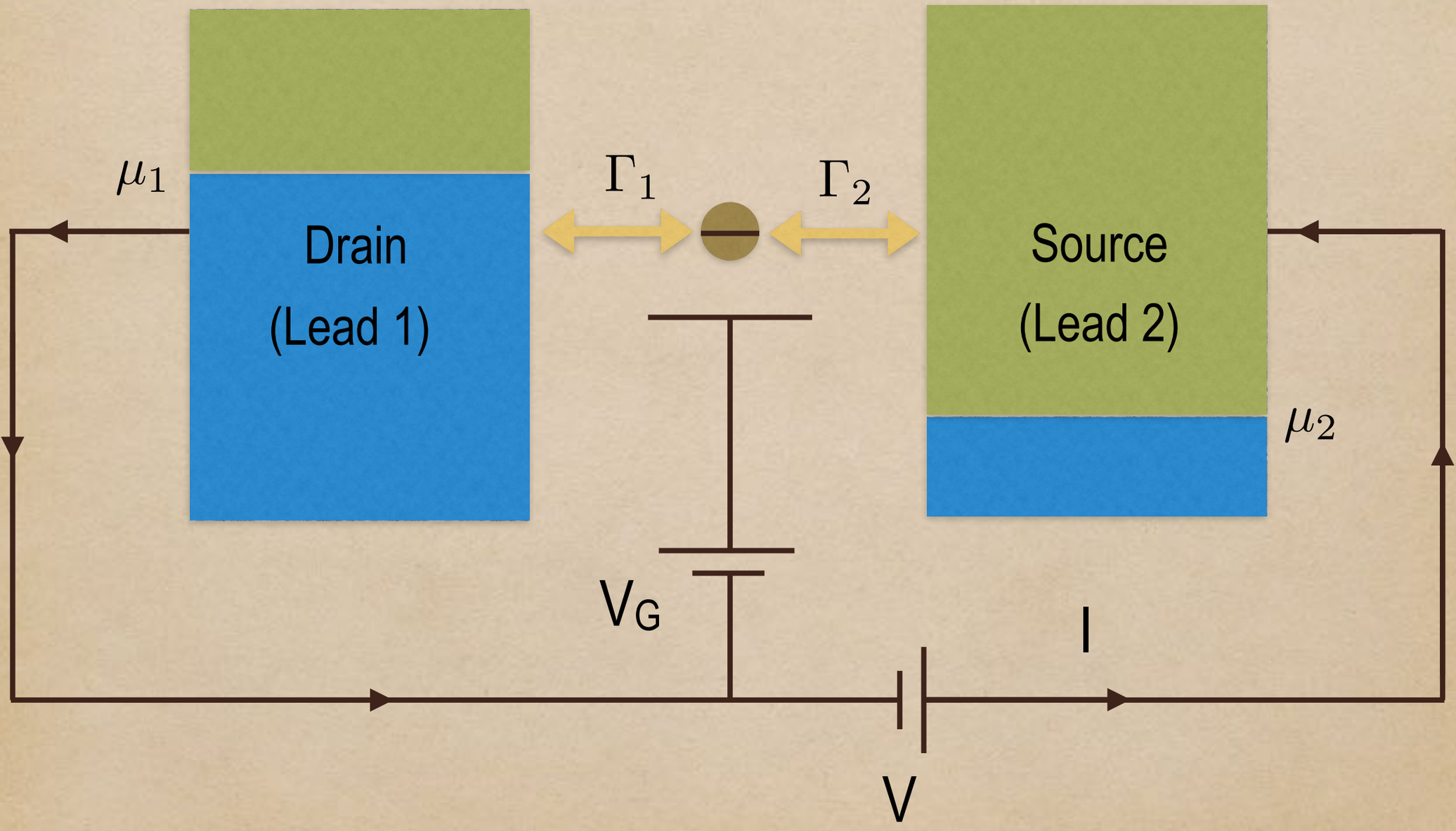
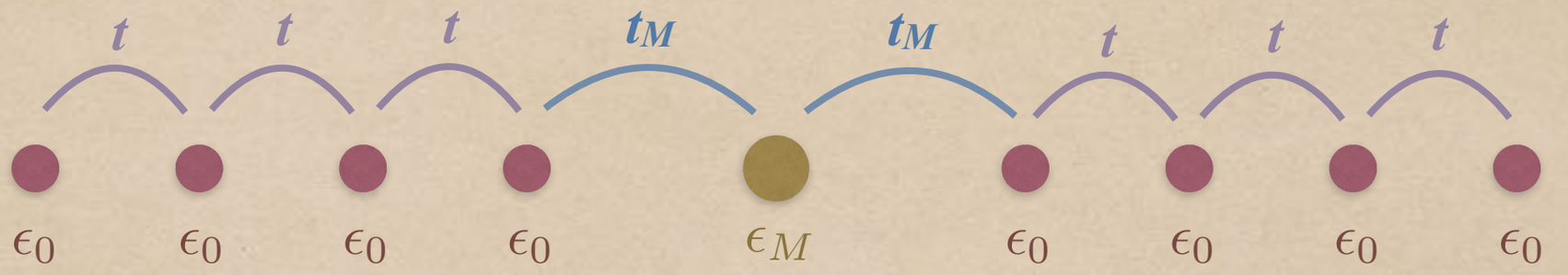
Quick start: single level model



