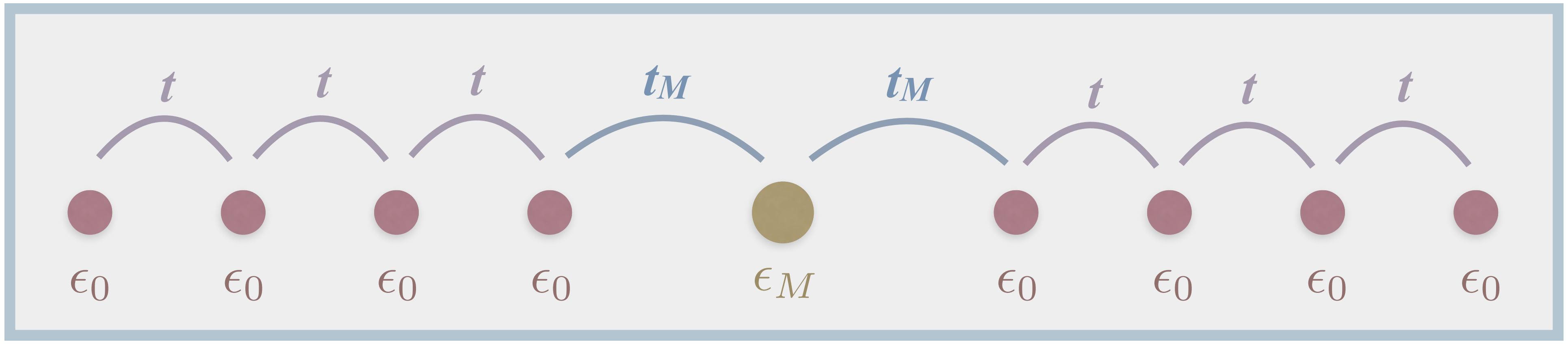
Single level bridging two atomic chains



Objectives

- Compute the transmission T(E) and see how it shows a Breit-Wigner resonance at ϵ_M
- Move the resonance by applying a gate voltage
- Compute the current-voltage curve to see the transistor effect

