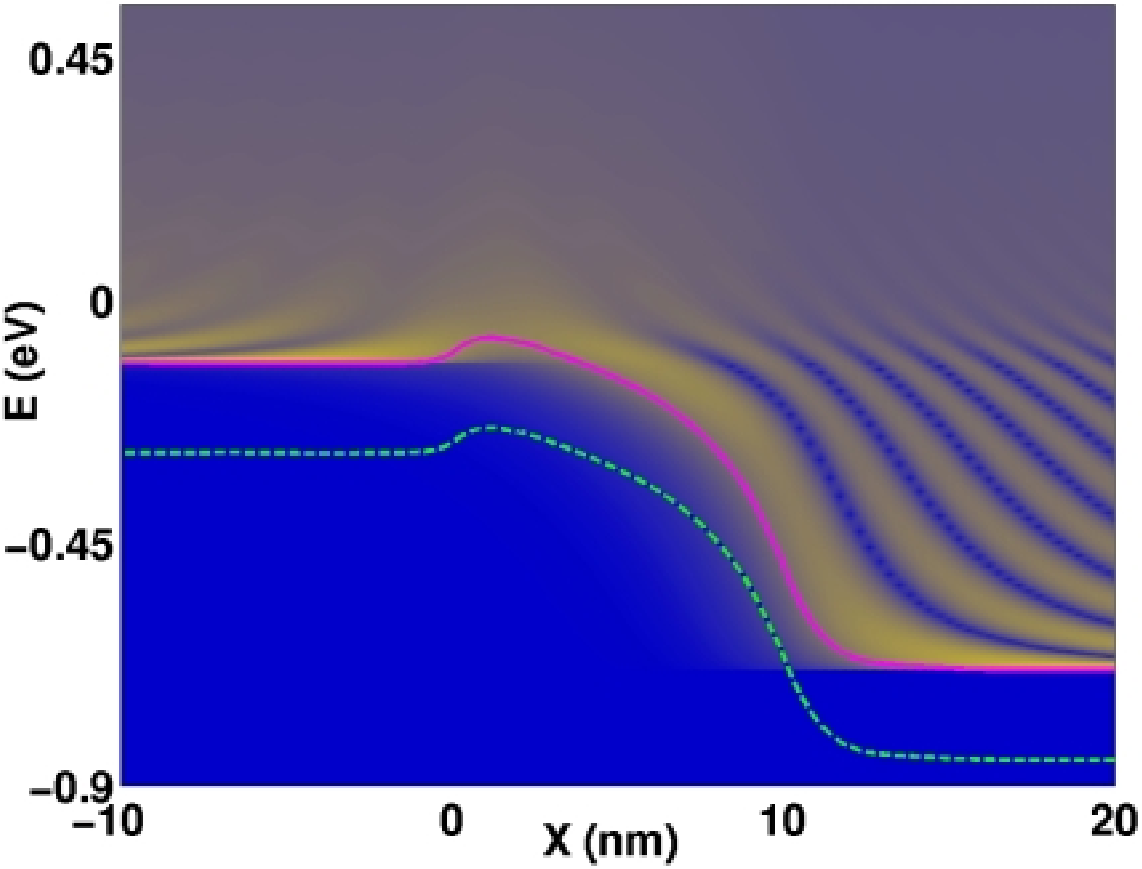
nanoMOS lab-II
NEGF formalism



Summary

- Quantum ballistic transport (qbte model).
- Density of States (DOS) plots.
- Transmission coefficient.
- Low temperature simulations
- Scattering simulations using Buttiker probes.

Getting Started

- Open a browser and go to nanohub.purdue.edu
- Login by clicking in nanoMOS 2.0 in the nanotools list.
- Click on Modify/Create input file
- Go to examples folder, select the appropriate exercise: lab-1…etc and copy it to the working folder.
- Go back to the working folder

Getting Started

- On top of the page go to “Step 2: Execute”
- Select your input deck from the pull-down button.
- Choose a name for the output folder and output file.
- Run the simulation by clicking on the “Run nanoMOS” button.
- Once simulation is done, go to “Step 3: output”, select an output file and open it….
- Congratulations you ran a nanoMOS simulation through the nanoHUB !!!!

