Transport calculations via the NEGF method

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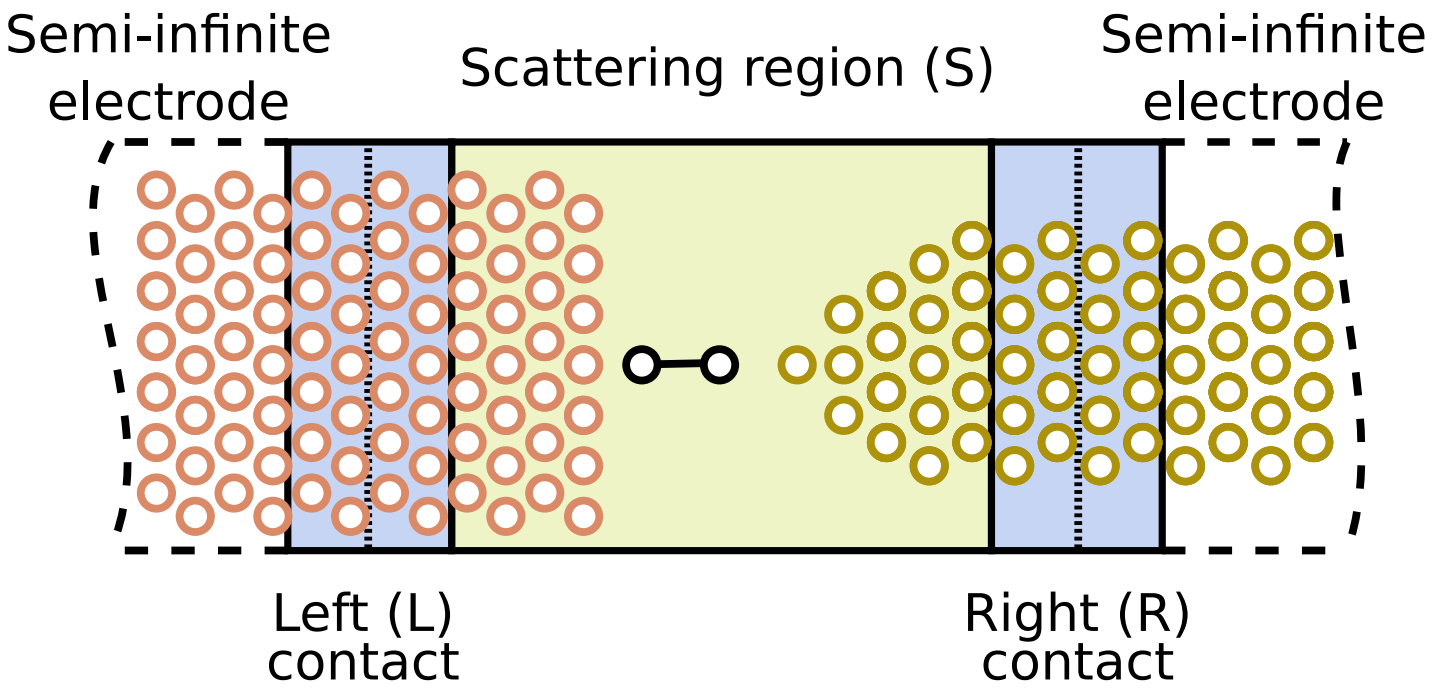
Aim of this talk

- ✓ Introduce the Non-Equilibrium Green's Function (NEGF) method;
- ✓ Show how to set up NEGF calculation in CP2K.