Results

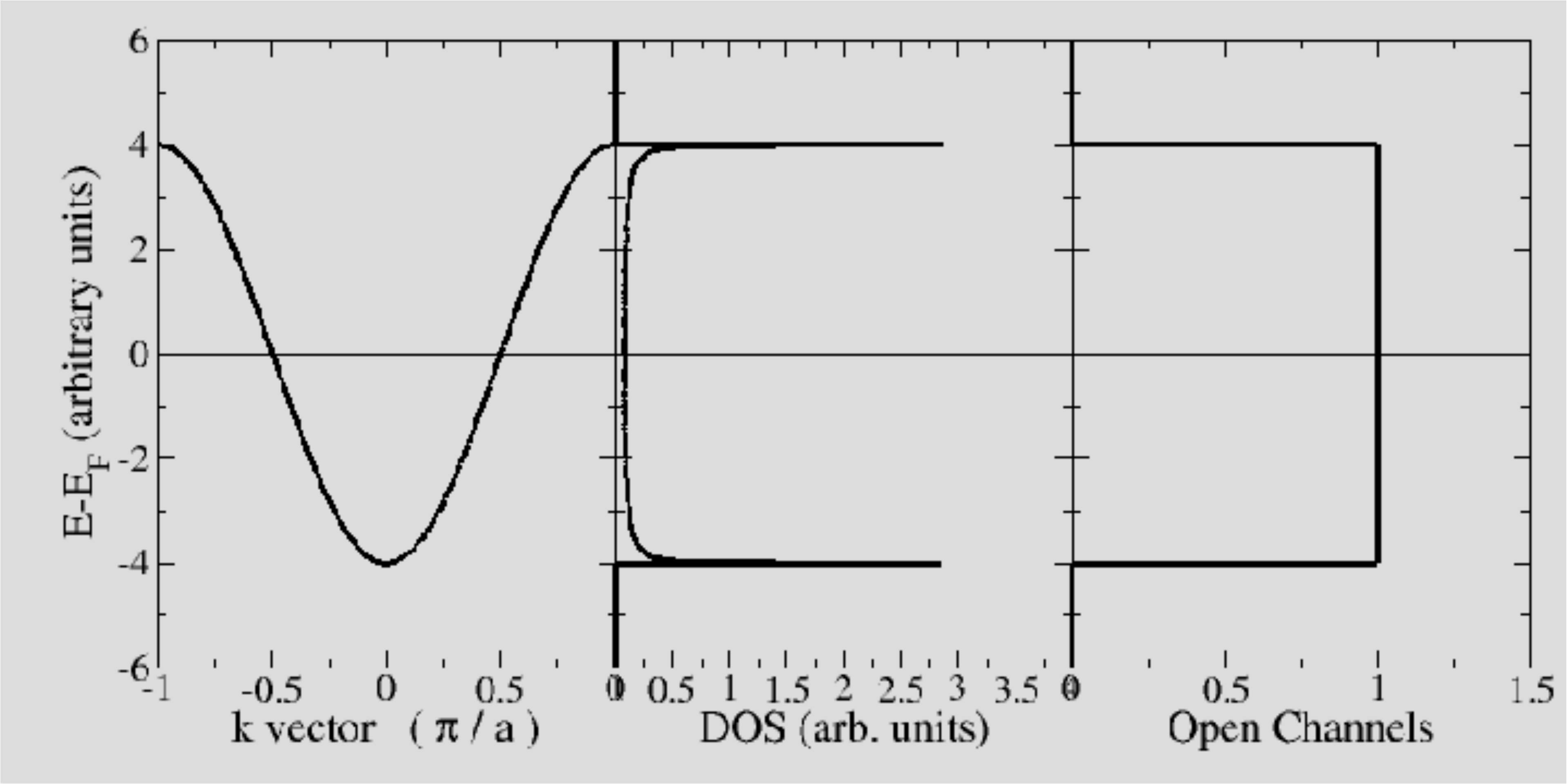
- For Mode 0
  Check the electronic structure of the leads: bands, Density of States & Open Channels
- For Mode 1
  Display the Breit-Wigner transmission resonance and move it by applying a Gate Voltage
- For Mode 4

Compute the current-voltage curve and see steps in current when the bias voltage obeys $\frac{eV}{2} = \epsilon_M$