Exercise 1

- Thin body (1.5 nm) DG MOSETS at Vds=Vdd.
- Interpretation of the DOS plot and transmission coefficient plot.
- The simulation will take 5 minutes
- Input deck in the example folder is uiuc-2.1

Ex-1 input deck

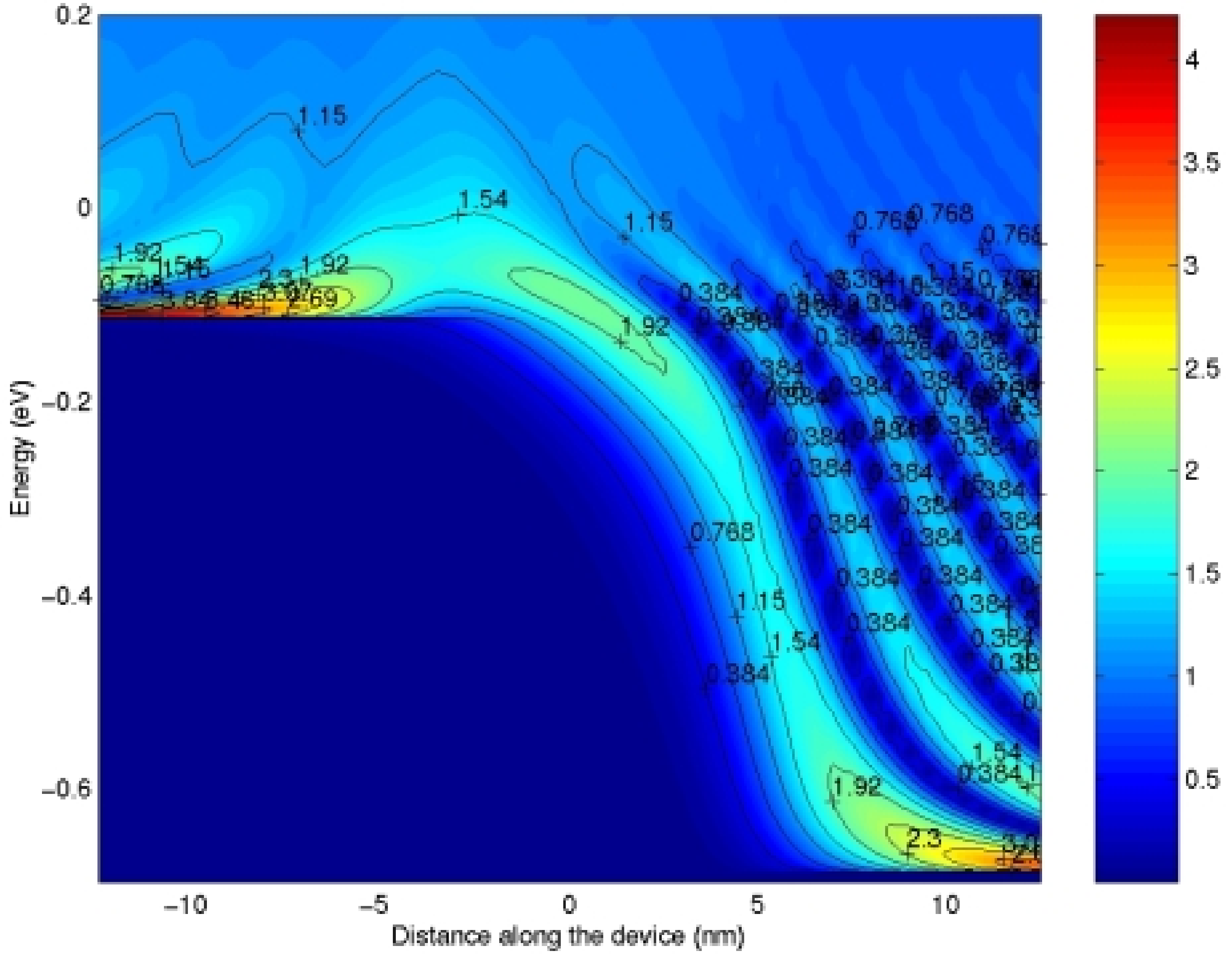
```
$ DEVICE DIRECTIVE
device  nsd=1e20, nbody=0, lgtop=10, lgbot=10, lsd=7.5,
+         overlap_s=0, overlap_d=0,
+       dopslope_s=0, dopslope_d=0,
+         tsi=1.5, tox_top=1.5, tox_bot=1.5, temp=300,

 $ TRANSPORT DIRECTIVE
transport model=qbte, mu_low=500, beta=2, vsat=1e7,
+         ELE_TAUW=1e-13, ELE_CQ=1

$ BIAS DIRECTIVE
bias vgtop=0.6, vgbot=0.6, vs=0.0, vd=0.6, vgstep=0.0, vdstep=0.0,
+    ngstep=0, ndstep=0, vd_initial=0.0
```