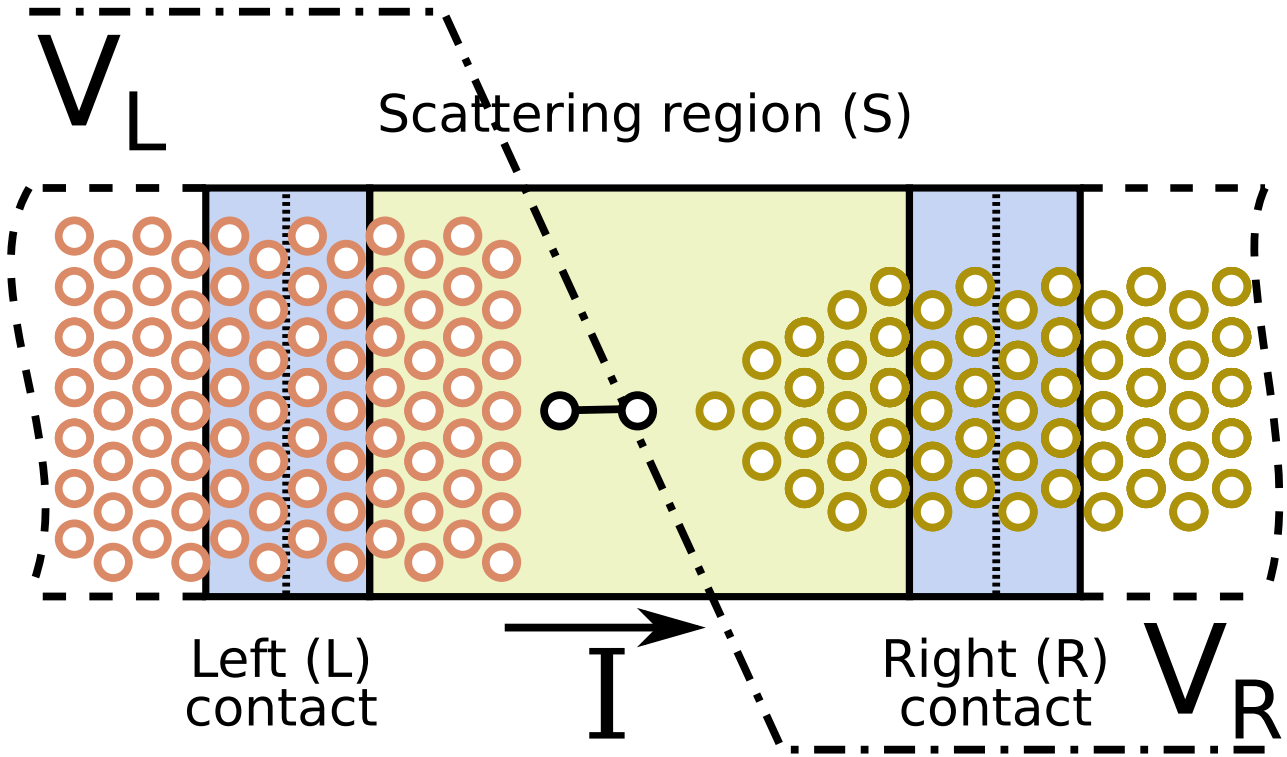
Literature:

1. S. Doniach and E. Sohdheimer "*Green's Functions for Solid State Physicists*", Frontiers in Physics Lecture note series 44 (1974);
2. H. Haug, A.-P. Jauho "Quantum Kinetics in Transport and Optics of Semiconductors", Springer Series in Solid State Sciences 123 (1998).