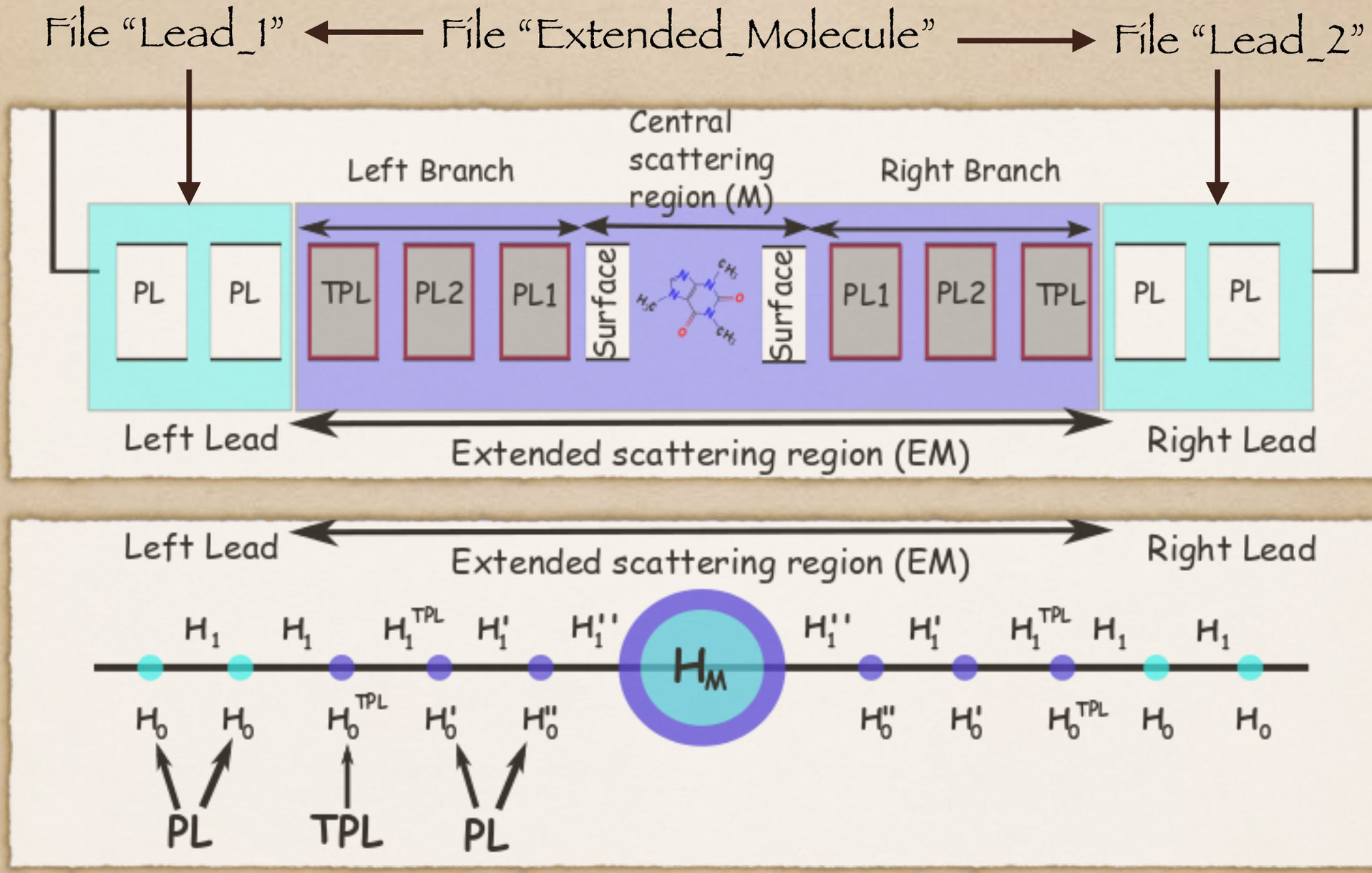
SINGLE LEVEL BRIDGING TWO ATOMIC CHAINS



OBJECTIVES

- COMPUTE THE TRANSMISSION T(E)
- SEE HOW T(E) SHOWS A RESONANCE
- MOVE THE RESONANCE BY APPLYING A GATE VOLTAGE
- CHECK THE TRANSISTOR EFFECT BY COMPUTING I(V)