Thin body

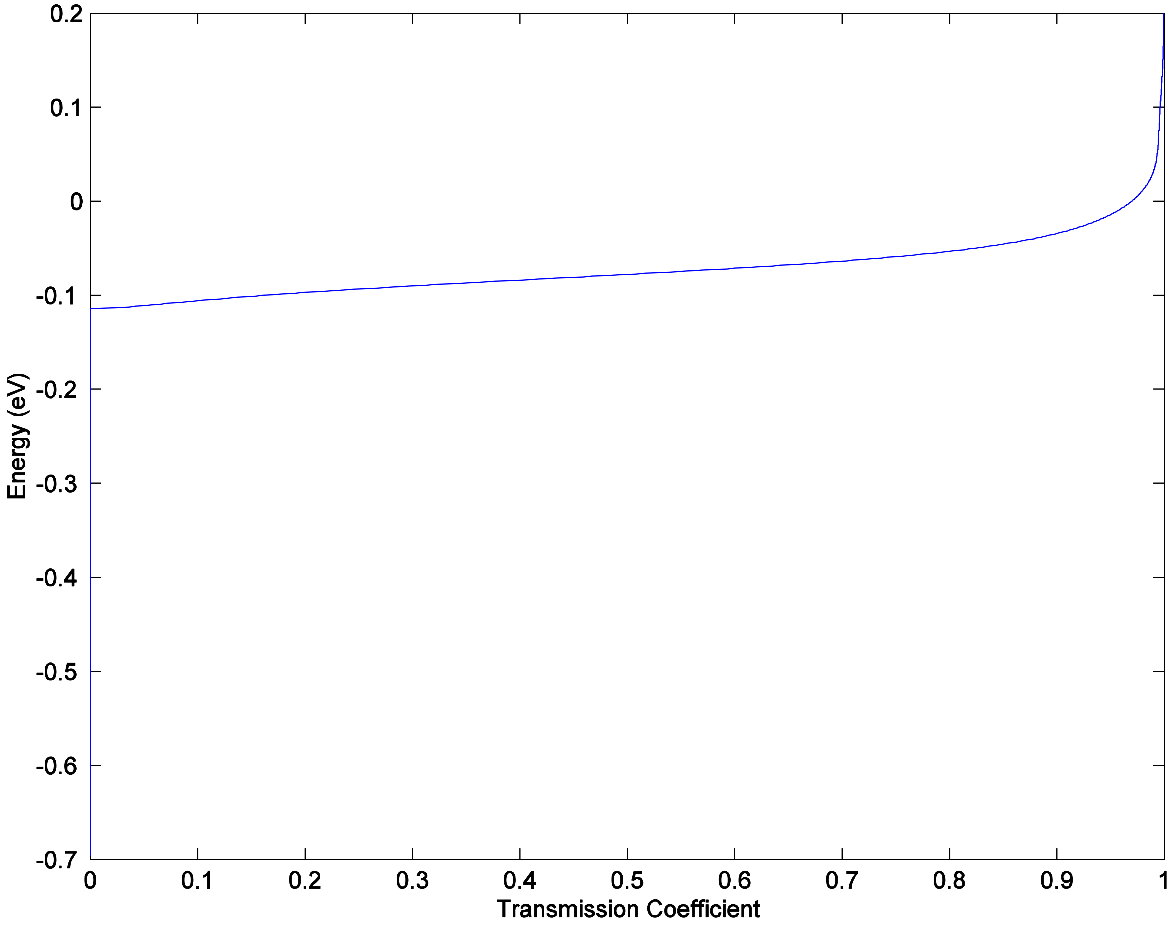
NEGF ballistic

On state

Outputs-DOS


Energy (eV)
Distance along the device (nm)
0.2
0
−0.2
−0.4
−0.6
−10
−5
0
5
10
4
3.5
3
2.5
2
1.5
1
0.5

