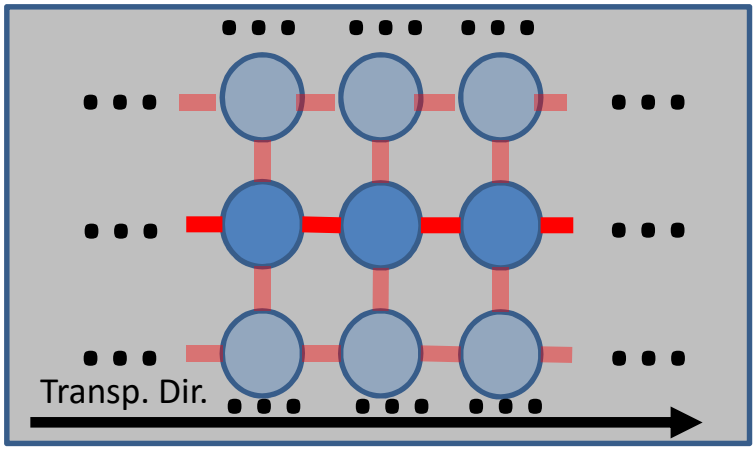
5.TB - Square lattice

Objectives

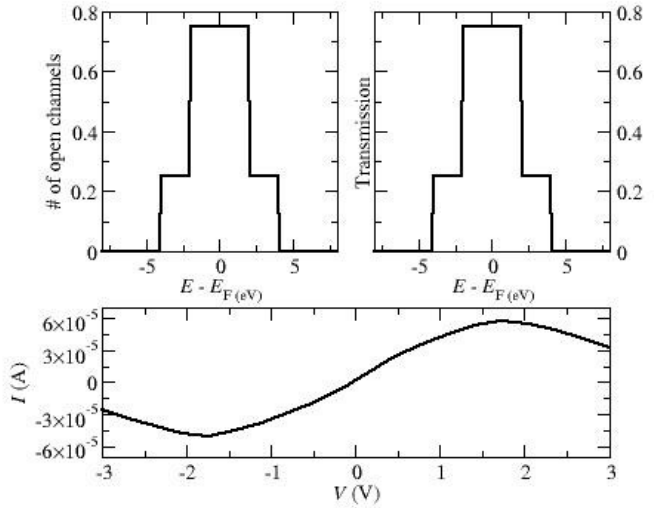
- Simulate two-dimensional (2D) system with perfect transmission (equal to the number of open channels or bands at a certain energy).
- Check that the transmission exactly coincides with the number of open channels.



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 hast 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.



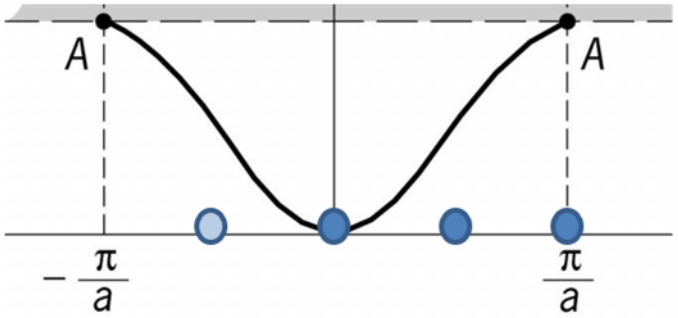
Current as a function of voltage.
Calculated with **Mode 4** of Gollum.

5.TB - Hamiltonian

***k*-points** $\Psi_{\vec{k}_\parallel}(\vec{r}) = \sum_{\vec{R}_\parallel} e^{i\vec{k}_\parallel \cdot \vec{R}_\parallel} \phi(\vec{r} - \vec{R}_\parallel)$ $\quad \hat{H}_{\vec{k}_\parallel} = \sum_{\vec{R}_\parallel} e^{i\vec{k}_\parallel \cdot \vec{R}_\parallel} \hat{H}_{\vec{R}_\parallel}$

4 k-points in the BZ:

Because of symmetry, they can be reduced to only 3.



Leads $\hat{H}_{\mathrm{L/R},1} = \begin{pmatrix} \varepsilon_1 & \gamma \\ \gamma & \varepsilon_1 \end{pmatrix}$ $\quad \hat{H}_{\mathrm{L/R},2} = \begin{pmatrix} \varepsilon_2 & \gamma \\ \gamma & \varepsilon_2 \end{pmatrix}$ $\quad \hat{H}_{\mathrm{L/R},3} = \begin{pmatrix} \varepsilon_3 & \gamma \\ \gamma & \varepsilon_3 \end{pmatrix}$

5.TB - 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 1000 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.