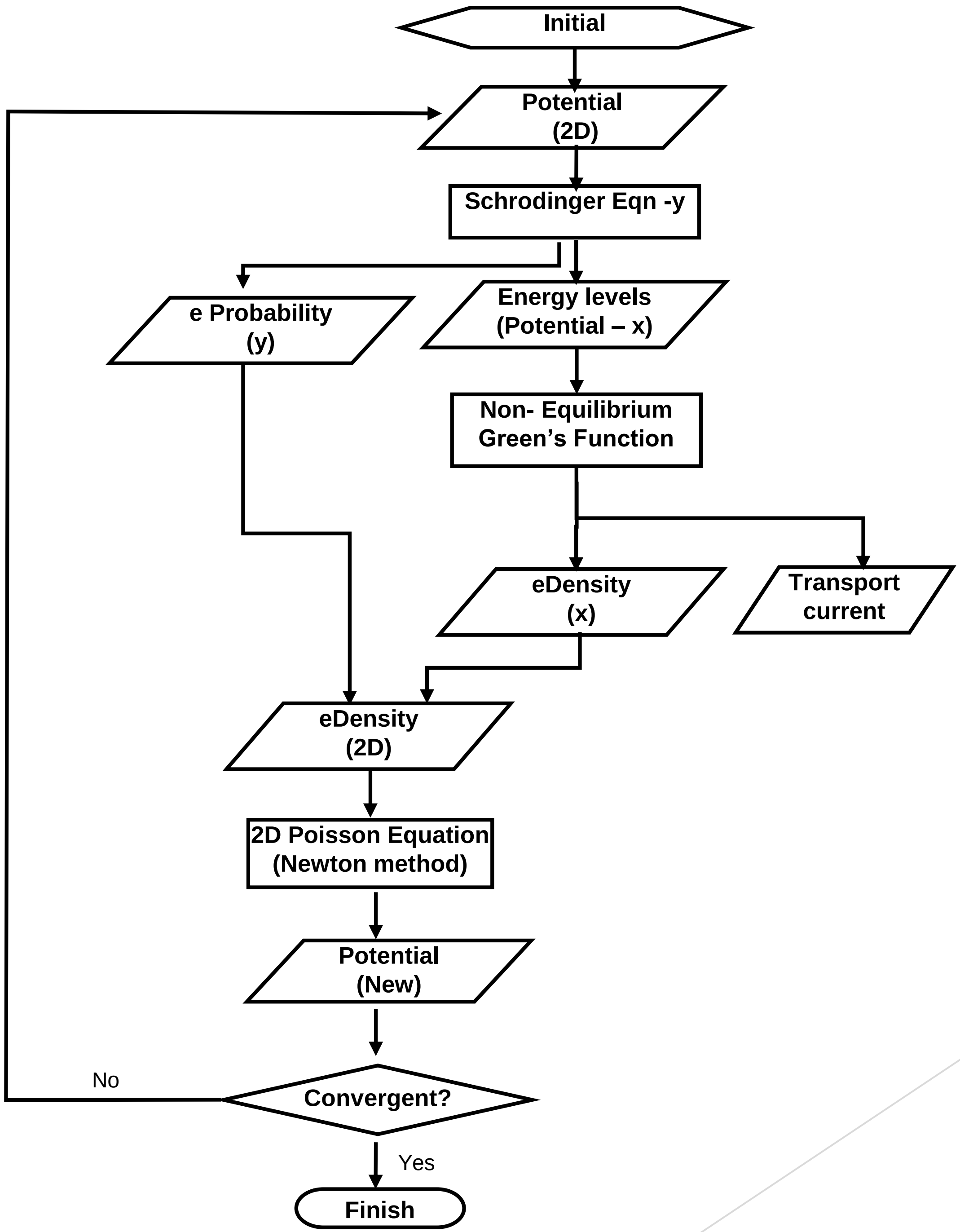


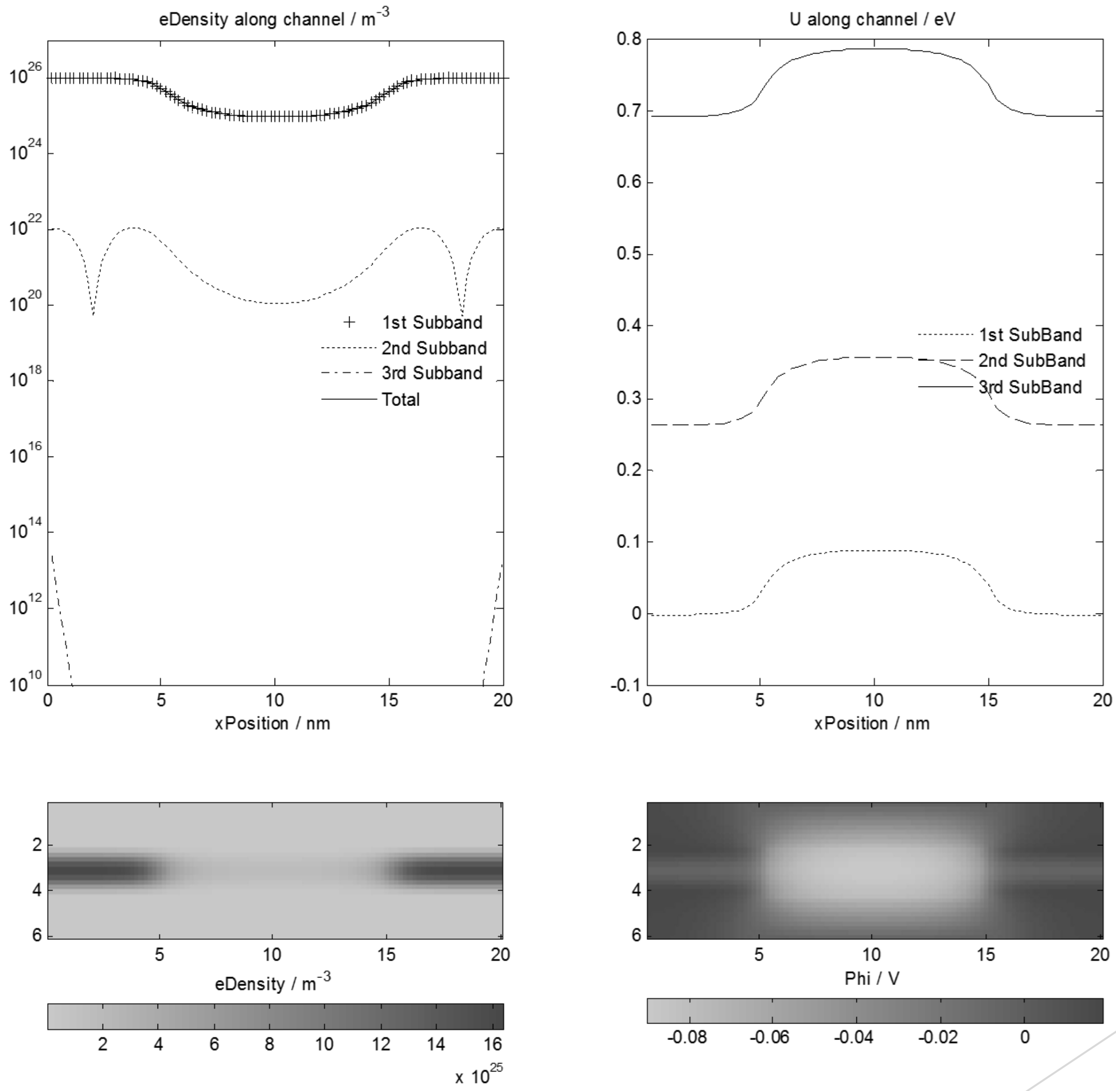