Output-Transmission



Remarks

- In quantum ballistic simulation we compute the density of states.
- Forbidden regions can be identified and tunneling can be seen.
- Simulation time is more expensive than classical simulation

Exercise 2

- Underlapped device exhibits a quantum well in the off-state.
- DOS plot and transmission coefficient exhibit tunneling phenomena.
- The simulation will take 3 minutes
- Input deck in the example folder is uiuc-2.2

Ex-2 input deck

```
$ DEVICE DIRECTIVE
device  nsd=1e20, nbody=0, lgtop=10, lgbot=10, lsd=15,
+         overlap_s=-7, overlap_d=-7,
+       dopslope_s=0, dopslope_d=0,
+         tsi=1.5, tox_top=1.5, tox_bot=1.5, temp=300,
```

Gate underlap

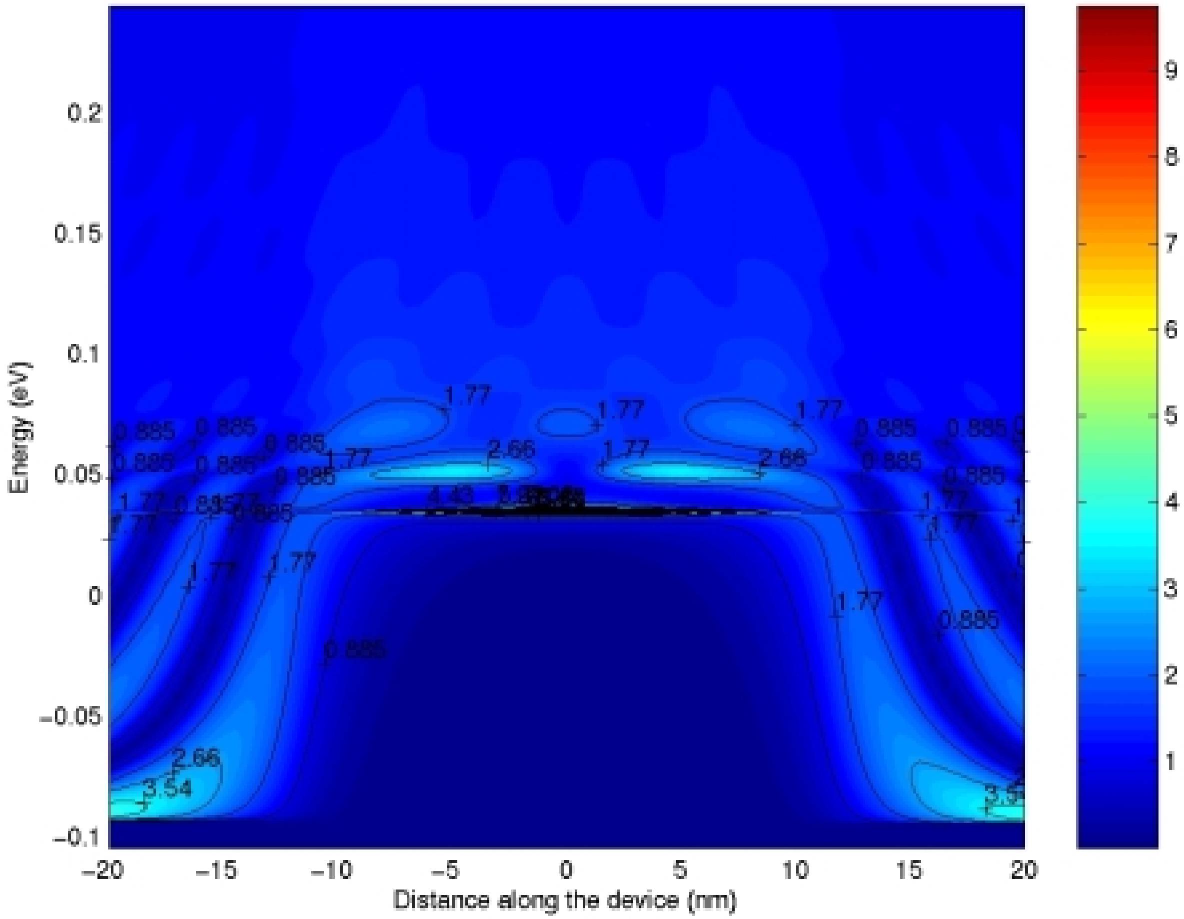
```
 $ TRANSPORT DIRECTIVE
transport model=qbte, mu_low=500, beta=2, vsat=1e7,
+         ELE_TAUW=1e-13, ELE_CQ=1
```