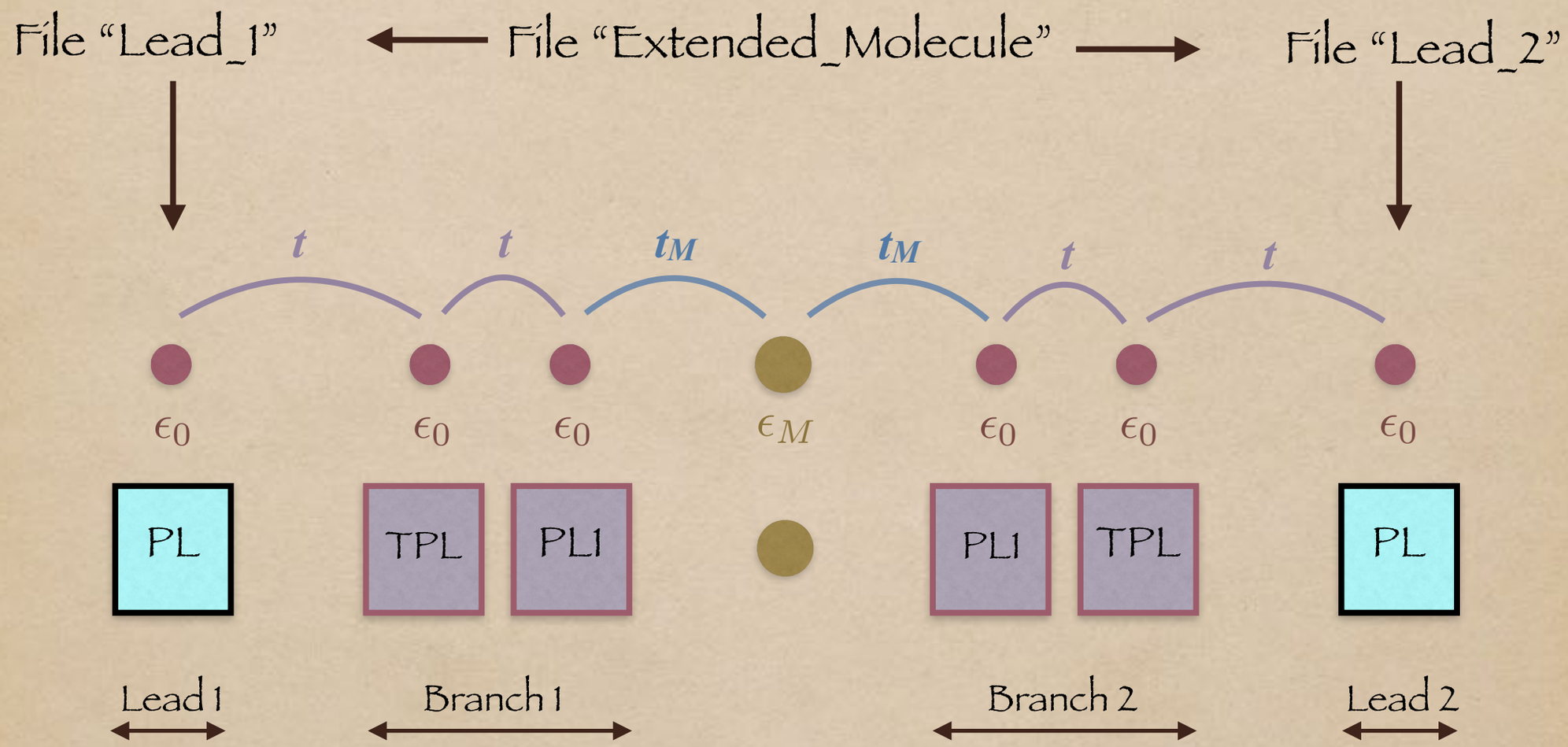
SOME FIGURES AND JARGON



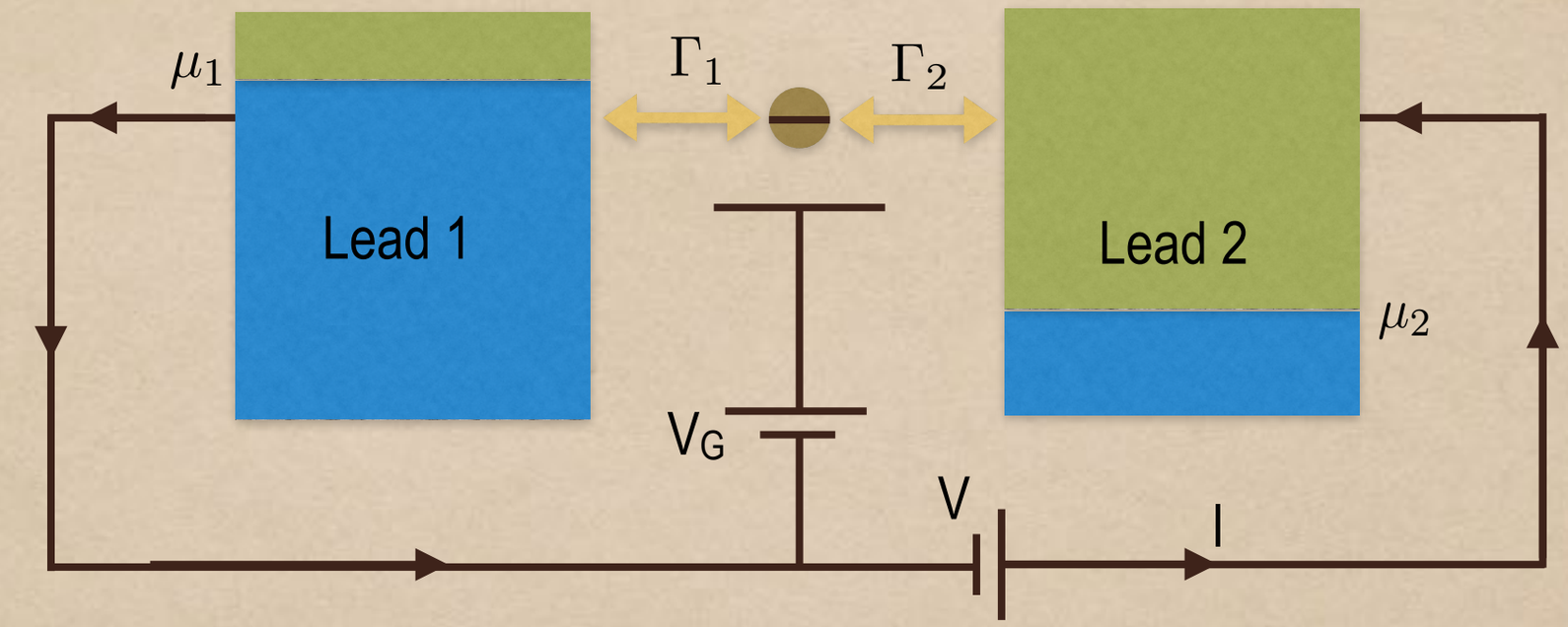
PL ≈ PRINCIPAL LAYER

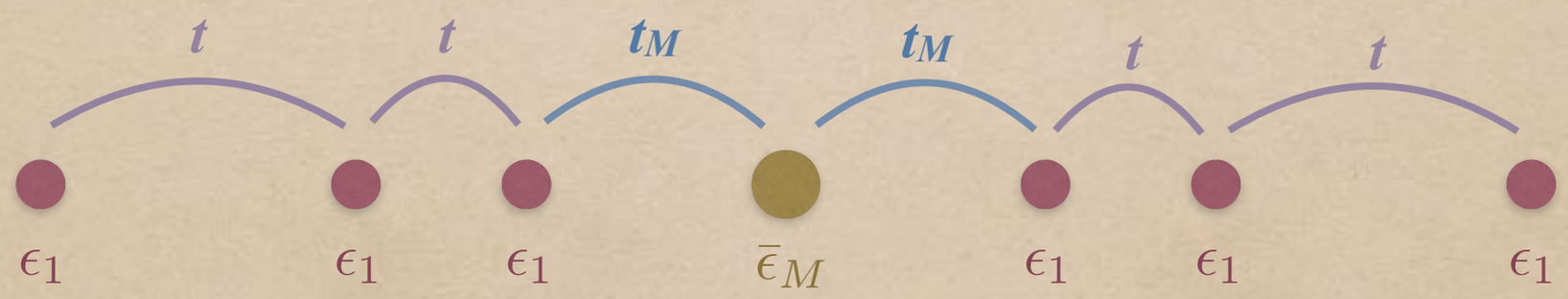
TPL ≈ TERMINATING PRINCIPAL LAYER

GOLLUM SETUP



PHYSICAL SETUP UNDER BIAS & GATE VOLTAGES





$$\mu_{1,2} = \mu_{eq} \pm eV/2$$

$$\epsilon_{1,2} = \epsilon_0 \pm eV/2$$

$$\bar{\epsilon}_M = \epsilon_M - eV_G$$

FILE "INPUT": COMMON FEATURES

Select mode (0 - 5)

```
# name: Mode
# type: scalar
 0
```

```
# name: HamiltonianProvider
# type: string
# rows: 1
tbm
```

Select Hamiltonian (tbm OR dft)

Select path to EM file

```
# name: Path_EM
# type: string
# rows: 1
../Extended_Molecule
```

```
# name: Path_Leads
# type: string
# rows: 1
1 ../Lead_2
```

Select path to each lead's file

Branches' features

```
# name: leadp
# type: matrix
# rows: 1
# columns: 3
 2       2       1
```

TPL PL1

Branch 2

```
# name: atom
# type: matrix
# rows: 5
# columns: 6
 1       1       2       0.00    0.00    0
 2       1       1       0.00    0.00    0
 3       0       1       0.00    0.00    1
 4       2       1       0.00    0.00    0
 5       2       2       0.00    0.00    0
```

Geometry of Extended Molecule

mode 0: CHECK LEAD'S DETAILS

BANDS, DENSITY OF STATES (DOS) & OPEN CHANNELS

Select mode 0

```
# name: Mode
# type: scalar
 0
```

```
# name: ERange
# type: matrix
# rows: 1
# columns: 3
 -6.00     6.00    10000.00
```

Choose energy range for DOS & OC

```
# name: kRange
# type: matrix
# rows: 1
# columns: 3
 -1.00     1.00    10000.00
```

