Boundary treatments of quantum transport in non-equilibrium Green's function and Wigner distribution methods for RTD

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CASCAMM, U. of Maryland, March 8-11, 2010

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Outline

1. Introduction
   - Structure of the RTD (Resonant Tunneling Diode)
   - NEGF & Wigner Models

2. Quantum Transport Models
   - 1D Non-equilibrium Green Function (NEGF)
   - 1D Wigner Equation
   - Self-consistent model and algorithm

3. Numerical Results

4. Conclusion

5. Further Work

Introduction

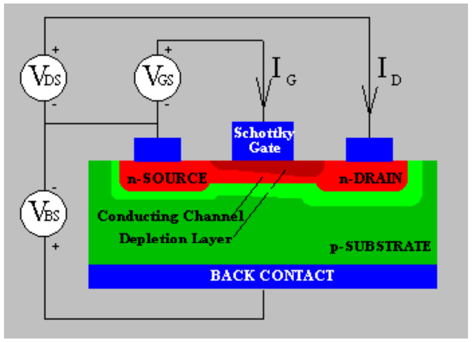
Basics on Quantum Transport in Nano-Devices

- Device length vis the mean free path

$$L << l_{mpf}$$

Channel Length $L = 20nm$

Mean free path $l_{mpf} = 100nm$



- Electron maintains coherence

$\Longrightarrow$ Quantum interference

Ballistic Transport

- Schrodinger wave description needed

Transport beyond Boltzman Equations

Intra-collusion Effects

Mean Free Path Time t_{mfp}

Collusion Duration Time t_{col} Fermi Golden Rule

$$t_{mfp} \approx t_{col}$$

- Incomplete Collusions
- nonlocality of scattering
- Memory effects
- multiple Scatterings

Transport beyond Boltzmann Equations

--- Effects from Non-Markovian processes

An Hierarchy of Models for Micro-to-NanoDevices

- Micro-Devices: $L > 1\mu m$

Drift-Diffusion models, $L < 0.1\mu m$

- submicron devices:
  non equilibrium, semi-classical Boltzmann, hydrodynamics models

- Nanodevices:

  ✓ **quantum interference (time and spatial correlations)**
  ✓ **many body scattering effect**
  ✓ **time dependent external fields**

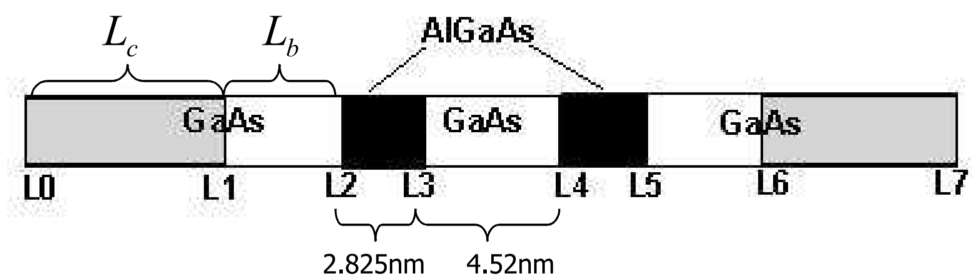
$G(r,t,r',t')$

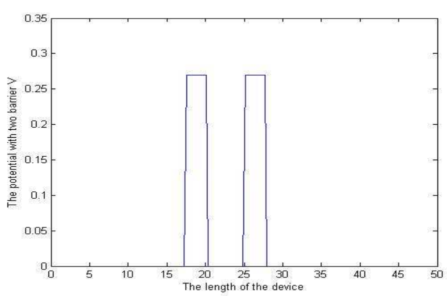
Nonequilibrium Green's function (quantum interference, many body scattering)

Density matrix $\rho(r,r',t) = \overline{\psi^*(r',t)\psi(r,t)}$

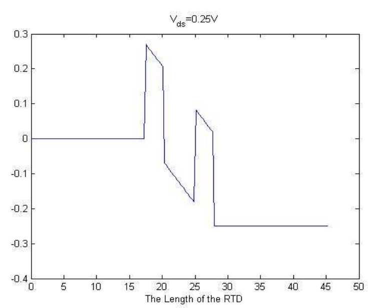
Wigner distributions (Spatial correlation) $f(R,k,t)$

Resonant Tunneling Diode (RTD) (Tsu & Esaki, 1970)





No External Bias



with External Bias

Superlattice and negative differential conductivity in semiconductors L **Esaki**, R **Tsu** - IBMJ RES DEVELOP, 1970

Tunneling in a finite superlattice R **Tsu**, L **Esaki**, Applied Physics Letters 22, 562 (1973)]

Quantum Transport Models

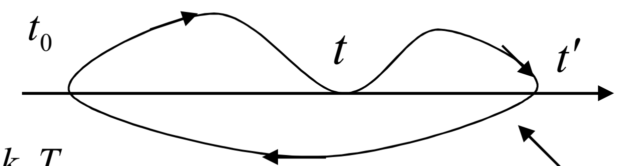
- Non-equilibrium Green’s Functions
- Wigner Distributions

Nonequilibrium Green's function for Many Body System

$$G(1,1') \equiv G(x,t,x',t') = -i < T_C \Psi_H(1)\Psi_H^+(1') >$$

Second quantization

Contour ordered



Time Contour C

$$H = H_0 + H'(t)$$

$$< O > = Tr[\rho_0 O_H] \qquad \rho_0 = \frac{\exp(-\beta H_0)}{Tr[\exp(-\beta H_0)]}, \beta = 1/k_B T$$

$$G(1,1') = \theta(t-t')G^>(1,1') + \theta(t'-t)G^<(1,1')$$

Correlation Functions

$$G^<(1,1') = +i < \Psi_H^+(1')\Psi_H(1) >$$ Correlation function

$$G^>(1,1') = -i < \Psi_H(1)\Psi_H^+(1') >$$

Dyson Equation

$$\{i\frac{\partial}{\partial t} - h(x,\nabla_x)\}G(x,t,x',t') = \delta(1-1') + \int_C d\sigma \int d^3y \Sigma(x,t,y,\sigma)G(y,\sigma,x',t')$$

$$h(x,\nabla_x) = -\frac{1}{2}\nabla_x^2 + V(x,t)$$

Quantum Boltzmann Equation (Kadanoff-Baym formulation)

$$[i\frac{\partial}{\partial t} - h(x,\nabla_x)]G^<(x,t,x',t') - [-i\frac{\partial}{\partial t'} - h(x',\nabla_{x'})]G^<(x,t,x',t') = Coll.$$

$$h(x,\nabla_x) = -\frac{1}{2}\nabla_x^2 + V(x,t)$$

$$Coll = \{G^>\Sigma^< - \Sigma^> G^<\} - G^R\Sigma^< + \cdots$$

$$[i\frac{\partial}{\partial t} - h(x,\nabla_x)]G^R(x,t,x',t') = \delta(1-1') + \int_C d\sigma \int d^3y \Sigma^R(x,t,y,\sigma)G^R(y,\sigma,x',t')$$

Key Quantity: Self Energy

Σ = Effects of Scattering events and Geometry

$G^<(x,t,x',t')$ Correlation function (fluctuations)

$A = -i\,\mathrm{Im}\{G^R\}$ Spectral density (dissipations)

Wigner Equations

Center of Mass System $R = \frac{1}{2}(x + x')$ $r = x - x'$

$T = \frac{1}{2}(t + t')$ $\tau = t - t'$

$$(r,\tau) \to (k,\omega)$$

$$G^{<}(R,T,r,\tau) \to F(R,T,k,\omega) \equiv G^{<}(R,T,k,\omega)$$

Wigner Equation

$$[i\frac{\partial}{\partial T} + i\frac{k}{m}\nabla_R + qV_W]F(R,T,k,\omega) = Coll$$

$$V_W(f) = [V(R + i\frac{1}{2}\nabla_k, T - i\frac{1}{2}\frac{\partial}{\partial\omega}) - V(R - i\frac{1}{2}\nabla_k, T + i\frac{1}{2}\frac{\partial}{\partial\omega})]f(R,T,k,\omega)$$

$\tau \to 0$ $F(R,T,k,\omega) \to f_W(R,k,T)$ Wigner Distribution

Quantum tunneling

2.Quantum transport models

- 1D NEGF

3D Schrödinger equation

$$H\Psi = E\Psi, \quad H = -\frac{\hbar^2}{2m_x}\frac{\partial^2}{\partial x^2} - \frac{\hbar^2}{2m_y}\frac{\partial^2}{\partial y^2} - \frac{\hbar^2}{2m_z}\frac{\partial^2}{\partial z^2} + eV(x,y,z)$$

For RTD , it is reduced to an 1D Schrödinger equation

$$-\frac{\hbar^2}{2m_x}\frac{\partial^2\phi(x)}{\partial x^2} + v(x)\phi(x) = E\phi(x)$$

The potential of the form

$$v(x) = \begin{cases} v_1 & -\infty < x < X_1 \\ v(x) & X_1 < x < X_2 \\ v_2 & X_2 < x < +\infty \end{cases}$$