NEGF ballistic

```
$ BIAS DIRECTIVE
bias vgtop=0.4, vgbot=0.4, vs=0.0, vd=0.001, vgstep=0.0, vdstep=0.0,
+    ngstep=0, ndstep=0, vd_initial=0.0
```

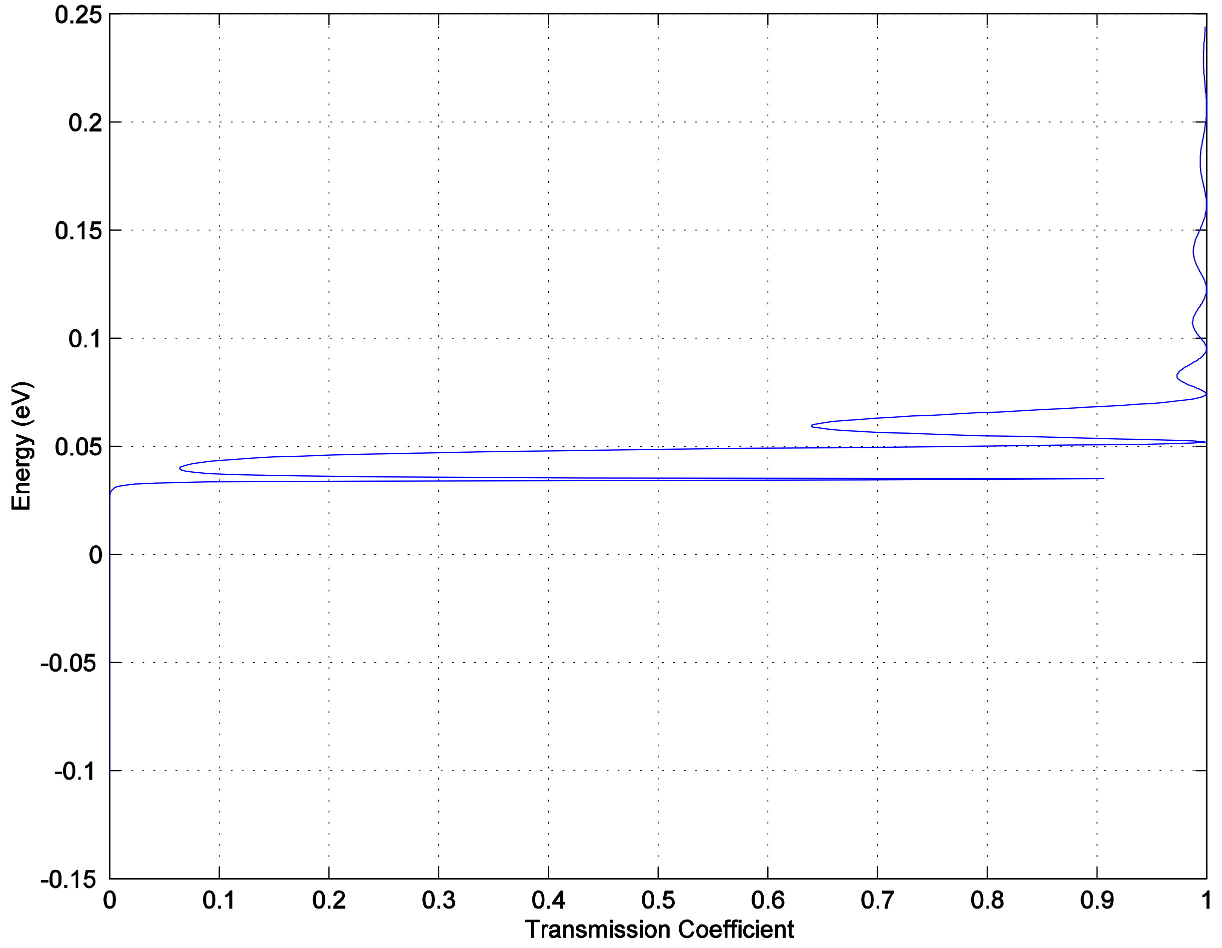
Off state

Outputs



Energy (eV)
Distance along the device (nm)
0.2
0.15
0.1
0.05
0
−0.05
−0.1
−20
−15
−10
−5
0
5
10
15
20
9
8
7
6
5
4
3
2
1

Outputs



0.25
0.2
0.15
0.1
0.05
0
-0.05
-0.1
-0.15
Energy (eV)
0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1
Transmission Coefficient

Remarks

- Underlapped structure can be simulated.
- In the off state this creates a quantum well along the device.
- The DOS shows quantized energy levels in the well.
- The transmission coefficient shows a peak below the top of the barrier.

Exercise 3

