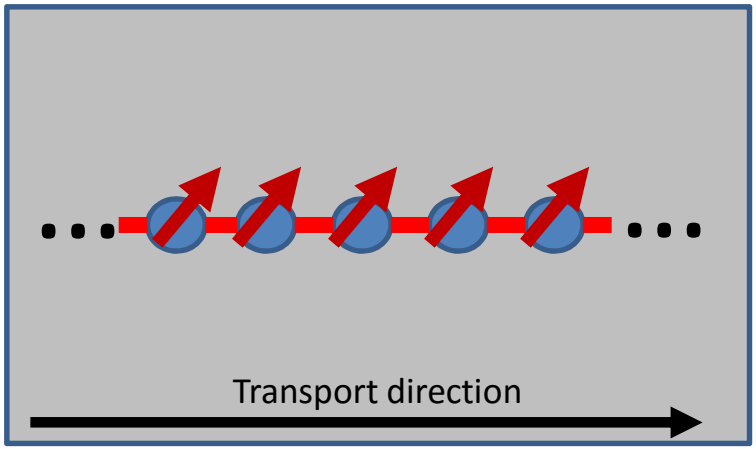
2.TB - Single-atom chain. Non-collinear magnetism

Objectives

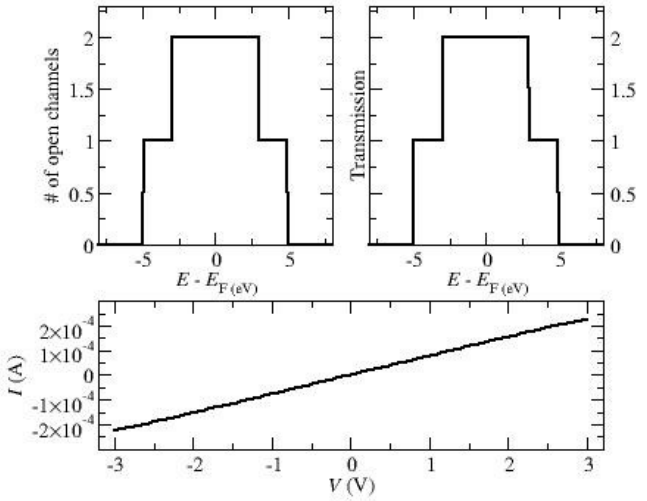
- Simulate a one-dimensional (1D) system with perfect transmission (equal to the number of open channels or bands at a certain energy) and non-collinear magnetic configuration.
- Check that the transmission exactly coincides with the number of open channels.



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

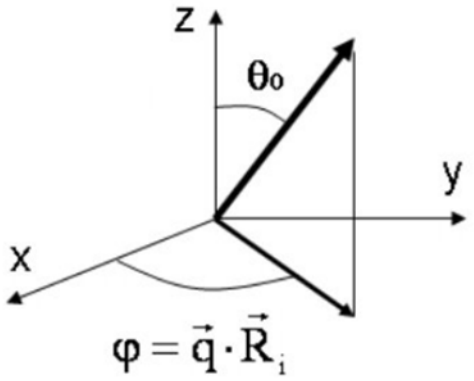
Results

- The transmission has a step-like shape which corresponds to the number of open channels resolved in spin.
- The exchange splitting along the spin *y* direction is 2 eV.
- The current linearly increases (as expected, since it is equal to the integral of a constant function) and does not saturate because the bias window does not reach the edges of the band.



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

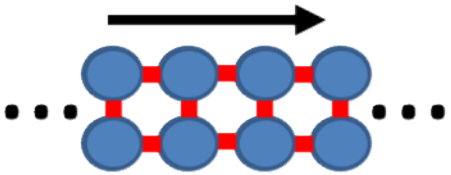
2.TB - Hamiltonian



$$\hat{U}_y(\theta) = \begin{pmatrix} \cos\theta/2 & \sin\theta/2 \\ -\sin\theta/2 & \cos\theta/2 \end{pmatrix}$$

$$\hat{U}_z(\varphi) = \begin{pmatrix} e^{i\varphi/2} & 0 \\ 0 & e^{-i\varphi/2} \end{pmatrix}$$

$$\begin{pmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{pmatrix} = \hat{U}_z^{+}(\varphi)\hat{U}_y^{+}(\theta) \begin{pmatrix} H_{\uparrow} & 0 \\ 0 & H_{\downarrow} \end{pmatrix} \hat{U}_y(\theta)\,\hat{U}_z(\varphi)$$



Leads

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

2.TB - System description and parameters

Leads

- Unit cell with just one atom. One orbital per atom.
- Single-atom chain with non-collinear magnetic configuration. The exchange splitting along the *y* direction 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 200 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 60 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): 0.0 eV on the ↑↑ and ↓↓ sites, -1.0i eV on the ↑↓ site and 1.0i eV on the ↓↑ site.
- Nearest-neighbour coupling matrix elements (both leads and EM) between the ↑↑ or the ↓↓ sites: -2.0 eV.