1D Green equation:

$$(E - v(x) - \frac{\hbar^2}{2m_x}\frac{\partial^2}{\partial x^2})G(x,x') = \delta(x - x')$$

left boundary condition :

$$G(x'_e, x') = e^{-ik_1(x'_e - X_1)}G(X_1, x'), x'_e \in (-\infty, X_1), x' \in [X_1, X_2]$$

right boundary condition:

$$G(x'_e, x') = e^{ik_2(x'_e - X_2)}G(X_2, x'), x'_e \in (X_2, -\infty), x' \in [X_1, X_2]$$

$$k_1 = \sqrt{\frac{2m_x(E - v_1)}{\hbar^2}}, \qquad k_2 = \sqrt{\frac{2m_x(E - v_2)}{\hbar^2}}$$

Finite Difference Method for the NEGF,

$$EI - H = \begin{pmatrix} \Delta_0 & t_x & 0 & \dots & \dots & \dots & \dots & \dots & \dots \\ t_x & \Delta_1 & t_x & 0 & \dots & \dots & \dots & \dots & \dots \\ 0 & t_x & \Delta_2 & t_x & \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots & t_x & \Delta_{N-2} & t_x & \dots \\ \dots & \dots & \dots & \dots & \dots & 0 & t_x & \Delta_{N-1} & t_x \\ \dots & \dots & \dots & \dots & \dots & \dots & 0 & t_x & \Delta_N \end{pmatrix}$$

where $t_x = \dfrac{\hbar^2}{2m_x a^2}$, and $\Delta_i = E - 2t_x - v(x_i)$

$$\Sigma_s(i,j) = -t_x e^{ik_1 a}\delta_{1,j}\delta_{1,i} \qquad \Sigma_d(i,j) = -t_x e^{ik_2 a}\delta_{N,j}\delta_{N,i}$$

$$\Gamma_s(i,j) = 2t_x \sin(k_1 a)\delta_{1,j}\delta_{1,i} \qquad \Gamma_d(i,j) = 2t_x \sin(k_2 a)\delta_{N,j}\delta_{N,i}$$

$$\left[EI - H - \Sigma_s - \Sigma_d\right]G = I$$

Green's function representation of electron density

Device Green function:

$$G = \left[EI - H - \Sigma_s - \Sigma_d\right]^{-1}$$

Spectral function:

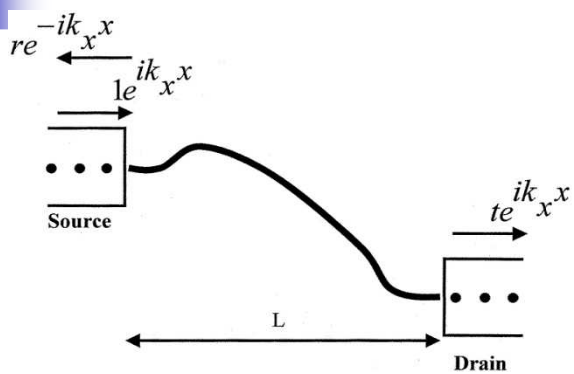
$$A_s = G\Gamma_s G^+, \qquad A_d = G\Gamma_d G^+$$

Self energy for environment (contacts) dissipation:

$$\Gamma_{s,d} = i(\Sigma_{s,d} - \Sigma_{s,d}^+)$$

$$\rho(x) = \frac{m^* k_B T}{2\pi^2 \hbar^2} \int \log(1 + e^{(\frac{\mu_s - E}{k_B T})}) A_s + \log(1 + e^{(\frac{\mu_s - E}{k_B T})}) A_d dE$$

Transmission Coefficients T & G



$$\phi(x) = \begin{cases} e^{ik_1 x} + re^{-ik_1 x}, x < X_1 \\ te^{ik_2 x}, x > X_2 \end{cases}$$

$$(EI - H - \Sigma_s - \Sigma_d)\begin{pmatrix} \phi(x_0) \\ \phi(x_1) \\ \vdots \\ \phi(x_N) \end{pmatrix} = \begin{pmatrix} i2t_x \sin(k_1 a) \\ 0 \\ \vdots \\ 0 \end{pmatrix}$$

$$\phi(x_0) = 2it_x \sin(k_1 a) G(1,1) \equiv iG(1,1)\Gamma_s(1,1)$$

electron current

$$j = \frac{\hbar}{2im_x}\left(\phi^*(x)\frac{\partial\phi(x)}{\partial x} - \phi(x)\frac{\partial\phi^*(x)}{\partial x}\right)$$

$$T^{s-d} = \frac{j_{transmitted}}{j_{incident}} = 1 - |r|^2 = 1 - |\phi(x_0) - 1|^2$$
$$= |G(1,1)|^2 \Gamma_s(1,1)\Gamma_d(N,N)$$

Transmission coefficient

In general

$$T^{s-d} = \mathrm{trace}(\Gamma_s \mathrm{G} \Gamma_\mathrm{d} \mathrm{G}^+)$$

Green's function representation of current density

Inflow current formula (Landauer or Tsu-Esaki formula)

$$I^{(\mathrm{in})} = \int I^{(\mathrm{in})}(E)dE = \frac{em^{*}k_B T}{2\pi^2\hbar^3}\int_0^{+\infty} \log(1+e^{(\frac{\mu-E}{k_B T})})\mathrm{T}^{\text{s-d}}(E)dE$$

$$I^{(\mathrm{in})}(E) = e\sum_{k_y\,k_z} T^{\text{s-d}}(E)F_f(\frac{\hbar^2 k_y^2}{2m_y} + \frac{\hbar^2 k_z^2}{2m_z} + E(k_x) - \mu)v_x(E(k_x))$$

Total current:

$$I = I^{(in)} - I^{(out)} \qquad I = \int_0^{+\infty} I(E)dE$$

$$I(E) = \frac{em^{*}k_B T}{2\pi^2\hbar^3}[\log(1+e^{(\frac{\mu_s-E}{k_B T})}) - \log(1+e^{(\frac{\mu_d-E}{k_B T})})]\mathrm{T}^{\text{s-d}}(E)$$

1D Wigner Equation

Density matrix:

$$\rho(x,x') = \frac{m^* k_B T}{\pi \hbar^2} \sum_{k_x} \log(1 + e^{(\frac{\mu - E(k_x)}{k_B T})}) \varphi(x, E(k_x)) \varphi^*(x', E(k_x))$$

Weyl transform:

$$R = \frac{x + x'}{2}, \quad r = x - x'$$

Wigner function is defined as

$$f(R,k) = \int_{-\infty}^{+\infty} \rho\left(R + \frac{r}{2}, R - \frac{r}{2}\right) e^{-ikr} dr$$

For a plane wave :

$$f^{\alpha}(R,k) = \int_{-\infty}^{+\infty} \varphi\left(R + \frac{r}{2}, E_{\alpha}\right) \varphi^*\left(R + \frac{r}{2}, E_{\alpha}\right) e^{-ikr} dr$$

Wigner equation:

$$-\frac{q\hbar^2}{m_x}\frac{\partial}{\partial x}f(x,k)-\frac{1}{2\pi}\int_{-\infty}^{\infty}V_w(x,k-k')f(x,k')dk'=0$$

Wigner potential:

$$V_w(x,k)=\int_{-\infty}^{+\infty}[v(x+\frac{r}{2})-v(x-\frac{r}{2})]e^{ikr}dr$$

Density function described by Wigner Function:

$$\rho\ (x)=\frac{1}{2\pi}\int_{-\infty}^{\infty}f_w(x,k)dk$$

Current density :

$$I(x)=e\int_{-\infty}^{+\infty}\frac{\hbar k}{m_x}f_w(x,k)dk$$

Truncations in the definition of Wigner potential

The original form of the second term in Wigner equation

$$\int_{-\infty}^{+\infty}[v(x+\frac{r}{2})-v(x-\frac{r}{2})]\rho(x+\frac{r}{2},x-\frac{r}{2})e^{-ikr}dr$$

Assumming $\rho(x+\frac{r}{2},x-\frac{r}{2})\rightarrow 0,\quad \text{as} \quad r\rightarrow\infty$

Truncate in Coherence length L_{coh} $\quad r \in (-\infty,+\infty)\rightarrow[-\frac{L_{coh}}{2},\ \frac{L_{coh}}{2}]$

$$\int_{-\frac{L_{coh}}{2}}^{+\frac{L_{coh}}{2}}[v(x+\frac{r}{2})-v(x-\frac{r}{2})]\rho(x+\frac{r}{2},x-\frac{r}{2})e^{-ikr}dr$$

Effective Wigner potential

$$\tilde{V}_w(x,k)=\int_{-\frac{L_{coh}}{2}}^{\frac{L_{coh}}{2}}[v(x+\frac{r}{2})-v(x-\frac{r}{2})]e^{ikr}dr$$

Mass conservation with full momentum k-space

$$\frac{\partial}{\partial t} f(x,k,t) + \frac{\hbar k}{m} \frac{\partial}{\partial x} f(x,k,t) + \int_{-\infty}^{+\infty} \tilde{V}_w(x,k-k') f(x,k',t) dk' = 0$$

- Electron density

$$\mathrm{n}(x,t) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} f(x,k,t) \mathrm{d}k.$$