Mode 0

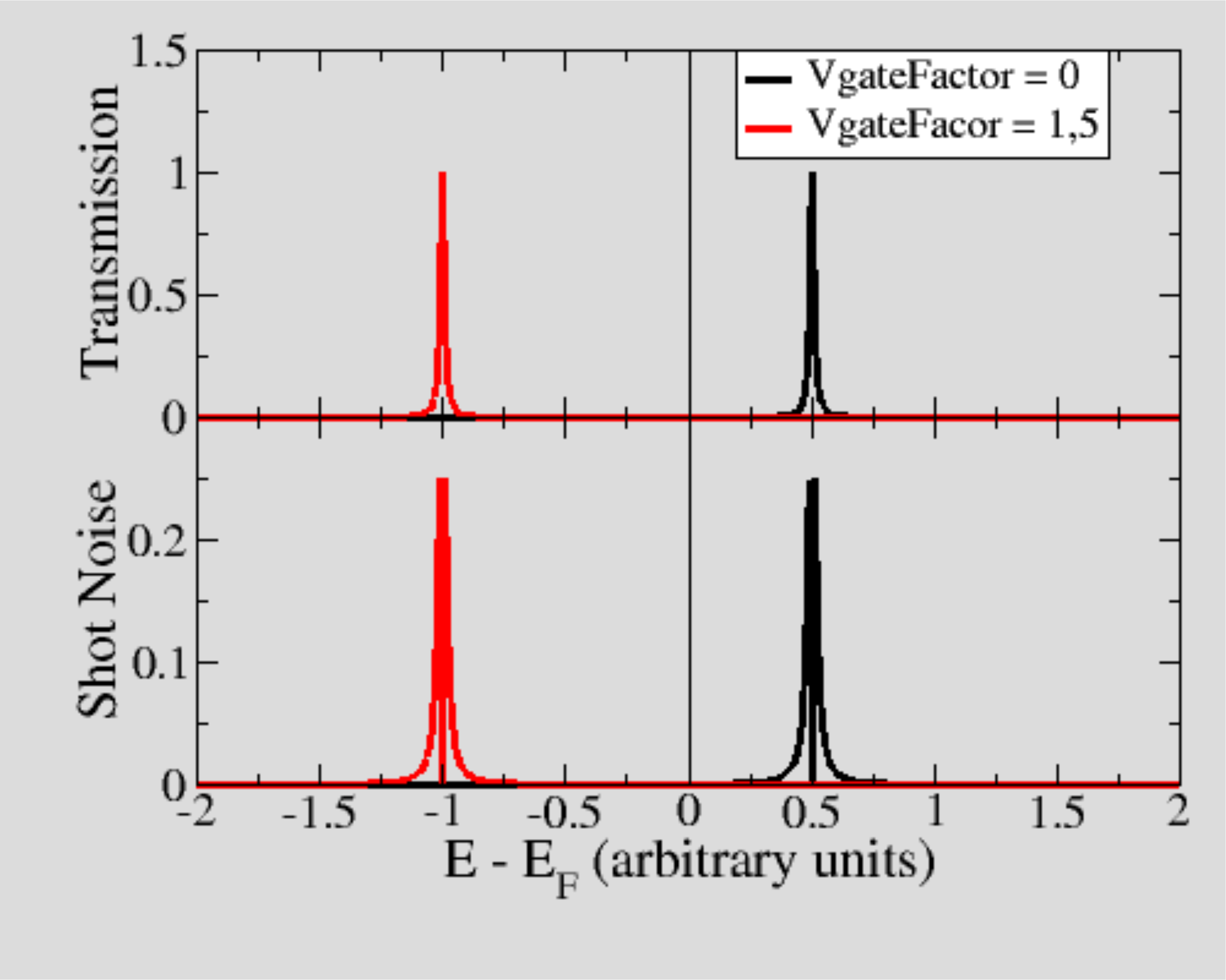
Check lead's details: Bands, Density of States and Open Channels

Lead 2 checked only, according to input file
Energy units are arbitrary in this example