- Low temperature (100 K) NEGF simulation of the device simulated in Lab-I exercise 3.
- For comparison, run a classical simulation of Lab-1 exercise 3 at low temperature (100 K).
- Demonstrates source-drain tunneling.
- The simulation will take 12 minutes
- Input deck in the example folder is uiuc-2.3

Ex-3 input deck

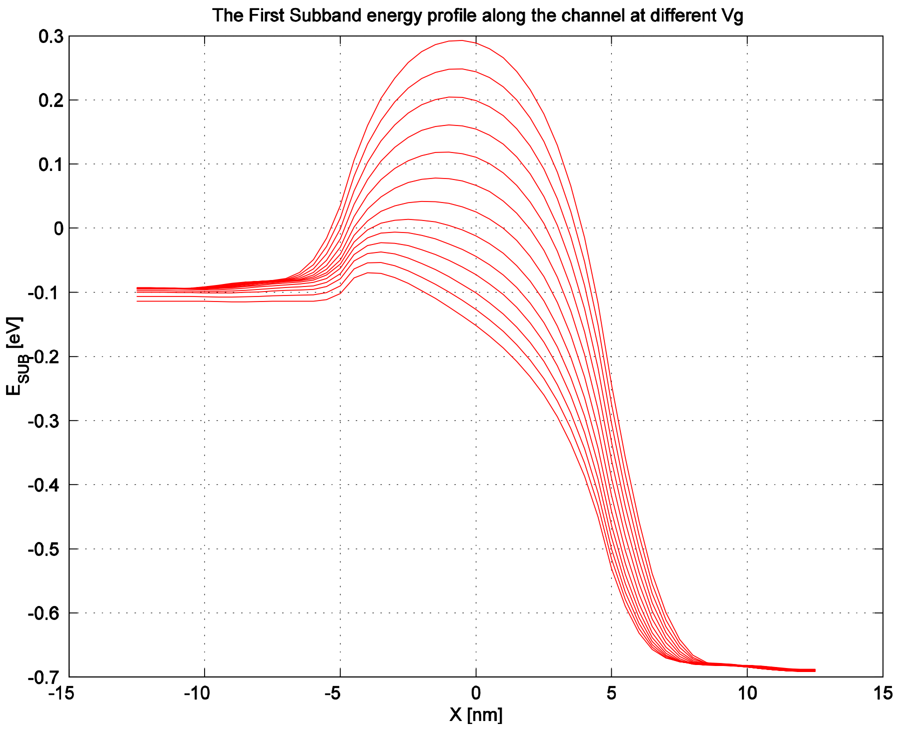
```
$ DEVICE DIRECTIVE
device  nsd=1e20, nbody=0, lgtop=10, lgbot=10, lsd=7.5,
+          overlap_s=0, overlap_d=0,
+        dopslope_s=0, dopslope_d=0,
+          tsi=1.5, tox_top=1.5, tox_bot=1.5, temp=100,

 $ TRANSPORT DIRECTIVE
transport model=qbte, mu_low=500, beta=2, vsat=1e7,
+          ELE_TAUW=1e-13, ELE_CQ=1

$ BIAS DIRECTIVE
bias vgtop=0.0, vgbot=0.0, vs=0.0, vd=0.6, vgstep=0.05, vdstep=0.0,
+    ngstep=12, ndstep=0, vd_initial=0.0
```