- Current density

$$\mathrm{j}(x,t) = \frac{\hbar}{2\pi m} \int_{-\infty}^{+\infty} k f(x,k,t) \mathrm{d}k.$$

- we define

$$p(x,t) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} dk \int_{-\infty}^{+\infty} dk' \tilde{V}_w(x,k-k') f(x,k',t) = 0$$

- Noting ***$V_w(x,k)$* is odd in *k*,** we have the continuity equation

$$\frac{\partial}{\partial t} n(x,t) + \frac{\partial}{\partial x} j(x,t) = -p(x,t) \equiv 0$$

Truncation in phase space (x, k)

- Computation domain in k-space: $\Omega_k = [-\frac{L_k}{2}, \frac{L_k}{2}]$

$$n(x,t) = \frac{1}{2\pi}\int_{-\frac{L_k}{2}}^{\frac{L_k}{2}} f(x,k,t)dk \qquad j(x,t) = \frac{\hbar}{2\pi m}\int_{-\frac{L_k}{2}}^{\frac{L_k}{2}} kf(x,k,t)dk$$

$$p(x,t) = \frac{1}{2\pi}\int_{-\frac{L_k}{2}}^{\frac{L_k}{2}} dk \int_{-\frac{L_k}{2}}^{\frac{L_k}{2}} dk'\tilde{V}_w(x,k-k')f(x,k',t)$$

$$\frac{\partial}{\partial t}f(x,k,t) + \frac{\hbar k}{m}\frac{\partial}{\partial x}f(x,k,t) + \int_{-\frac{L_k}{2}}^{\frac{L_k}{2}} \tilde{V}_w(x,k-k')f(x,k',t)dk' = 0$$

$$\Downarrow$$

$$\frac{\partial}{\partial t}n(x,t) + \frac{\partial}{\partial x}j(x,t) = -p(x,t) = 0$$

Selection of Mesh h_k in k-space

$$k_j = jh_k$$

$$\tilde{V}_w(x,k_j) = \int_{-\frac{L_{coh}}{2}}^{\frac{L_{coh}}{2}} [v(x+\frac{r}{2}) - v(x-\frac{r}{2})] e^{ik_j r} dr$$

$$= 2\int_0^{\frac{L_{coh}}{2}} [v(x+\frac{r}{2}) - v(x-\frac{r}{2})] \sin(rk_j) dr$$

$$\approx h_{coh} \sum_{l=1}^{\frac{N_{coh}}{2}-1} \sin(r_l k_j)[*] + \frac{h_{coh}}{2} \sin(\frac{L_{coh}}{2} k_j)[*]$$

To use Fast Discrete Fourier Transform:

$$r_l k_j = l h_{coh} k_j = j \frac{l L_{coh} h_k}{N_{coh}}$$

$$h_k L_{coh} = 2\pi$$

Selection of Mesh h_{coh} in Wigner Potentials

Conservation condition:

$$p(x) = \frac{1}{2\pi}\int_{-\frac{L_k}{2}}^{\frac{L_k}{2}} dk \int_{-\frac{L_k}{2}}^{\frac{L_k}{2}} dk' \tilde{V}_w(x, k-k') f(x, k', t) = 0$$

$$\tilde{V}_w(x, k-k') = h_{coh} \sum_{l=1}^{\frac{N_{coh}}{2}-1} \sin(r_l(k-k'))[*] + \frac{h_{coh}}{2}\sin(\frac{L_{coh}}{2}(k-k'))[*]$$

$$\rightarrow \quad \int_{-\frac{L_k}{2}}^{\frac{L_k}{2}} \sin\left((k-k')r_l\right) dk = 0$$

$$\cos\left((\frac{L_k}{2} - k')r_l \right) - \cos\left((\frac{L_k}{2} - k')r_l - L_k r_l \right) = 0 \quad \rightarrow \quad \boxed{L_k h_{coh} = 2\pi}$$

$$L_{coh} h_k = 2\pi, \quad L_k h_{coh} = 2\pi, \quad N_k = \frac{L_k}{h_k} = \frac{L_{coh}}{h_{coh}} = N_{coh}$$

L_k Truncation in the k-space

L_{coh} Truncation in the coherence length

Frensley inflow boundary condition (1987) – a heuristic view

According to free electron (plane wave) source injection, the Wigner function is:

$$\varphi_m(x) = \begin{cases} e^{ik_1 x} + re^{-ik_1 x}, x < 0 \\ te^{ik_2 x}, x > L_x \end{cases}$$

$$f^m(x,q) = \int_{-\infty}^{+\infty} \varphi_m(x+\frac{r}{2})\varphi_m(x-\frac{r}{2})e^{-iqr}dr$$
$$= \delta(k_1 - q) + |r|^2 \delta(k_1+q) - i2r\sin(k_1 x)\delta(q)$$
$$(x < 0, k_1 > 0)$$

Boundary Condition:

$$f(X_1,q) = \frac{m^* k_B T}{\pi\hbar^2}\log\left(1+\exp(\frac{\mu_s - \frac{\hbar^2 q^2}{2m} - v_1}{k_B T})\right), q > 0$$

$$f(X_2,q) = \frac{m^* k_B T}{\pi\hbar^2}\log\left(1+\exp(\frac{\mu_s - \frac{\hbar^2 q^2}{2m} - v_2}{k_B T})\right), q < 0$$

The scheme of the Wigner equation

Upwind scheme:

$$\frac{\hbar q_j}{m_x}\frac{f_w(x_i,q_j)-f_w(x_{i-1},q_j)}{h_x}+\frac{1}{\pi\hbar}\sum_{j'=0}^{N_q-1}V_w(x_i,q_j-q'_{j'})f_w(x,q'_{j'})=0,\quad q_j>0$$

$$\frac{\hbar q_j}{m_x}\frac{f_w(x_{i+1},q_j)-f_w(x_i,q_j)}{h_x}+\frac{1}{\pi\hbar}\sum_{j'=0}^{N_q-1}V_w(x_i,q_j-q'_{j'})f_w(x,q'_{j'})=0,\quad q_j<0$$

By trapezoidal rule

$$V_w(x_i,q_j-q'_{j'})=h_{coh}\sum_{k=1}^{\frac{N_{coh}}{2}-1}\sin(kh_{coh}(q_j-q_{j'}))[v(x_{i+k})-v(x_{i-k})]$$

$$+\frac{h_{coh}}{2}\sin(\frac{L_{coh}}{2}(q_j-q_{j'}))[v(x_{i+N_r/2})-v(x_{i+N_r/2})]$$

Density formula:

$$\rho(x) = \frac{1}{2\pi} \sum_{j=0}^{N_q} f_w(x, q_j) h_q$$

Current formula:

$$j(x + \frac{h_x}{2}) = \frac{h_q}{2\pi} \left[\sum_{q_j < 0} \frac{\hbar q_j}{m_x} f_w(x + h_x, q_j) + \sum_{q_j > 0} \frac{\hbar q_j}{m_x} f_w(x, q_j) \right]$$

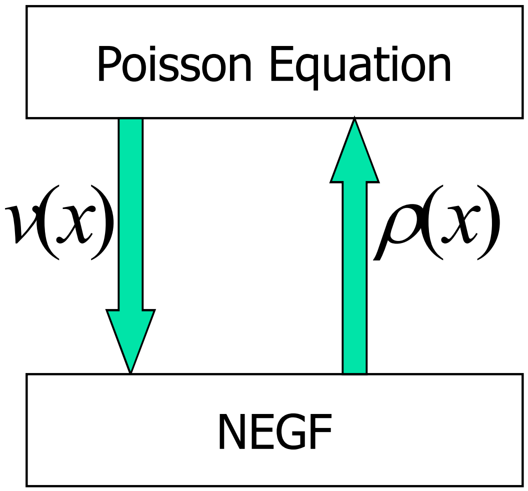
Self-consistent model and algorithm

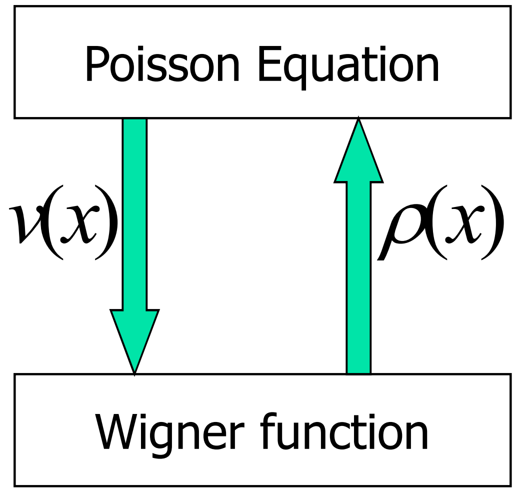
Poisson equation

$$-\frac{\partial}{\partial x}\left(\varepsilon(x)\frac{\partial}{\partial x}\right)v(x) = e(-\rho(x) + N_d(x))$$

