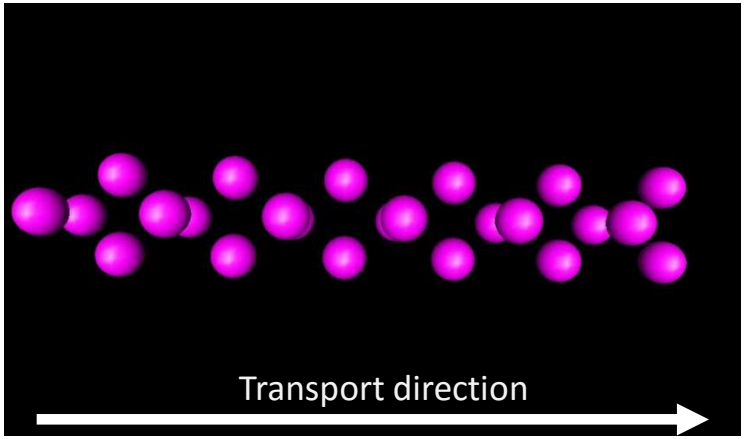
4.DFT - (001) bulk nickel. Spin-polarized

Objectives

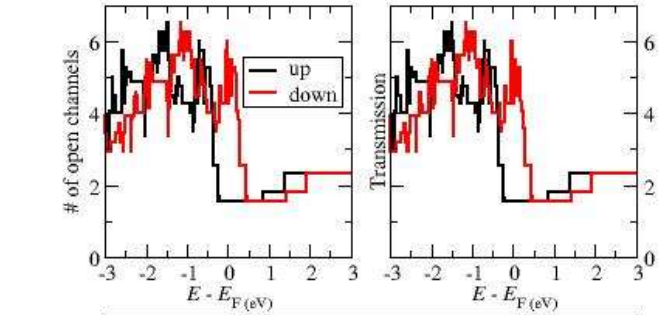
- Simulate a magnetic three-dimensional (3D) system (transverse periodic boundary conditions and *k*-points) with perfect transmission (equal to the number of open channels or bands at a certain energy) and various channels.
- Check that the transmission exactly coincides with the number of open channels.

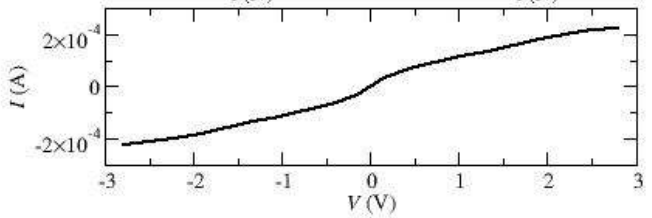


Results

- The transmission has a step-like shape which indicates the number of open channels. We have s and d orbitasl in the valence of nickel. The presence of atoms in the transverse directions can produce transmissions larger than 6 (1-s + 5-d).
- Since the system is spin-polarized the transmission and channels are different for spin up-and spin-down electrons.
- The transmission and channels can have non-integer values due to the inclusion of perpendicular *k*-points.
- The current linearly increases until it slightly saturates. Changes in the slope are due to the appearance or disappearance of new bands.

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.

4.DFT - System description and parameters

Leads

- Ni leads made of 8 Ni atoms (4 layers) to avoid second-nearest-neighbour interactions.
- Lattice vectors along the transverse directions that replicate a fcc lattice.

Extended molecule (EM)

- 24 atoms (12 layers). The same transverse lattice vectors of the leads that replicate a fcc lattice.
- The system is also periodic along the transport direction (*z*) to avoid finite size effects.

Gollum parameters

- Transmission coefficients calculated between -3.0 eV and 3.0 eV in 2000 energy points.
- 1 principal layers on each electrode. Electronic structure obtained from the leads calculation.
- No SAINT correction or Fermi level shift.
- Bias voltage between -2.8 V and 2.8 V calculated in 20 voltage points. The bias shift is applied just in the middle of the chain (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.

Ab-initio (Siesta) parameters

- Basis set: Single-ζ (SZ); s and d orbitals in the Pt valence.
- LDA exchange and correlation functional. CA parametrization.
- Mesh cut-off: 300 Ry.
- 30 *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). 4x4 *k*-point along the perpendicular directions.
- Spin-polarized calculation. It is possible to distinguish between spin-up and spin-down electrons.

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