Choose k range for bands

```
# name: DOS
# type: scalar
1
```

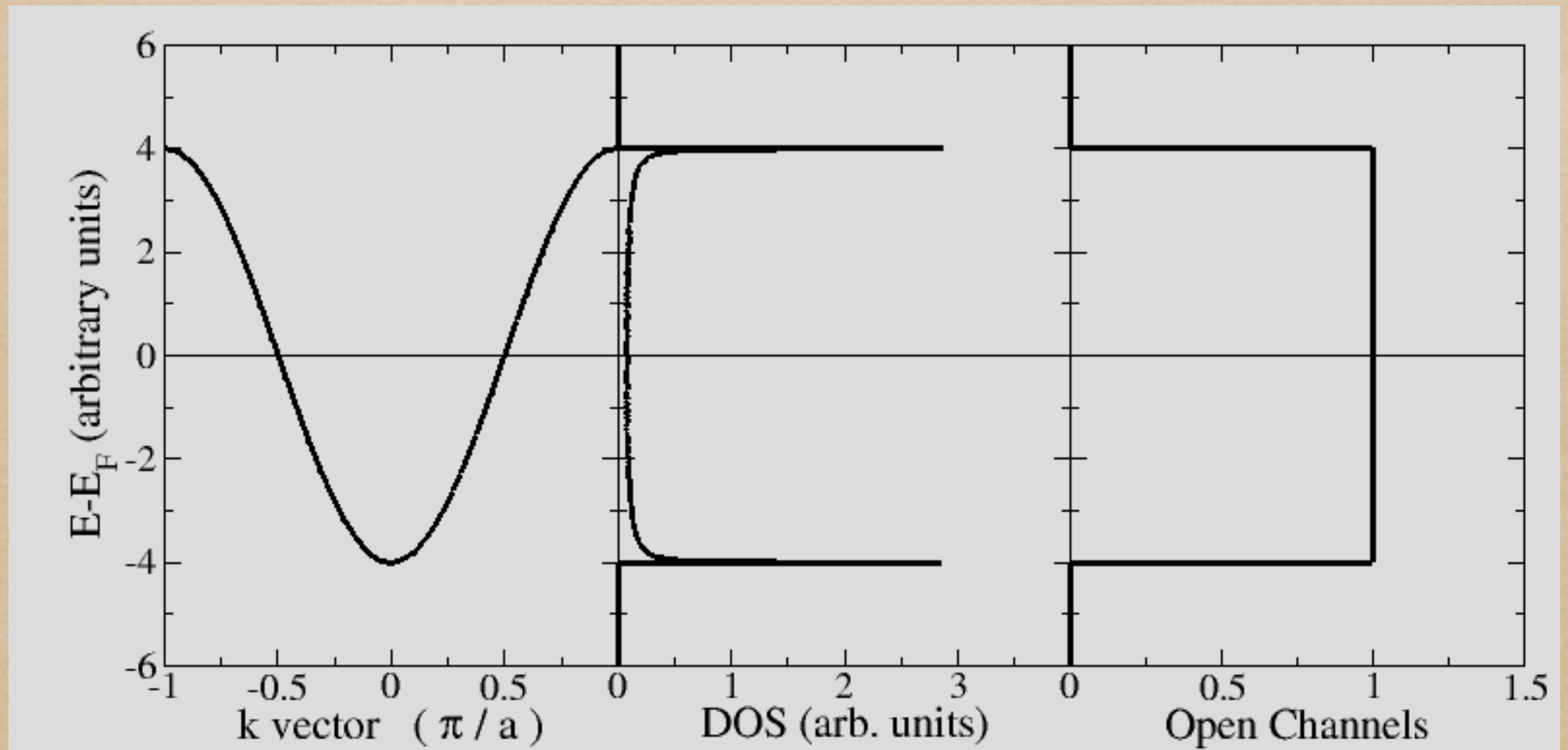
Decide if you want to compute DOS

```
# name: Path_Leads
# type: string
# rows: 1
1 ../Lead_2
# name: leadp
# type: matrix
# rows: 1
# columns: 3
 2         2         1
```

Decide which leads to check

mode 0: CHECK LEAD'S DETAILS

BANDS, DENSITY OF STATES (DOS) & OPEN CHANNELS



Lead 2 checked only, according to input file

Energy units are arbitrary in this example

mode 1: Transmission & Shot noise

Select mode 0

```
# name: Mode
# type: scalar
 1
```

```
# name: ERange
# type: matrix
# rows: 1
# columns: 3
 -6.00     6.00    500.00
```