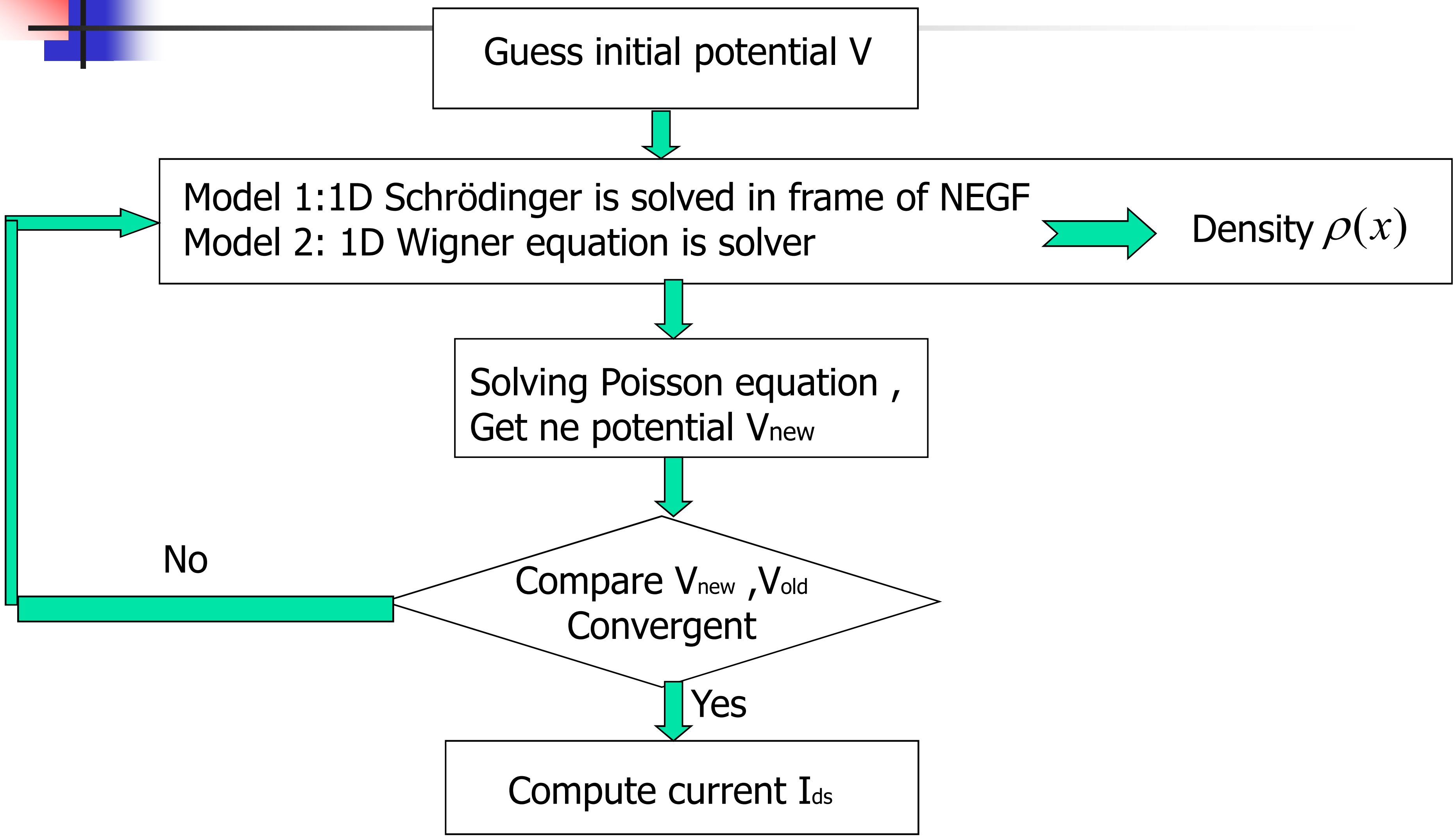
$$v(0) = 0, v(L) = -v_b$$

Self-consistent model



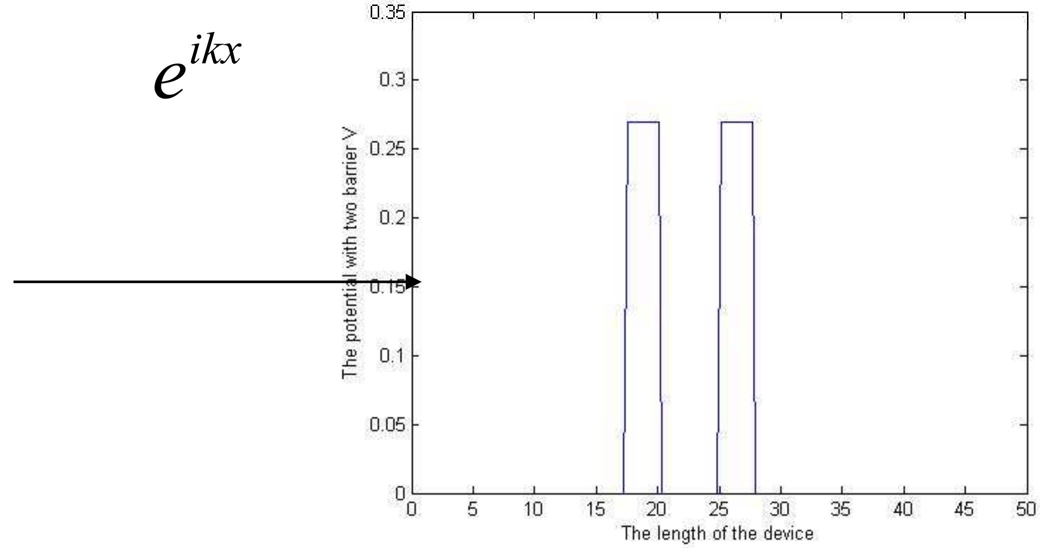


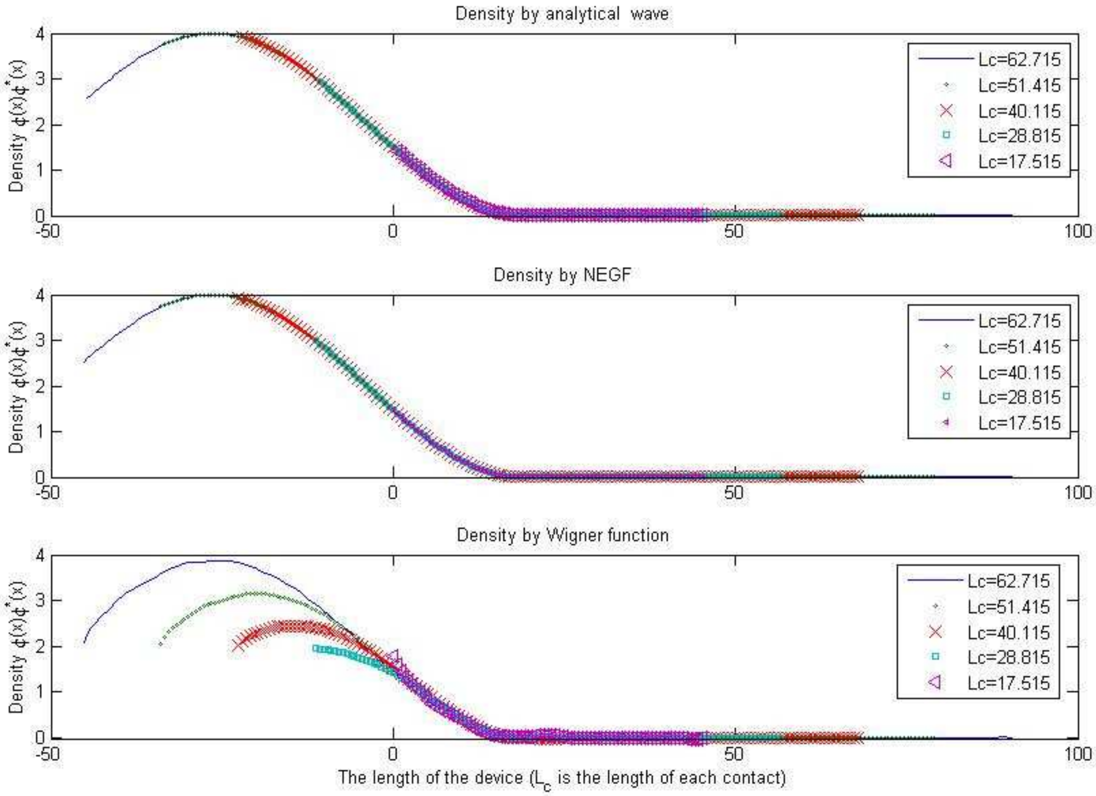
Self-consistent algorithm



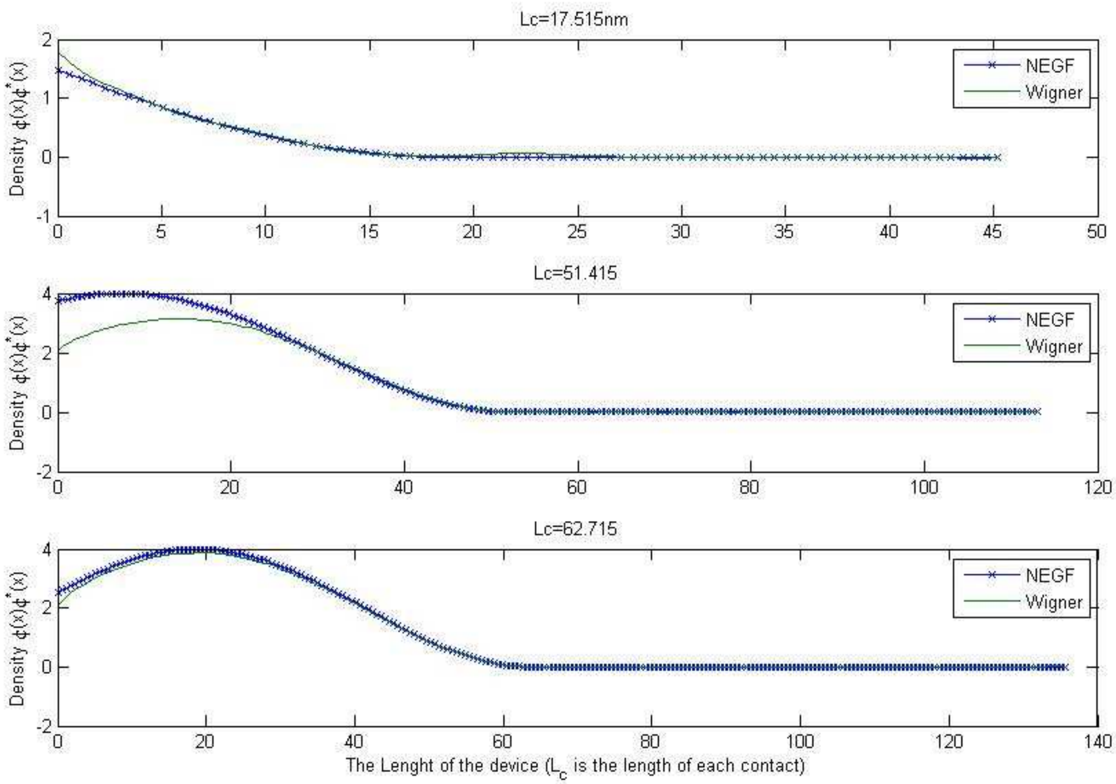
3. Numerical result

