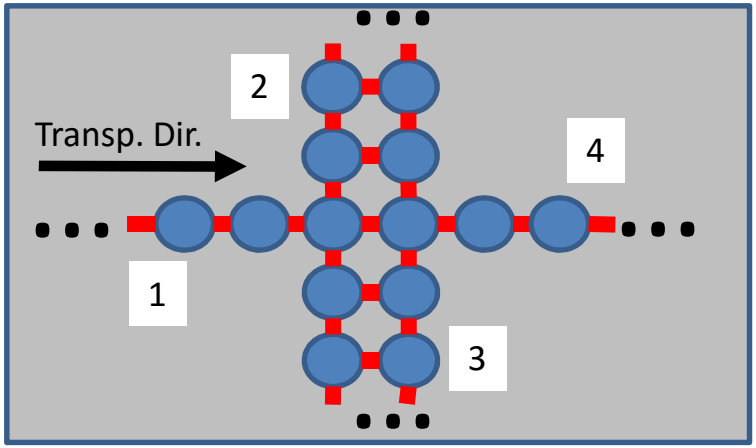
6.TB - Four-probe system

Objectives

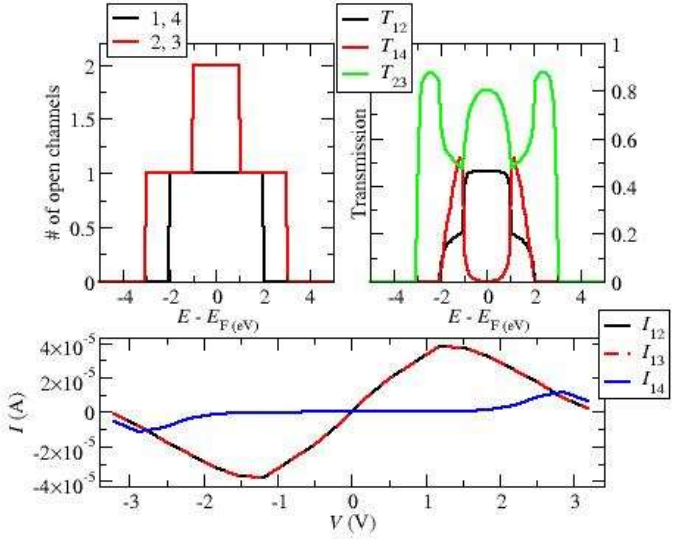
- Simulate a four-probe system with two types of electrodes.
- Calculate the transmissions from one to other electrodes.
- See the effect of including a bias voltage on one of the electrodes. Calculate the currents.



Results

- There is one open channel in electrodes 1 and 4 and a maximum of two in electrodes 2 and 3.
- The transmission between electrodes 1 and 4, T_{14}, is not perfect because the presence of the other electrodes (part of the probability is diverted towards them). The same for T_{23}.
- $T_{12} = T_{13} = T_{24} = T_{34}$.
-The voltage in ramped up only in the first electrode. The current towards electrodes 2 and 3 is much larger than that towards electrode 4 because the transmission in 2 and 3 is larger.
- NDR appears because the transmission is dramatically affected by the voltage.

Transmission and number of open channels as a function of energy. Calculated with **Mode 1** of Gollum.



Current as a function of voltage.
Calculated with **Mode 4** of Gollum.

6.TB - Hamiltonian

Leads 1 and 4

$$\hat{H}_{\mathrm{L/R}} = \begin{pmatrix} \varepsilon_0 & \gamma \\ \gamma & \varepsilon_0 \end{pmatrix} \qquad \hat{H}_{\mathrm{L/R},0} = (\varepsilon_0) \qquad \hat{H}_{\mathrm{L/R},1} = (\gamma)$$

Leads 2 and 3

$$\hat{H}_{\mathrm{L/R}} = \begin{pmatrix} \varepsilon_0 & \gamma & \gamma & 0 \\ \gamma & \varepsilon_0 & 0 & \gamma \\ \gamma & 0 & \varepsilon_0 & \gamma \\ 0 & \gamma & \gamma & \varepsilon_0 \end{pmatrix} \quad \hat{H}_{\mathrm{L/R},0} = \begin{pmatrix} \varepsilon_0 & \gamma \\ \gamma & \varepsilon_0 \end{pmatrix} \quad \hat{H}_{\mathrm{L/R},1} = \begin{pmatrix} \gamma & 0 \\ 0 & \gamma \end{pmatrix}$$

Extended molecule (EM): In this particular example we include the leads calculation in that of the extended molecule, so that we do not have to carry out two simulations.

6.TB - System description and parameters

Leads

- 1 and 4: unit cell with just one atom. 2 and 3: unit cell with two atoms. One orbital per atom.
- Single-atom (1 and 4) and two-atom (2 and 3) chains connected in the middle of the EM.

Extended molecule (EM)

- 14 atoms in the calculation.
- Same parameters as in the leads (correspondingly).

Gollum parameters

- Transmission coefficients calculated between -5.0 eV and 5.0 eV in 1000 energy points.
- 2 principal layers on each electrode. The terminating principal layer is the second on each. Electronic structure obtained from the leads calculation.
- No SAINT correction or Fermi level shift.
- Bias voltage between -5.0 V and 5.0 V calculated in 20 voltage points. The bias shift is applied on the first terminating layer of each electrode only (4th column of the `atom` variable set to different from 0). This is an approximation since the voltage should not fall (or at least fall very slowly) on a perfect infinite system.

Tight-binding parameters

- Orthogonal basis set (overlap matrix = identity matrix).
- On-site matrix elements (both leads and EM): 0.0 eV.
- Coupling between atoms (everywhere): 1.0 eV.