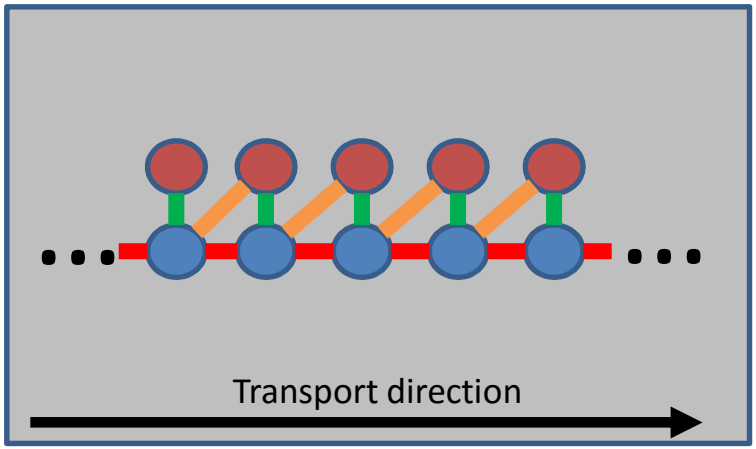
4.TB - Two-level chain

Objectives

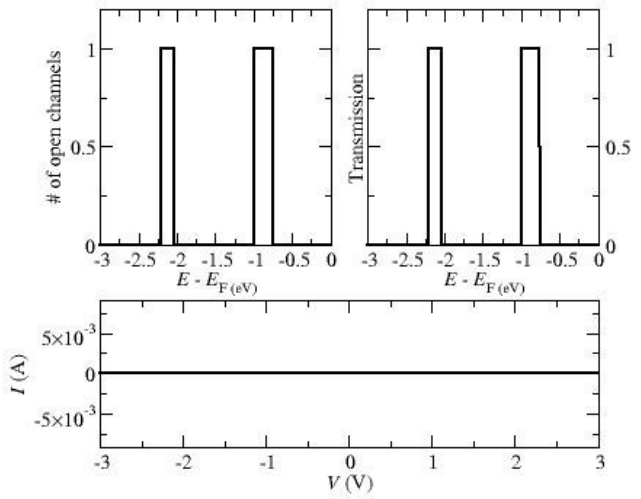
- Simulate one-dimensional (1D) system with different orbitals and perfect transmission (equal to the number of open channels or bands at a certain energy).
- Check that the transmission exactly coincides with the number of open channels.



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

Results

- The transmission has a step-like shape which corresponds to the number of open channels at a given energy.
- There are two separated bands whose center is located near the on-site energy of each type of orbital.
- The width and final position of the band depends on the couplings through the chain and between both types of orbitals.
- The current is zero because the bias window does not reach the nearest band at low voltages and the transmission is destroyed at large voltages.



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

4.TB - Hamiltonian

Leads $\hat{H}_{\mathrm{L/R}} = \begin{pmatrix} \varepsilon_0 & \delta & \gamma & \zeta \\ \delta & \varepsilon_1 & 0 & 0 \\ \gamma & 0 & \varepsilon_0 & \delta \\ \zeta & 0 & \delta & \varepsilon_1 \end{pmatrix}$ $\hat{H}_{\mathrm{L/R,0}} = \begin{pmatrix} \varepsilon_0 & \delta \\ \delta & \varepsilon_1 \end{pmatrix}$ $\hat{H}_{\mathrm{L/R,1}} = \begin{pmatrix} \gamma & \zeta \\ 0 & 0 \end{pmatrix}$

Extended molecule (EM): A repetition of the leads (periodic system)

Singular coupling matrix between unit cells. It is necessary to decimate in order to obtain a matrix that can be inverted.

4.TB - System description and parameters

Leads

- Unit cell with just one atom. Two different orbitals per atom.
- Two-level chain with different couplings between orbitals in the same unit cell and orbitals in different unit cells.

Extended molecule (EM)

- Five atoms in the calculation.
- Same parameters as in the leads

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 -3.0 V and 3.0 V calculated in 20 voltage points. The bias shift is applied on the first terminating layer of the left and right electrodes 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): -2.0 eV and -1.0 eV for each type of orbital.
- Coupling between both types of orbitals: -3.0 eV.
- Coupling between orbitals in different unit cells: H_{11} = 0.1 eV, H_{12} = -0.2 eV, H_{21} = 0.0 eV and H_{22} = 0.0 eV.