- Comparison of the boundary conditions:
  Analytic test case





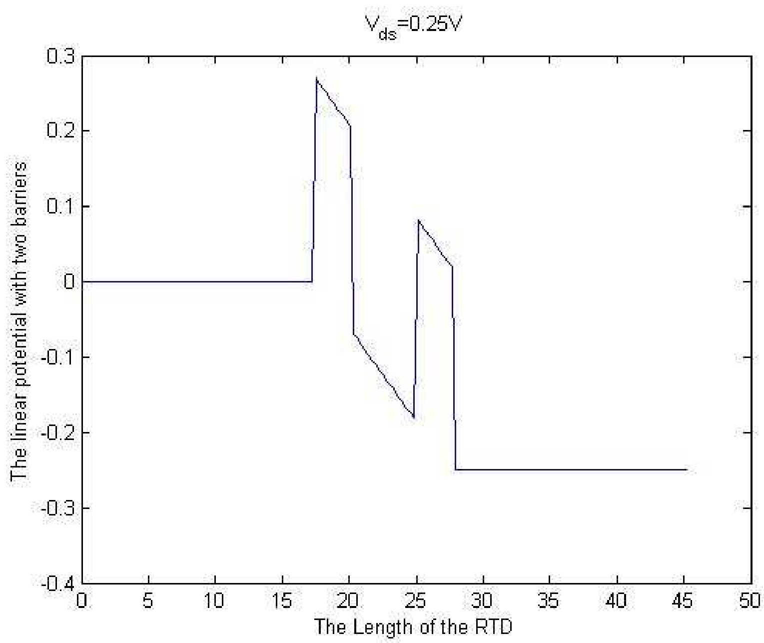
Density comparison of the Wave function, Green function and Wigner function methods



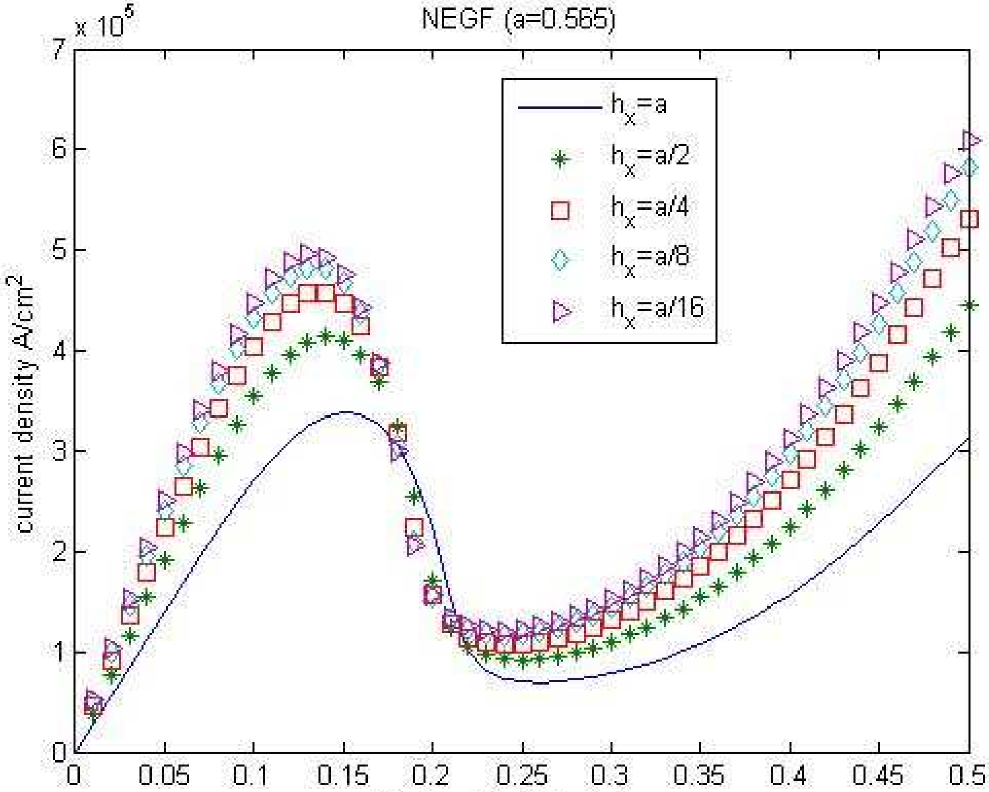
Density comparison of Green function and Wigner function method

