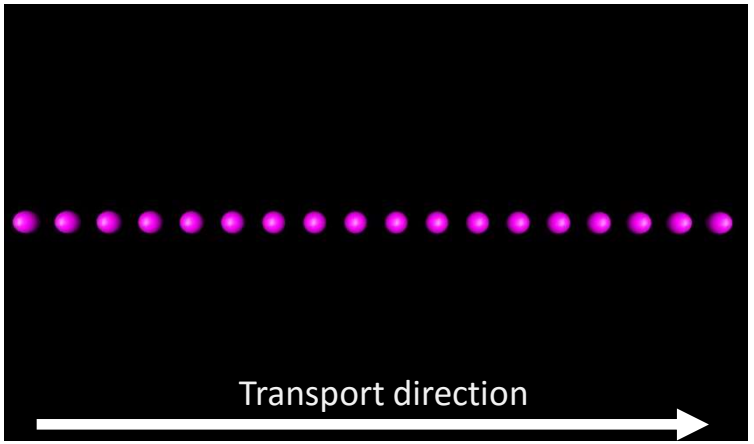
1.DFT - Gold linear chain

Objectives

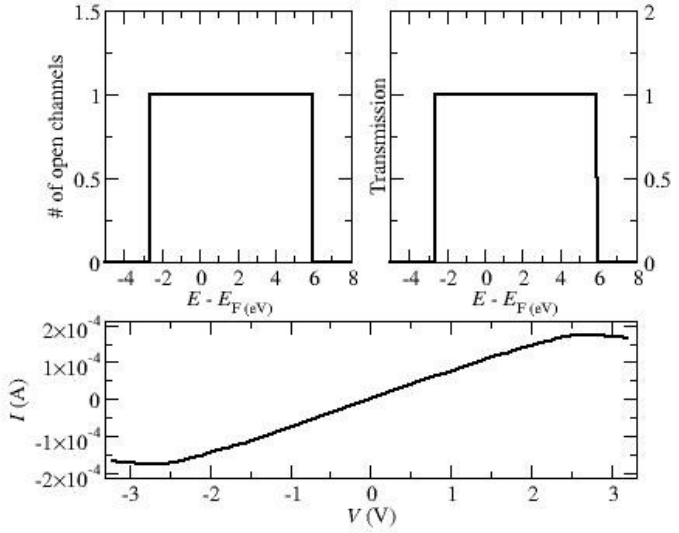
- Simulate a one-dimensional (1D) system with perfect transmission (equal to the number of open channels or bands at a certain energy).
- Check that the transmission exactly coincides with the number of open channels.



Results

- The transmission has a step-like shape which corresponds to the number of open channels. In this case there is only one s orbital in the valence of gold (the rest of states are included in the pseudopotential), so the transmission is equal to 1 in the range of energies that comprises the gold band.
- The current linearly increases (as expected, since it is equal to the integral of a constant function) until it saturates and slightly decreases (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.DFT - System description and parameters

Leads

- Au leads made of only 2 Au atoms.
- Lattice vectors long enough along the transverse directions to make sure the system is 1D.

Extended molecule (EM)

- Perfect gold chain made of 18 atoms (9 unit cells of the electrodes) and with the same transverse lattice vectors of the leads.
- The system is also periodic along the transport direction (*z*) to avoid finite size effects.

Gollum parameters

- Transmission coefficients calculated between -5.0 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 -3.2 V and 3.2 V calculated in 60 voltage points. The bias shift is applied on the first terminating layer of the left and right electrodes only (4^{th} 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.

Ab-initio (Siesta) parameters

- Basis set: Single-ζ (SZ); only the s orbital is included in the Au valence (the rest are hidden in the pseudopotential).
- LDA exchange and correlation functional. CA parametrization.
- Mesh cut-off: 150 Ry.
- 90 *k*-points along *z* in the lead calculation. 10 k-points in the EM calculation (to make sure the electronic structure exactly matches that of the leads). 1 *k*-point (Γ point) along the perpendicular directions.

Files necessary tor run the **leads** calculation: lead.fdf, Au.psf
Files necessary to run the **EM** calculation: emol.fdf, Au.psf