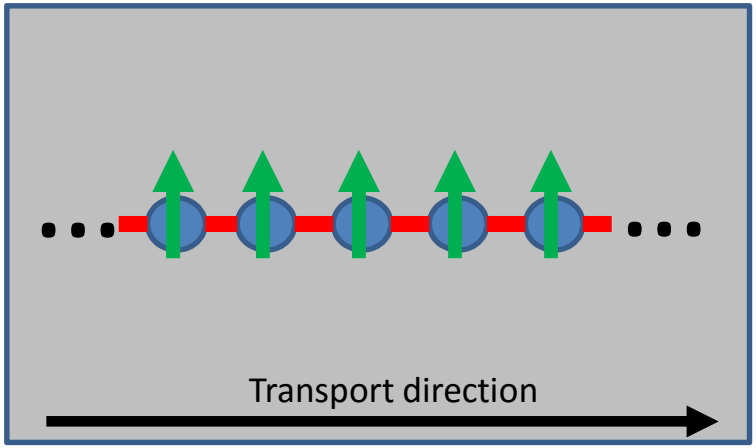
1.TB - Single-atom chain. Spin polarized

Objectives

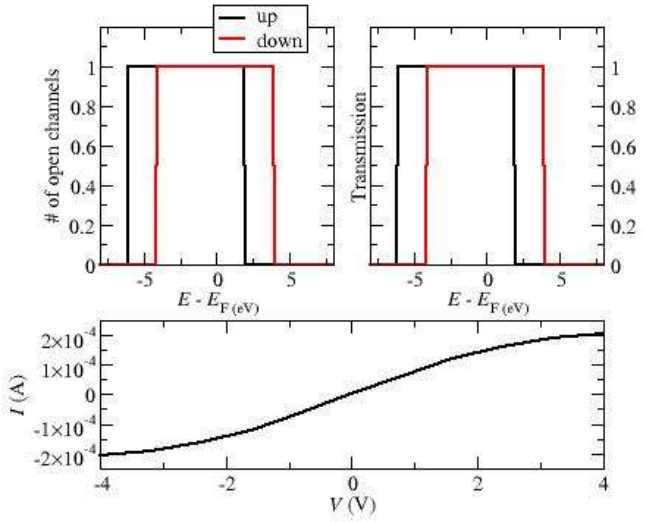
- Simulate a spin-polarized one-dimensional (1D) system with perfect transmission (equal to the number of open channels or bands at a certain energy).
- Check that the transmission exactly coincides with the number of open channels.



Results

- The transmission has a step-like shape which corresponds to the number of open channels.
- The spin-up and spin-down channels and transmissions have an exchange splitting of 2 eV.
- The current linearly increases (as expected, since it is equal to the integral of a constant function) until it saturates at large voltages (when the bias window starts covering the edges of the band, which are “rounded” by the effect of 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.

1.TB - Hamiltonian

Leads

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

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

Extended molecule (EM). 1 site.

Exchange splitting: $\Delta E = \varepsilon_\uparrow - \varepsilon_\downarrow$

$$\hat{H}_{\mathrm{EM},\uparrow} = \begin{pmatrix} \varepsilon_\uparrow & \gamma & 0 & 0 & 0 \\ \gamma & \varepsilon_\uparrow & \gamma & 0 & 0 \\ 0 & \gamma & \varepsilon_\uparrow & \gamma & 0 \\ 0 & 0 & \gamma & \varepsilon_\uparrow & \gamma \\ 0 & 0 & 0 & \gamma & \varepsilon_\uparrow \end{pmatrix} \qquad \hat{H}_{\mathrm{EM},\downarrow} = \begin{pmatrix} \varepsilon_\downarrow & \gamma & 0 & 0 & 0 \\ \gamma & \varepsilon_\downarrow & \gamma & 0 & 0 \\ 0 & \gamma & \varepsilon_\downarrow & \gamma & 0 \\ 0 & 0 & \gamma & \varepsilon_\downarrow & \gamma \\ 0 & 0 & 0 & \gamma & \varepsilon_\downarrow \end{pmatrix}$$

1.TB - System description and parameters

Leads

- Unit cell with just one atom. One orbital per atom.
- Single-atom chain with spin polarization. The exchange splitting between the spin-up and spin-down states is 2 eV.

Extended molecule (EM)

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

Gollum parameters

- Transmission coefficients calculated between -8.0 eV and 8.0 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 -4.0 V and 4.0 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 energies (both leads and EM): -1.0 eV (spin-up) and 1.0 eV (spin-down).
- Nearest-neighbour coupling matrix elements (both leads and EM): -2.0 eV.