Possibility $\Psi_x(y) = \psi_x(y)^+ \psi_x(y)$

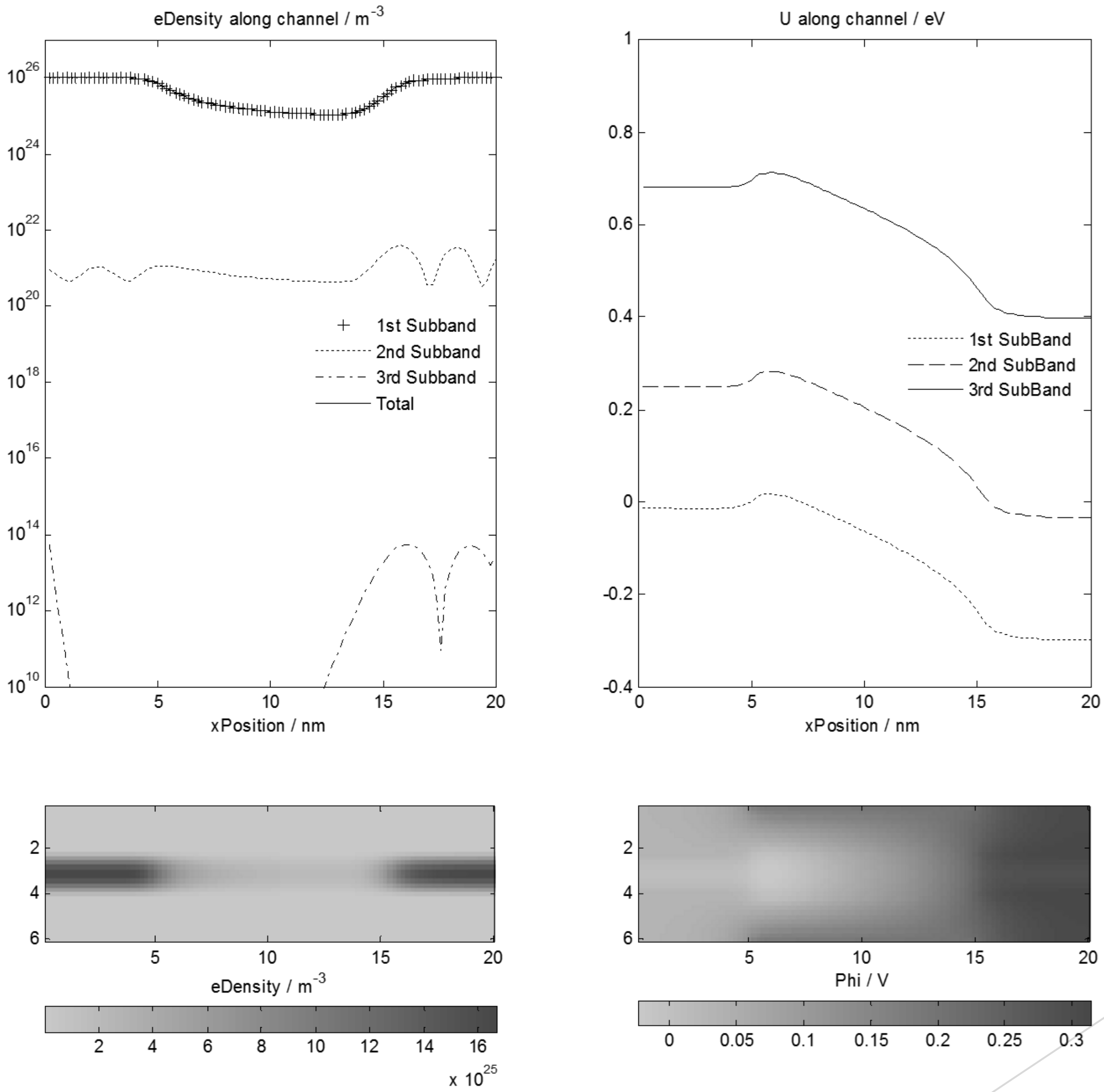
$$\int_{y\min}^{y\max} \Psi_x(y)dy = 1$$