Low temperature

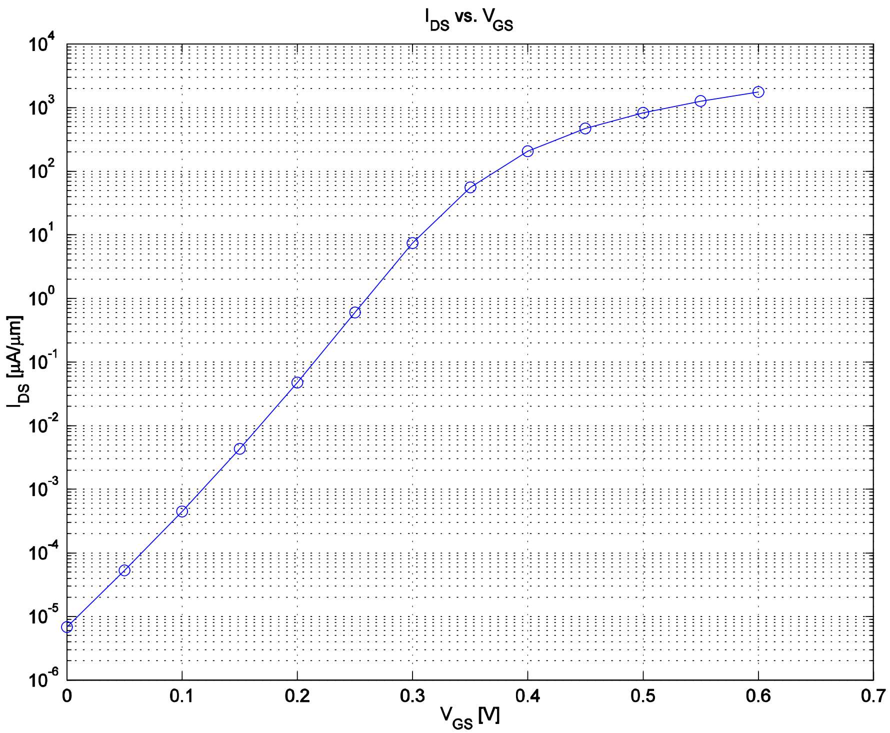
NEGF ballistic

Id-Vg simulation

Outputs



The First Subband energy profile along the channel at different Vg
E_{SUB} [eV]
X [nm]



I_{DS} vs. V_{GS}
I_{DS} [μA/μm]
V_{GS} [V]

Remarks

- What's different with what you get ?
- Comparison with lab-1 exercise 3: classical transport model.
- We see a higher off current due to source drain tunneling.
- The qbte model properly simulates source drain tunneling.

Exercise 4

- Do a scattering simulation..this will take time. (qdte)
- Examine the results available in the output example folder.
- Compare with quantum ballistic transport model.
- The simulation will take 40 minutes
- Input deck in the example folder is uiuc-2.4

Ex-4 input deck

```
$ DEVICE DIRECTIVE
device  nsd=1e20, nbody=0, lgtop=10, lgbot=10, lsd=7.5,
+         overlap_s=0, overlap_d=0,
+       dopslope_s=0, dopslope_d=0,
+         tsi=1.5, tox_top=1.5, tox_bot=1.5, temp=300,

 $ TRANSPORT DIRECTIVE
transport model=qdte, mu_low=500, beta=2, vsat=1e7,
+         ELE_TAUW=1e-13, ELE_CQ=1

$ BIAS DIRECTIVE
bias vgtop=0.6, vgbot=0.6, vs=0.0, vd=0.6, vgstep=0.0, vdstep=0.0,
+    ngstep=0, ndstep=0, vd_initial=0.0
```