Comparisons of IV curves of RTD by NEGF and Wigner Methods

IV curves with prescribed linear potential profile

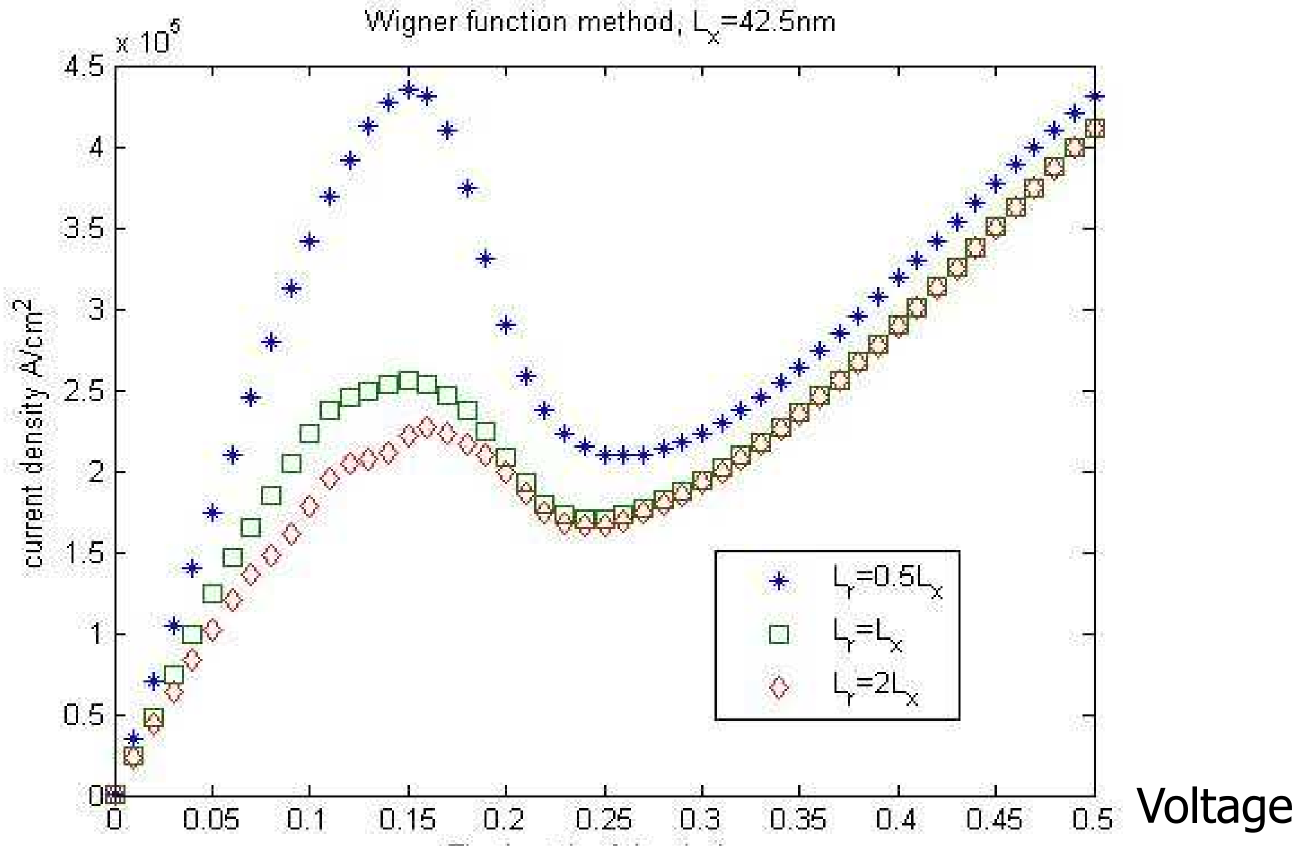


The convergence of the NEGF method – Mesh refinement



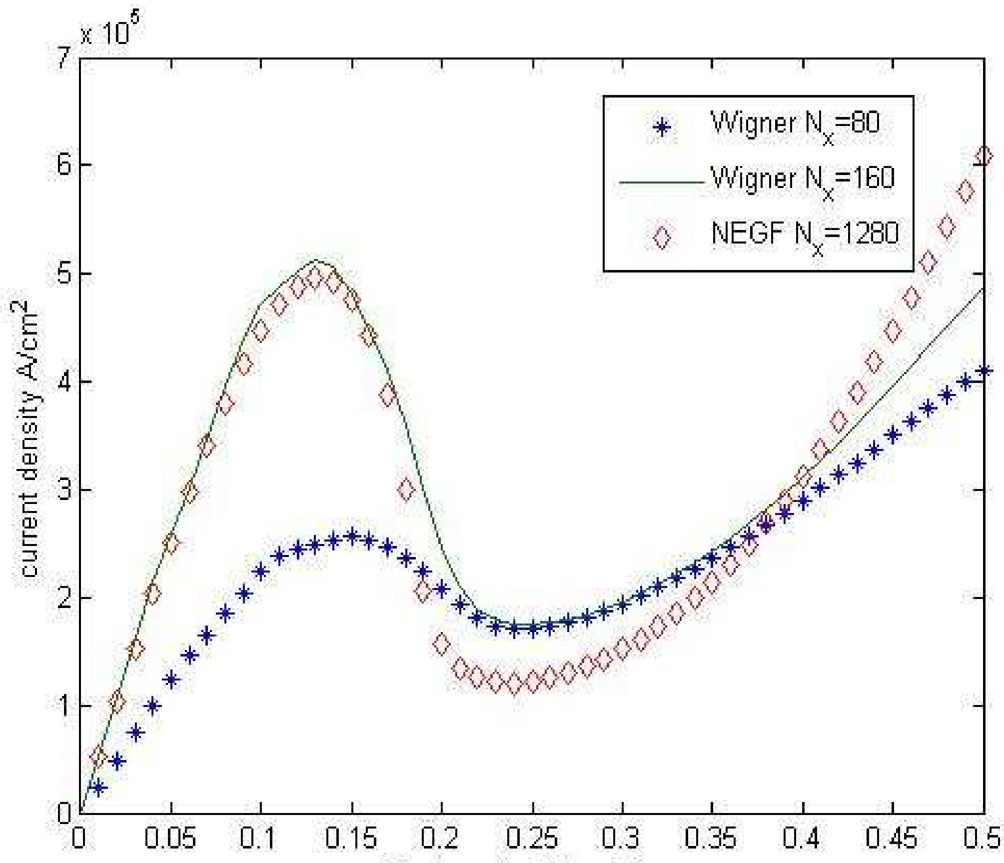
Voltage

Size of coherence length truncation h_{coh}, L_{coh}



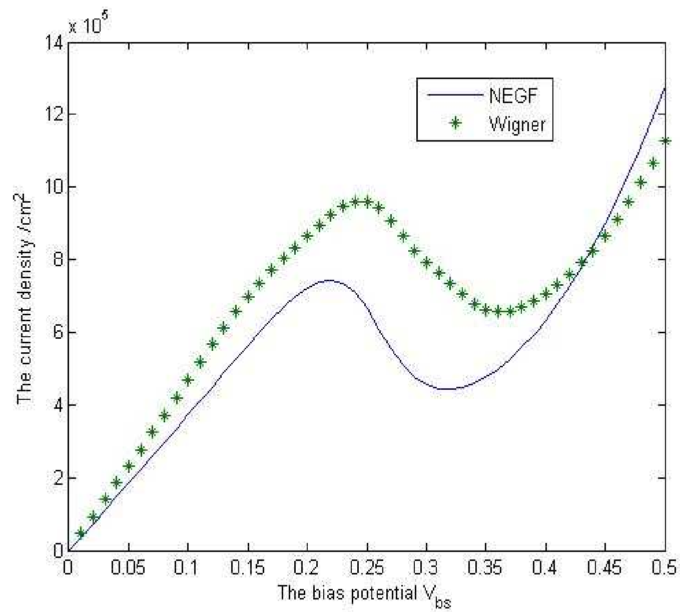
$$L_{coh} = 2L_x, h_{coh} = 1.3nm, h_x = 0.2825nm$$

Mesh Convergence of Wigner Method



Voltage

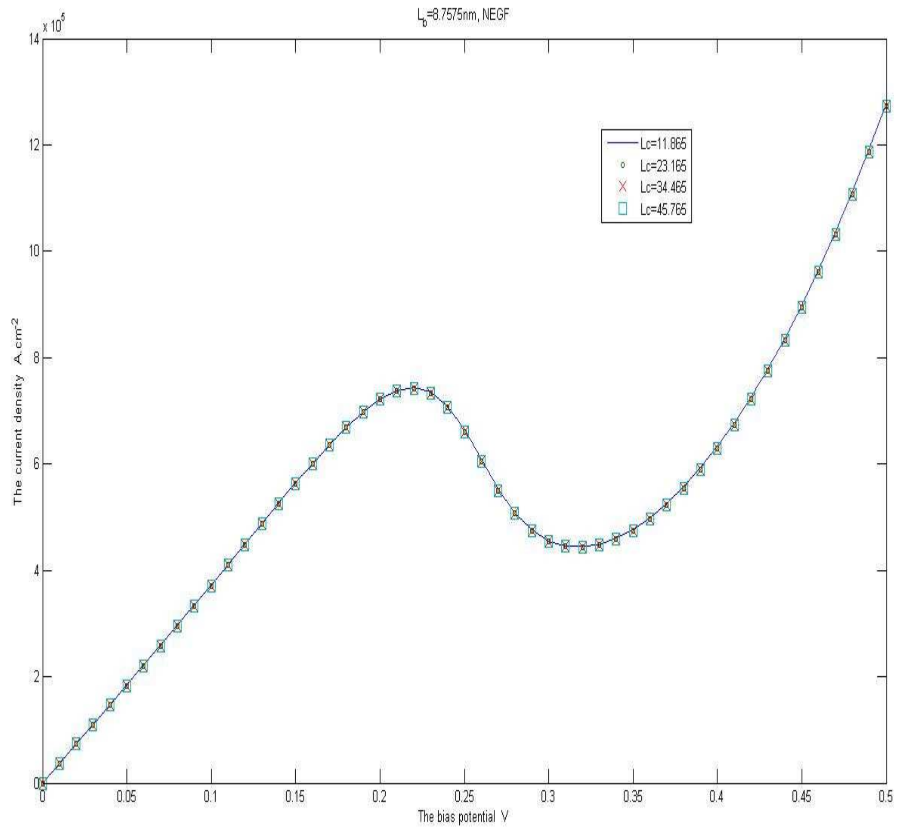
The self-consistent IV by the two transport methods