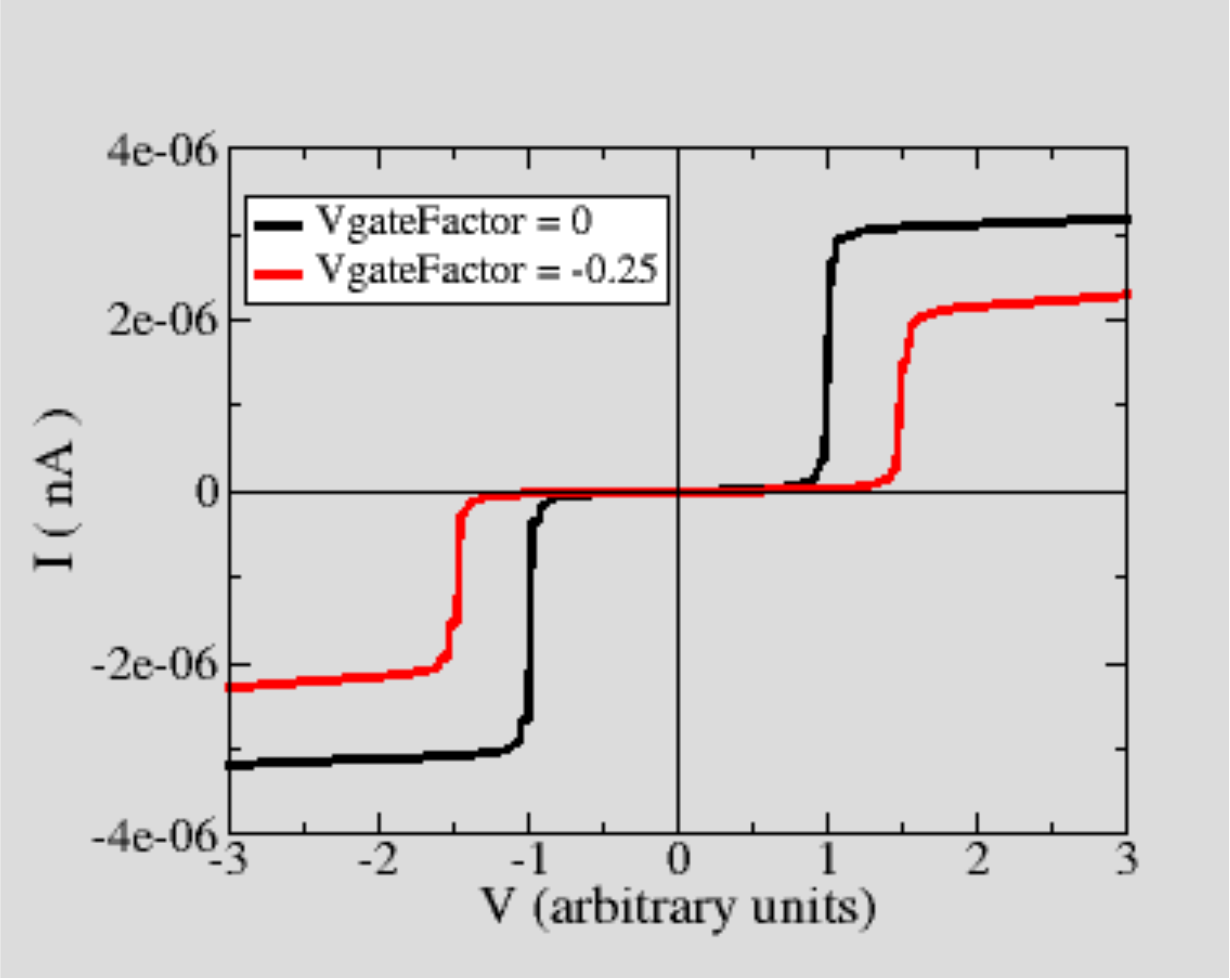
Mode 1

Compute Transmission and Shot Noise
See how a Breit-Wigner resonance develops
Move it by applying a Gate Voltage



Mode 4

Compute the Current - Voltage curves
Check the threshold Bias Voltage for Transistor effect
Change the threshold Bias Voltage by applying a Gate Voltage



System description and parameters

Leads

- Each lead is a single-atom semi-infinite chain, where each atom has a single orbital
- The unit cell consists of a single atom having a single orbital

Extended Molecule

- EM has 5 atoms.
- Four are identical with the leads
- The central is different

Tight-binding parameters

- An orthogonal basis set is used (Overlap matrix = Identity matrix). All energies in eV units
- On site energies $\epsilon_0 = 0, \;\; \epsilon_M = 0.5$
- Hopping integrals $t = -2, \;\; t_M = -0.1$

Gollum parameters

- Each of the four identical atoms in the Extended Molecule region makes 1 Principal Layer
- Mode 0: energies run in [-6,6] eV. K-points spand the 1-dimensional unit cell
- Mode 1: energies run in [-2,2] eV. Vgate is 0 or 1.5 volt
- Mode 4: Bias voltage runs in [-3,3] volt. Vgate is 0 or -0.25 volt.