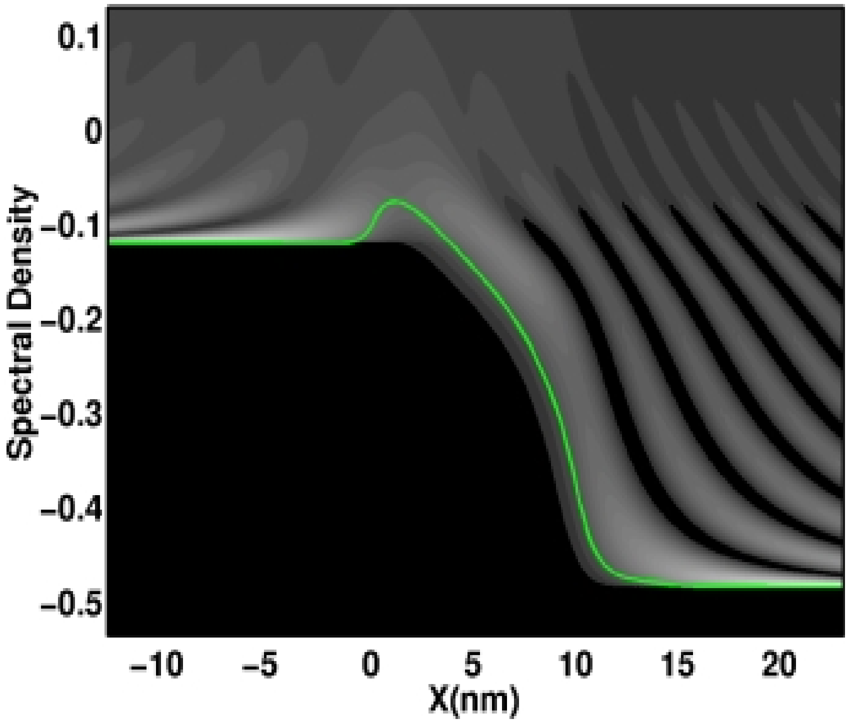
Thin body

NEGF with scattering

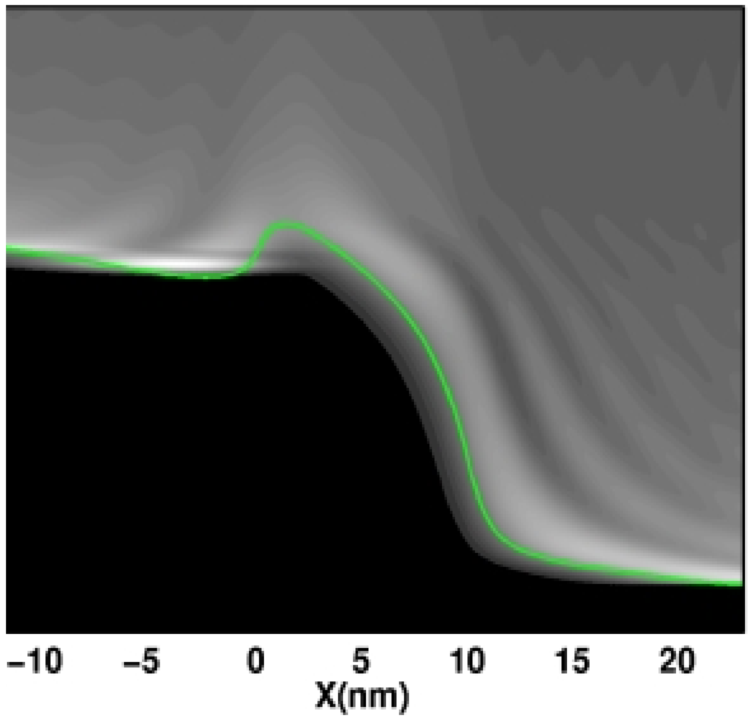
On state

Outputs

Ballistic



Scattering



Remarks

- Scattering broadens the energy levels and results in a loss of coherency
- Scattering results in potential drops in the source and drain
- Loss of coherency washes out the oscillations in the local density of states
- The probe model relaxes longitudinal energy correctly