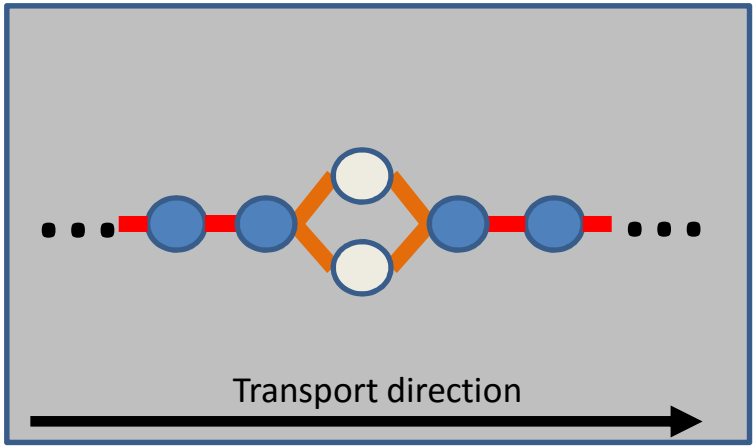
3.TB - Two-level system. SAINT + V_{gate}

Objectives

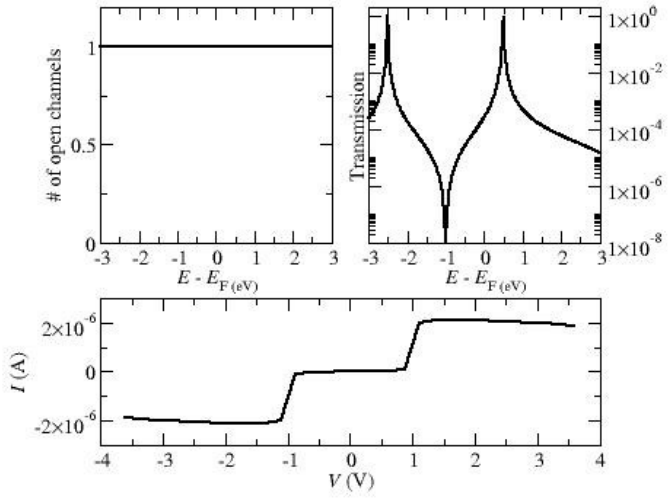
- Simulate a two level system (H2 molecule) coupled to metallic atomic chains.
- Check that the transmission has two peaks corresponding to the positions of the levels of the molecule.
- Apply a gate voltage to change the on-site energies and the SAINT correction to increase the separation between both molecular levels.



Results

- The transmission has two clear peaks that correspond originally to the position of the on-site levels. The width of the peaks, which is related to the hybridization with the leads, is small.
- There is a Fano resonance due to interference effects (lateral groups).
- The gate voltage, 1.0 V, moves the on-site levels to lower energies.
- The SAINT correction opens the gap from 1.0 eV to 3.0 eV.
- The current increases in steps whenever the bias window covers a molecular level.

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.

3.TB - Hamiltonian

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

Extended molecule (EM). 1 site. $\hat{H}_{\mathrm{EM}} = \begin{pmatrix} \varepsilon_0 & \delta & \delta & 0 \\ \delta & \varepsilon_1 & 0 & \delta \\ \delta & 0 & \varepsilon_1 & \delta \\ 0 & \delta & \delta & \varepsilon_0 \end{pmatrix}$

SAINT correction $\hat{H} = \hat{H}_0 + \Delta_{\mathrm{o}} \sum_{n_{\mathrm{o}}} |\Psi_{n_{\mathrm{o}}}><\Psi_{n_{\mathrm{o}}}| + \Delta_{\mathrm{u}} \sum_{n_{\mathrm{u}}} |\Psi_{n_{\mathrm{u}}}><\Psi_{n_{\mathrm{u}}}|$

3.TB - System description and parameters

Leads

- Unit cell with just one atom. One orbital per atom.
- Single-atom chain.

Extended molecule (EM)

- 6 atoms in the calculation. 2 atoms in the left electrode, 2 atoms in the molecule and 2 atoms in the right electrode.
- Same parameters as in the leads in the electrodes.

Gollum parameters

- Transmission coefficients calculated between -6.0 eV and 6.0 eV in 5000 energy points.
- 2 principal layers on each electrode. The terminating principal layer is the second on each. Electronic structure obtained from the leads calculation.
- Gate voltage of 1.0 V applied only on the molecular levels (1st column of the `atom` variable set to 0).
- SAINT correction of -1.0 eV on the occupied level and 1.0 eV on the unoccupied level. It is assumed a charge of 2 electrons in the molecule to define the occupied level.
- 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).

Tight-binding parameters

- Orthogonal basis set (overlap matrix = identity matrix).
- On-site matrix elements (ME) of the leads: 0.0 eV. On-site ME of the molecular atoms: -0.5 eV and 0.5 eV.
- Nearest-neighbour coupling in the leads: -2.0 eV. Coupling between the leads and the molecule: -0.1 eV.
- No coupling between the atoms in the molecule.