

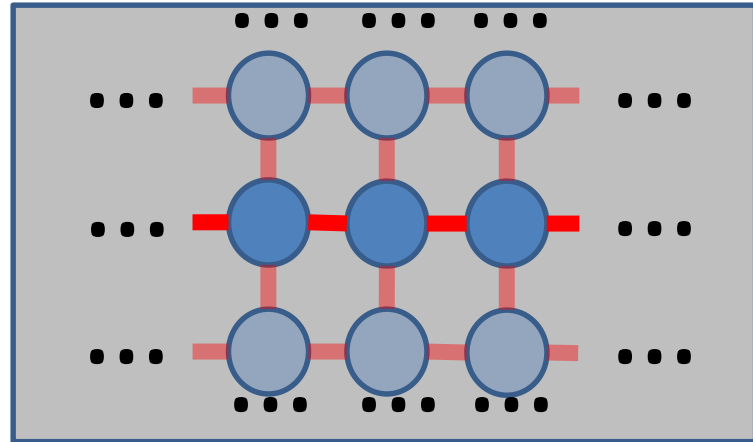
Square lattice

Objectives

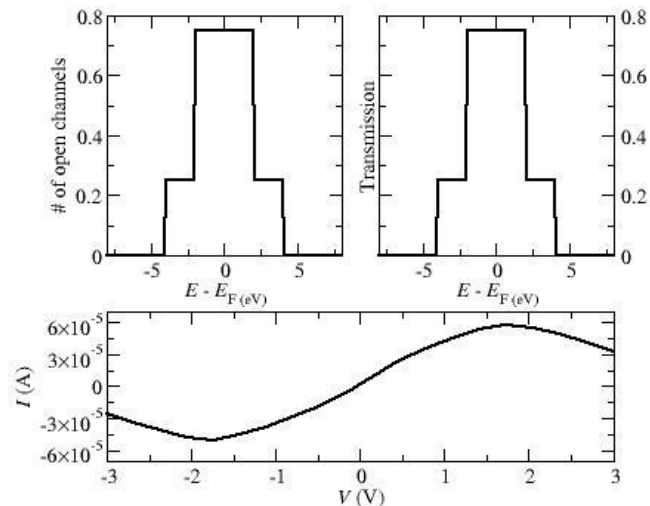
- Simulate two-dimensional (2D) system with perfect transmission (equal to the number of open channels or bands at a certain energy).
- Check that the transmission exactly coincides with the number of open channels.

Results

- The transmission has a step-like shape which corresponds to the number of open channels at a given energy.
- The number of open channels is not an integer because the results are normalized to the number of k -points.
- The central part has the largest contribution from the k -point with largest weight. The satellites and part of the central region correspond to the other k -points.
- The current linearly increases first and then decreases, giving rise to NDR, because the transmission is severely affected by 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.

System description and parameters

Leads

- Unit cell with just one atom. One orbital per atom.
- Single-atom chain replicated along one perpendicular direction with the same distances and coupling as along the z direction (square latt.).
- 4 Perpendicular k -points. Two are equivalent (only one of them is used with a double weight).

Extended molecule (EM)

- 3 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.
- 1 principal layer on each electrode. 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 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.
- Coupling between atoms: 1.0 eV.
- 4 perpendicular k -points. Only 3 are used (two of them are equivalent; only one of them is included with a double weight). There are 3 k -dependent Hamiltonians in the leads and EM.