Choose energy range for T & SN

Define Gate voltage

```
# name: VgateFactor
# type: scalar
 1
```

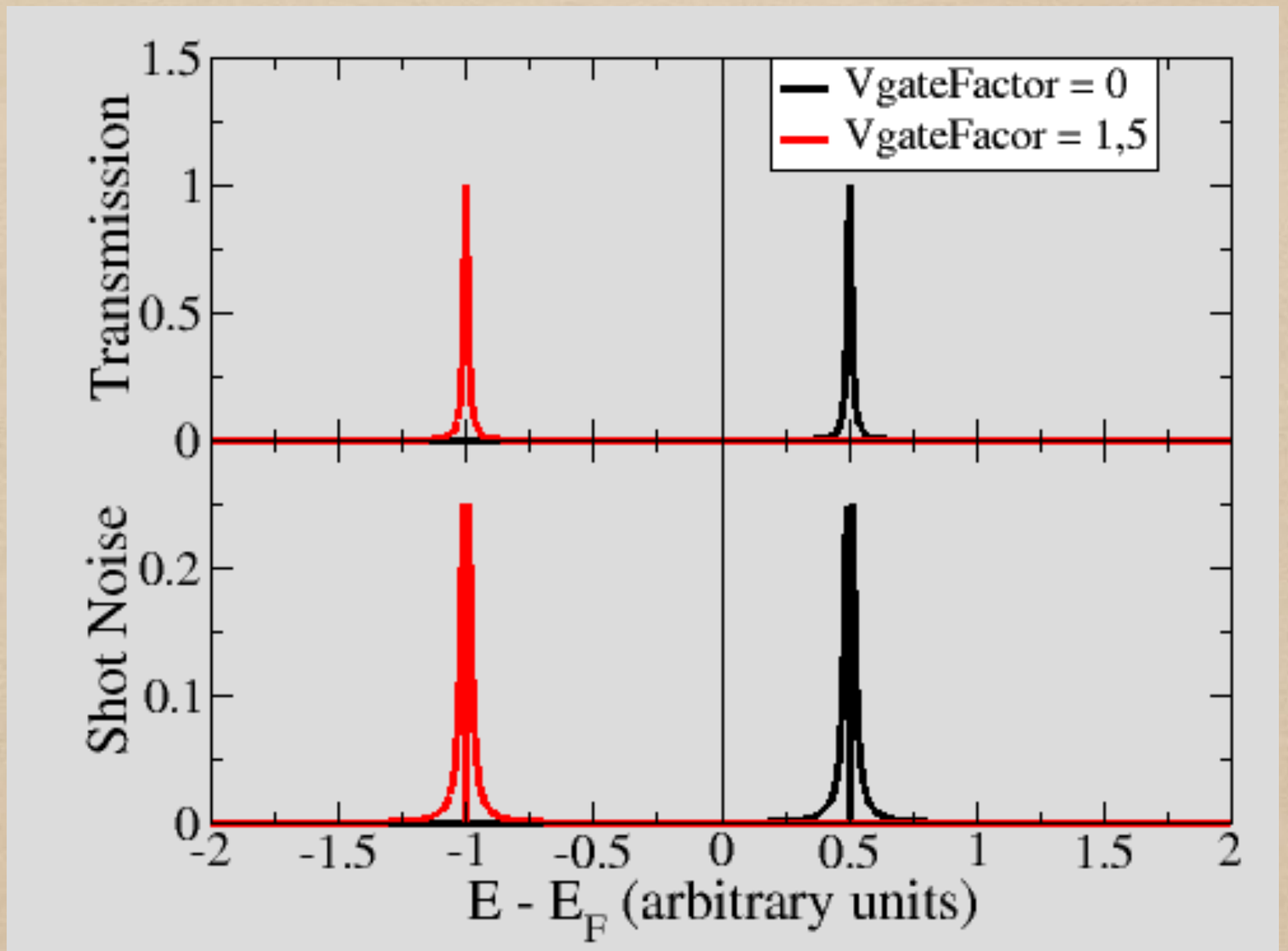
```
# name: leadp
# type: matrix
# rows: 2
# columns: 3
  2        2        -1
  2        2         1
```

Decide whether compute lead's GF from EM or from Leads Hamiltonians

Gate voltage profile at EM

```
# name: atom
# type: matrix
# rows: 5
# columns: 6
  1        1        2        0.00     0.00     0
  2        1        1        0.00     0.00     0
  3        0        0        0.00     0.00     1
  4        2        1        0.00     0.00     0
  5        2        2        0.00     0.00     0
```

mode 1: Transmission & Shot noise



mode 4: Current - Voltage characteristics

Select mode 0

```
# name: Mode
# type: scalar
 4
```

```
# name: Bias
# type: matrix
# rows: 2
# columns: 3
-3.0  3.0 200
 0    0    0
```

Electrode 1 voltage range

Constant voltage applied to Electrode 2

Energy integral accuracy

```
# name: Bias_accuracy
# type: scalar
0
```

```
# name: atom
# type: matrix
# rows: 5
# columns: 6
 1     1     2     1     1.0   0
 2     1     1     1     0.5   0
 3     0     0     0     0.0   1
 4     2     1     2     0.5   0
 5     2     2     2     1.0   0
```

Voltage drop profile

mode 4: Current - Voltage characteristics