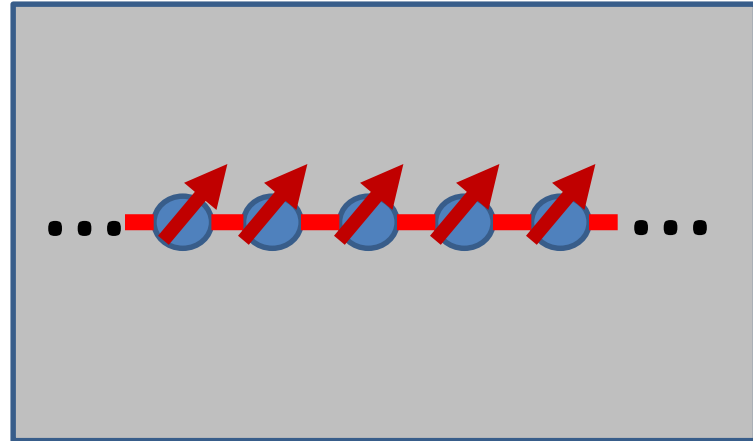


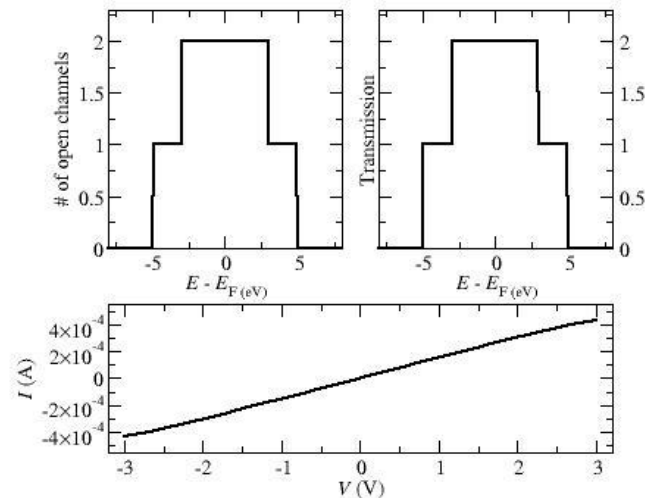
Single-atom chain. Non-collinear magnetism

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.



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

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 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): 0.0 eV on the $\uparrow\uparrow$ and $\downarrow\downarrow$ sites, -1.0i eV on the $\uparrow\downarrow$ site and 1.0i eV on the $\downarrow\uparrow$ site.
- Nearest-neighbour coupling matrix elements (both leads and EM) between the $\uparrow\uparrow$ or the $\downarrow\downarrow$ sites: -2.0 eV.