2.W90 - Sodium chain with a gap

Objectives

- Simulate a one-dimensional (1D) system with a defect (structural gap in the chain, i.e. two of the atoms have a large separation).

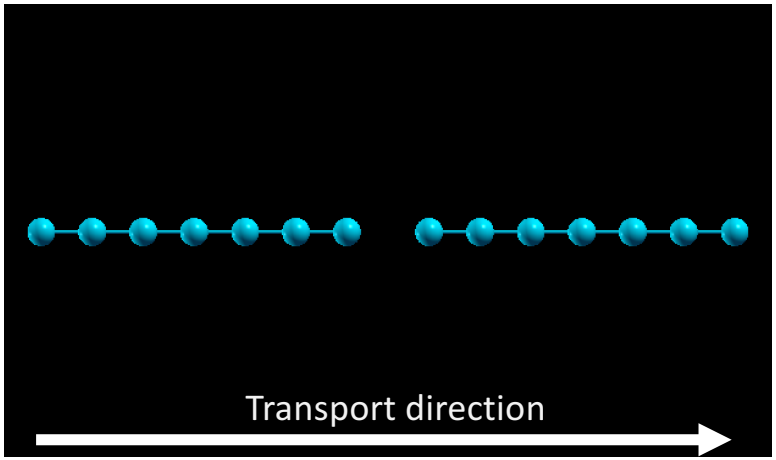
- Calculate the transmission and accurately obtain the current at finite voltages.

Results

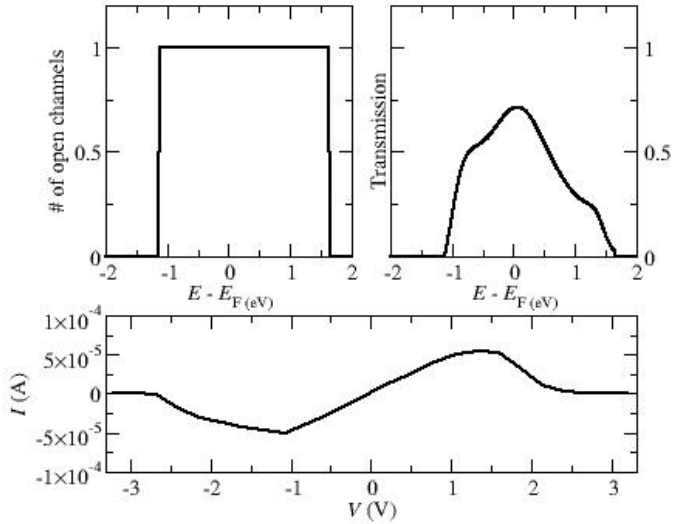
- The transmission has a rounded shape and is smaller than 1 due to scattering at the gap. There is only one Wannier function per atom, which corresponds to the s orbital in the valence of sodium. The transmission has then finite values in the range of energies that comprises the s band.

- The current linearly increases (as expected, since it is equal to the integral of a positive function) until it saturates and finally decreases (NDR) when the transmission is severely reduced by finite voltage effects (at high voltages the transmission is similar to the transmission of two asymmetric states with different energies).

- The current is also slightly asymmetric because the positions of the Wannier functions on both sides of the gap are not exactly the same.



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.

2.W90 - System description and parameters

Leads

- Na leads made of only 3 Na atoms.
- Lattice vectors long enough along the transverse directions to make sure the system is 1D.

Extended molecule (EM)

- Two Na chain with 7 atoms (2 unit cells of the electrodes on each side plus two additional atoms in the middle) separated 5.249 Å 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.

Ab-initio (QuantumEspresso-PW and Wannier90) parameters

- Basis set (PW) cutoff: ecutwfc = 30 (PW scf and nscf).
- LDA exchange and correlation functional. PZ parametrization (defined by the pseudopotential).
- Number of bands in the EM: nbnd = 39 (PW nscf and W90). Number of Wanniers in the EM: num_wann = 14 (W90).
- 2 (PW scf) and 4 (PW nscf and W90) *k*-points along *z* in the lead calculation. 1 *k*-point (Γ point) in the EM calculation and along the perpendicular directions.
- The number of Wannier functions coincides with the number of atoms in both the leads and the extended molecule; the number of Wannier groups also coincides with the number of atoms.

* Files necessary to run the **leads** calculation: Na_l.scf, Na_l.nscf, Na_l.pw2wan, Na_l.win, Na.pz-n-vbc.UPF
* Files necessary to run the **EM** calculation: Na_chain.scf, Na_chain.nscf, Na_chain.pw2wan, Na_chain.win, Na.pz-n-vbc.UPF

Gollum parameters

- Transmission coefficients calculated between -5.0 eV and 5.0 eV in 2000 energy points.
- 2 principal layers on each electrode. The terminating principal layer is the second (outermost) on each. Electronic structure obtained from the extended molecule or from the leads calculation.
- No SAINT correction or Fermi level shift.
- Bias voltage between -3.2 V and 3.2 V calculated in 25 voltage points. The bias shift is applied on the 7th and 8th atoms (4th column of the `atom` variable set to 1 or 2). This choice is accurate because the voltage should fall just in the gap.