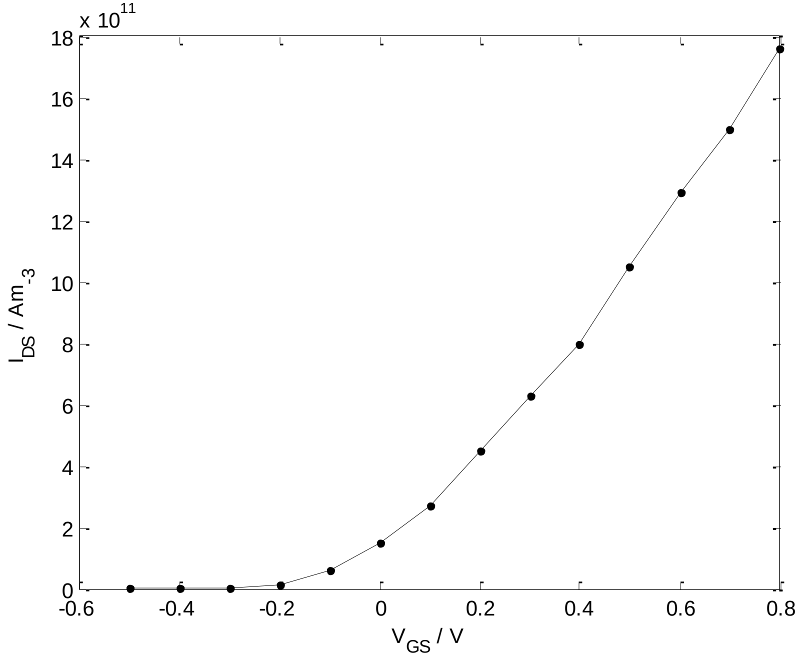

Initial
Potential
(2D)
Schrodinger Eqn -y
e Probability
(y)
Energy levels
(Potential – x)
Non- Equilibrium
Green's Function
eDensity
(x)
Transport
current
eDensity
(2D)
2D Poisson Equation
(Newton method)
Potential
(New)
No
Convergent?
Yes
Finish

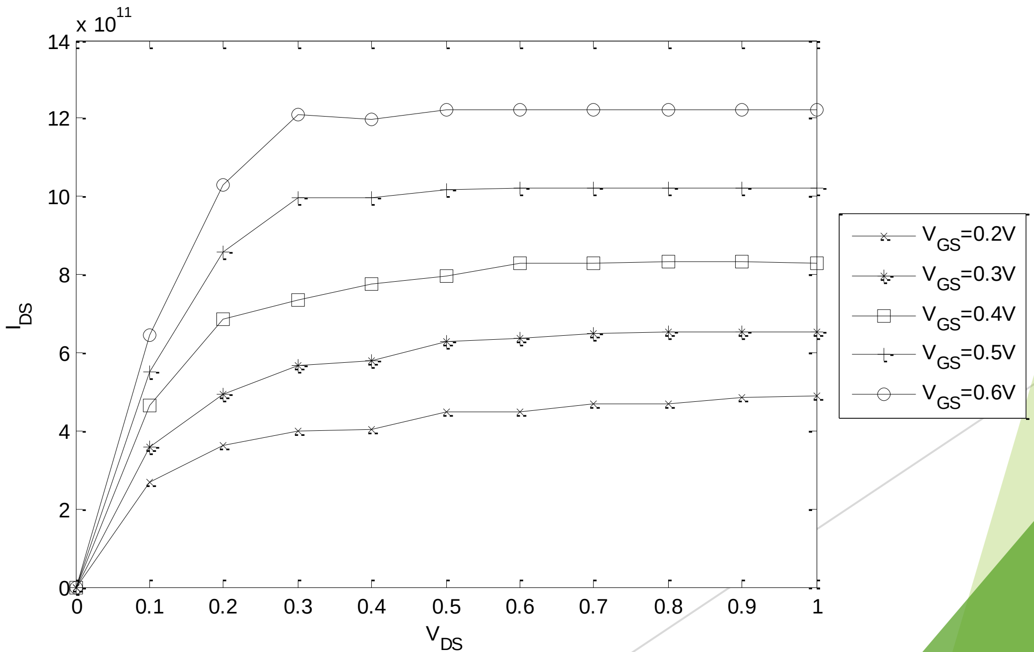


eDensity along channel / m^-3
1st Subband
2nd Subband
3rd Subband
Total
xPosition / nm
U along channel / eV
1st SubBand
2nd SubBand
3rd SubBand
xPosition / nm
eDensity / m^-3
x 10^25
Phi / V



eDensity along channel / m-3
1st Subband
2nd Subband
3rd Subband
Total
xPosition / nm
U along channel / eV
1st SubBand
2nd SubBand
3rd SubBand
xPosition / nm
eDensity / m-3
x 10^25
Phi / V


x 10^11
18
16
14
12
10
8
6
4
2
0
-0.6
-0.4
-0.2
0
0.2
0.4
0.6
0.8
I_DS / Am_-3
V_GS / V


x 10^11
14
12
10
8
6
4
2
0
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
I_DS
V_DS
V_GS=0.2V
V_GS=0.3V
V_GS=0.4V
V_GS=0.5V
V_GS=0.6V