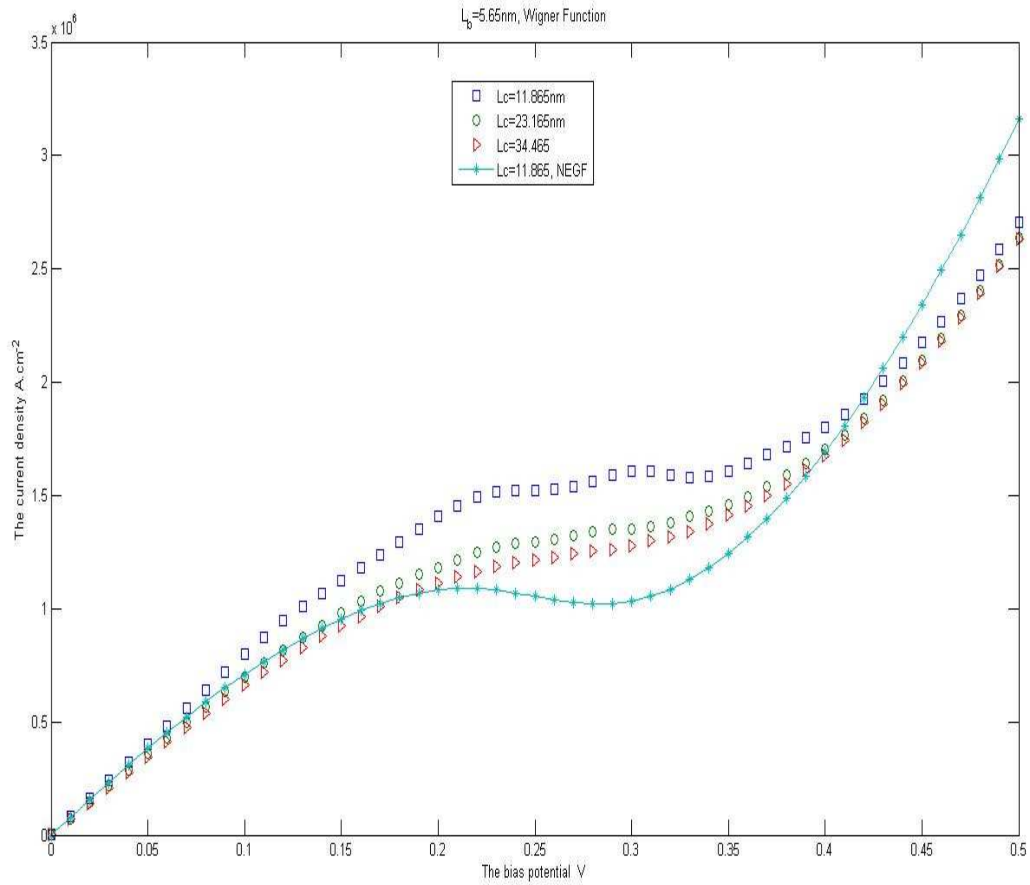
$$L_c = L_b = 8.7575nm$$

The current value computed by the Wigner equation is higher than that by the NEGF method.

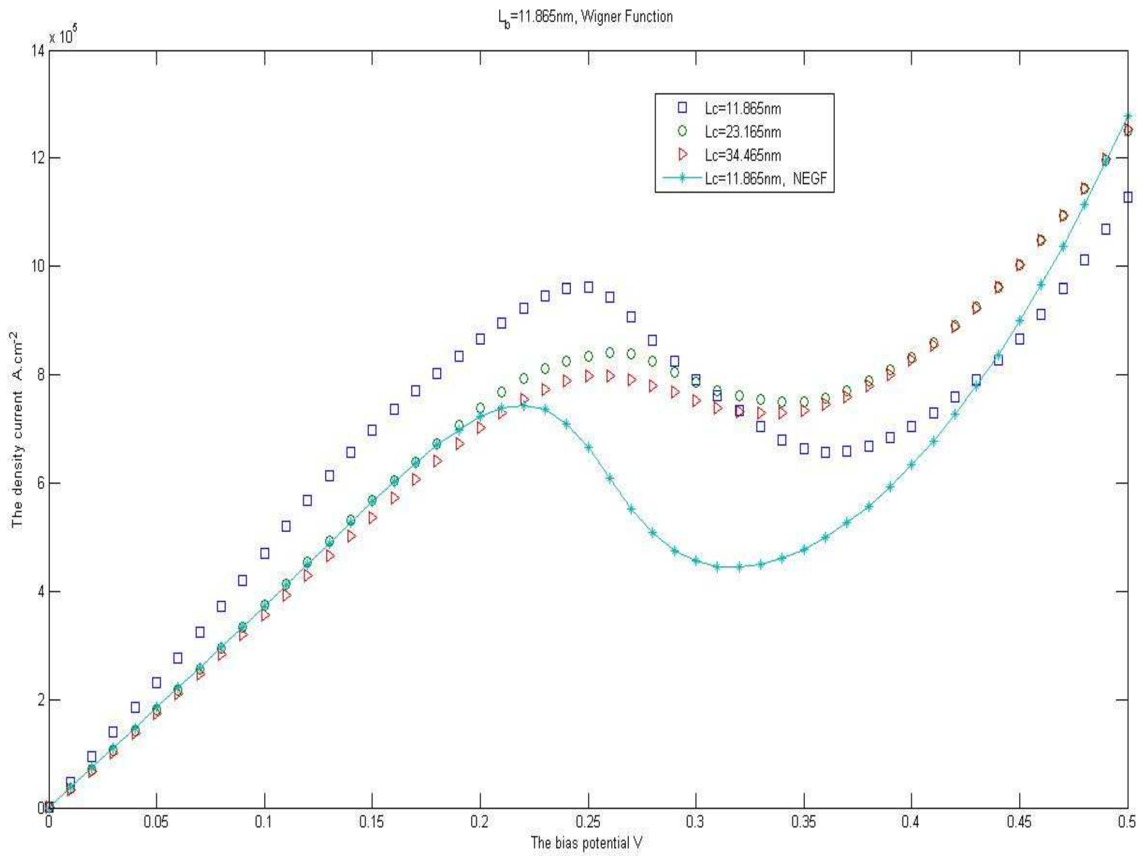
NEGF current and contact length L_c



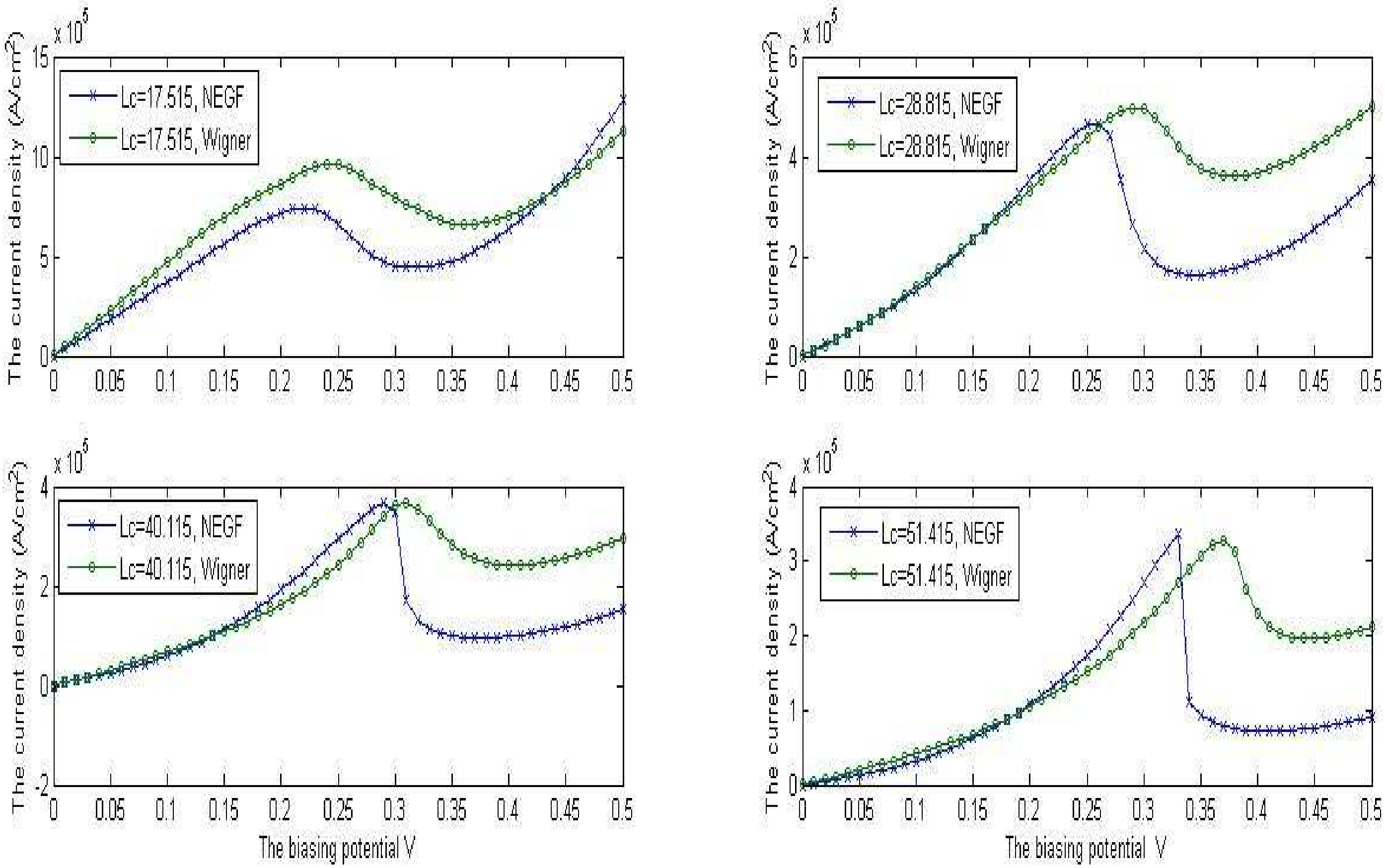
Wigner current & contact length L_c (1)



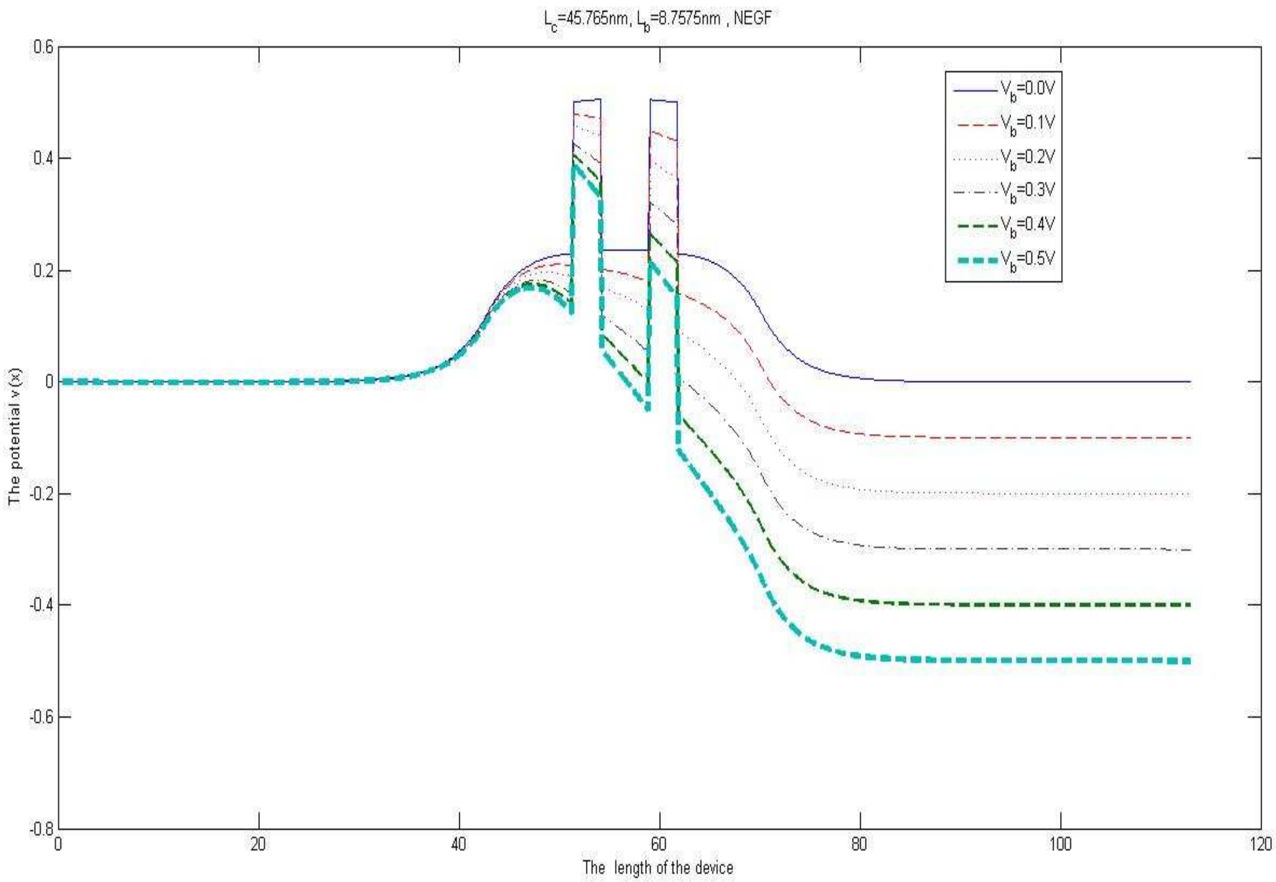
Wigner current & contact length L_c (2)



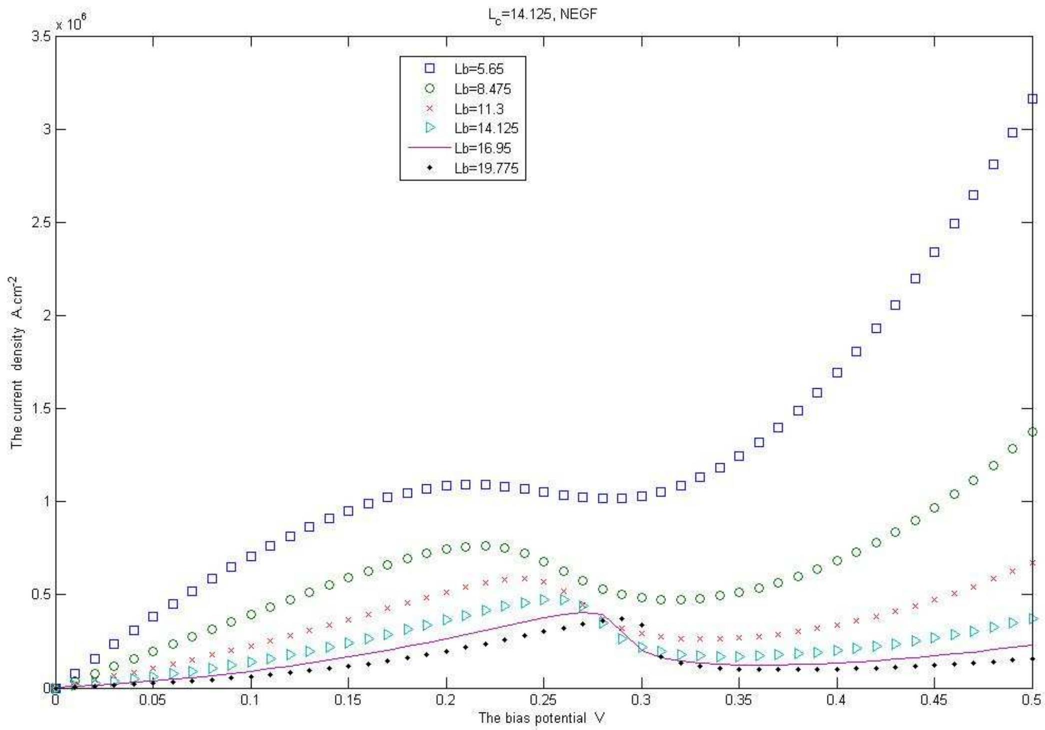
Comparison between NEGF & Wigner Currents



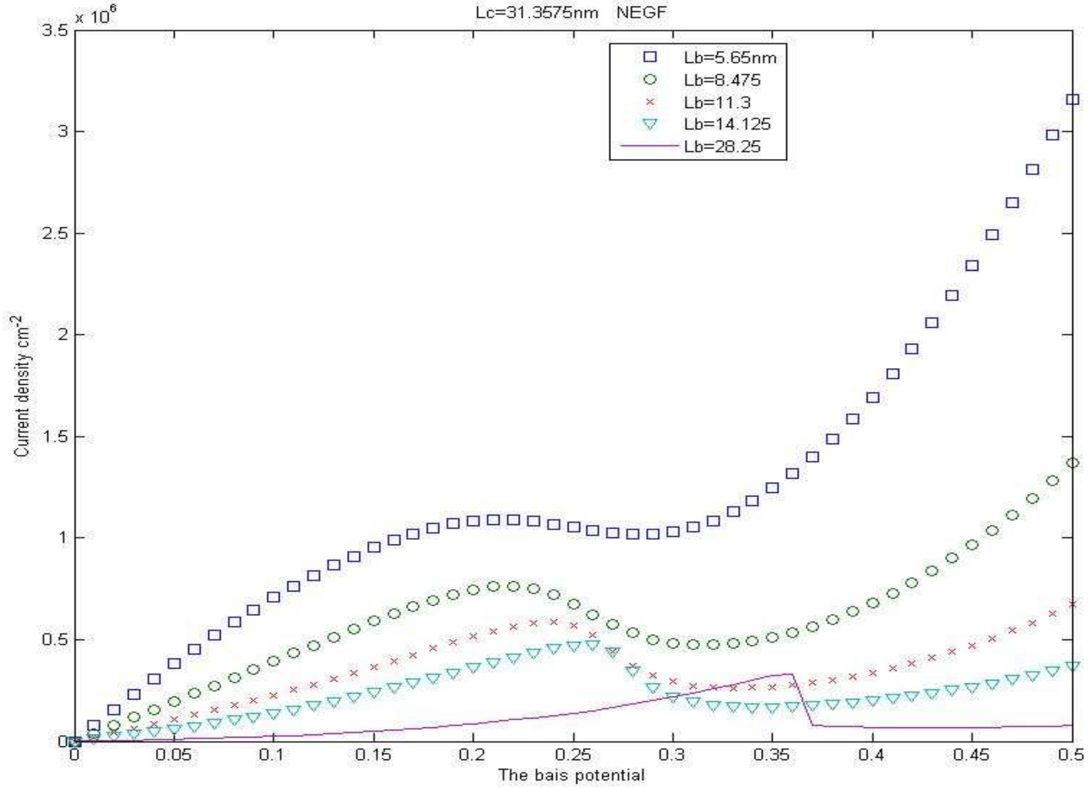
Self-Consistent Potentials in NEGF



Effect of the buffer size - NEGF



Effect of Buffer Size - Wigner



4 Conclusion

- The accuracy of the Frensley inflow boundary condition depends on the
  size of the contact region included in the the simulation and potential height in the RTD.

5. Further work & Acknowledgement

- Transient effect
- Scattering effect

Funding Provided by ARO

Thank You!