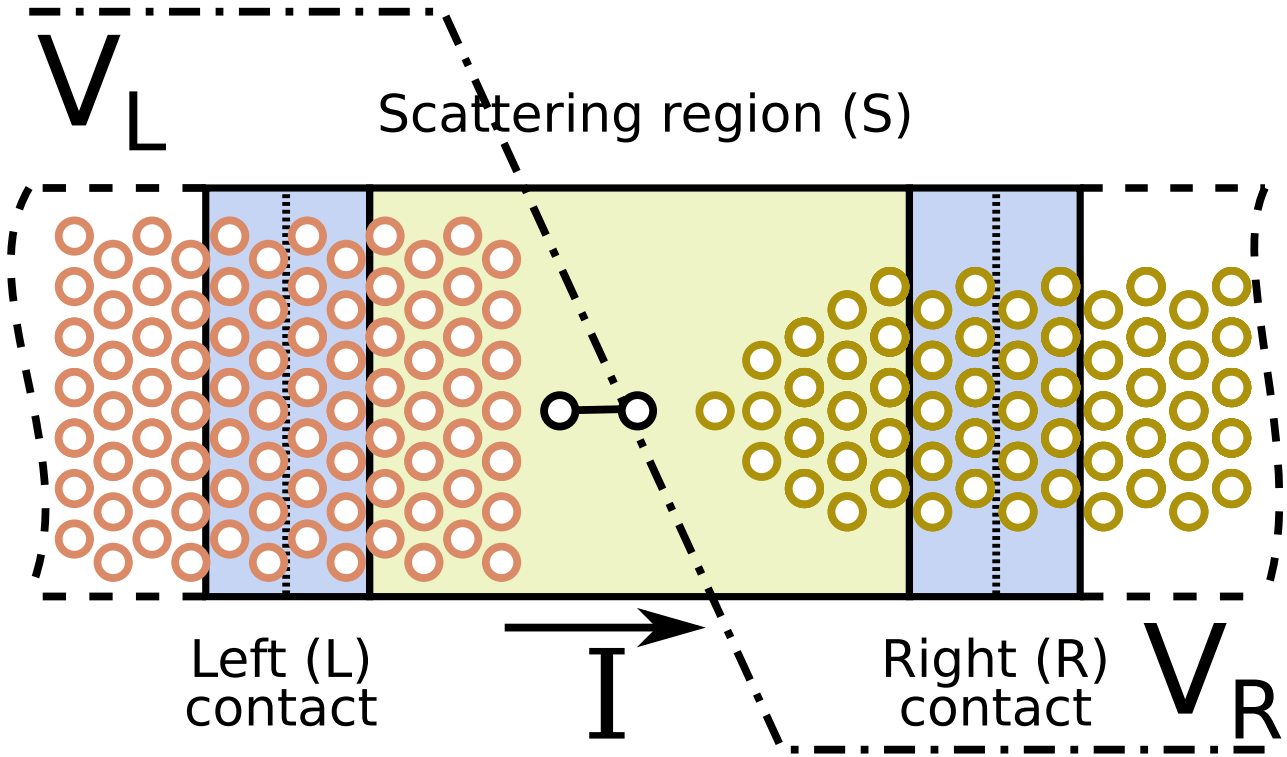
The simplest setup



The simplest setup



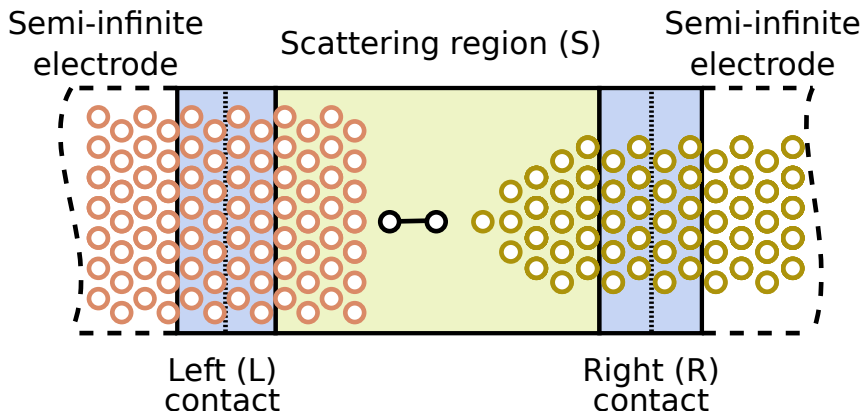
The simplest setup



Compute: $G_S^{ret.}$, $G_S^{adv.}$

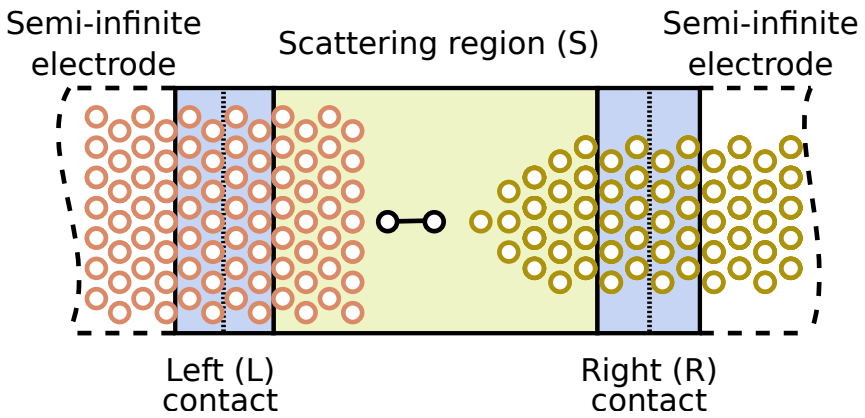
- Density of states
- Transmission
- Current

Assumption: Nearest-neighbour interaction



$$\mathbf{H} = \begin{pmatrix} \mathbf{H}_{\mathrm{L}} & \mathbf{H}_{\mathrm{LS}} & 0 \\ \mathbf{H}_{\mathrm{SL}} & \mathbf{H}_{\mathrm{S}} & \mathbf{H}_{\mathrm{SR}} \\ 0 & \mathbf{H}_{\mathrm{SR}} & \mathbf{H}_{\mathrm{R}} \end{pmatrix}$$

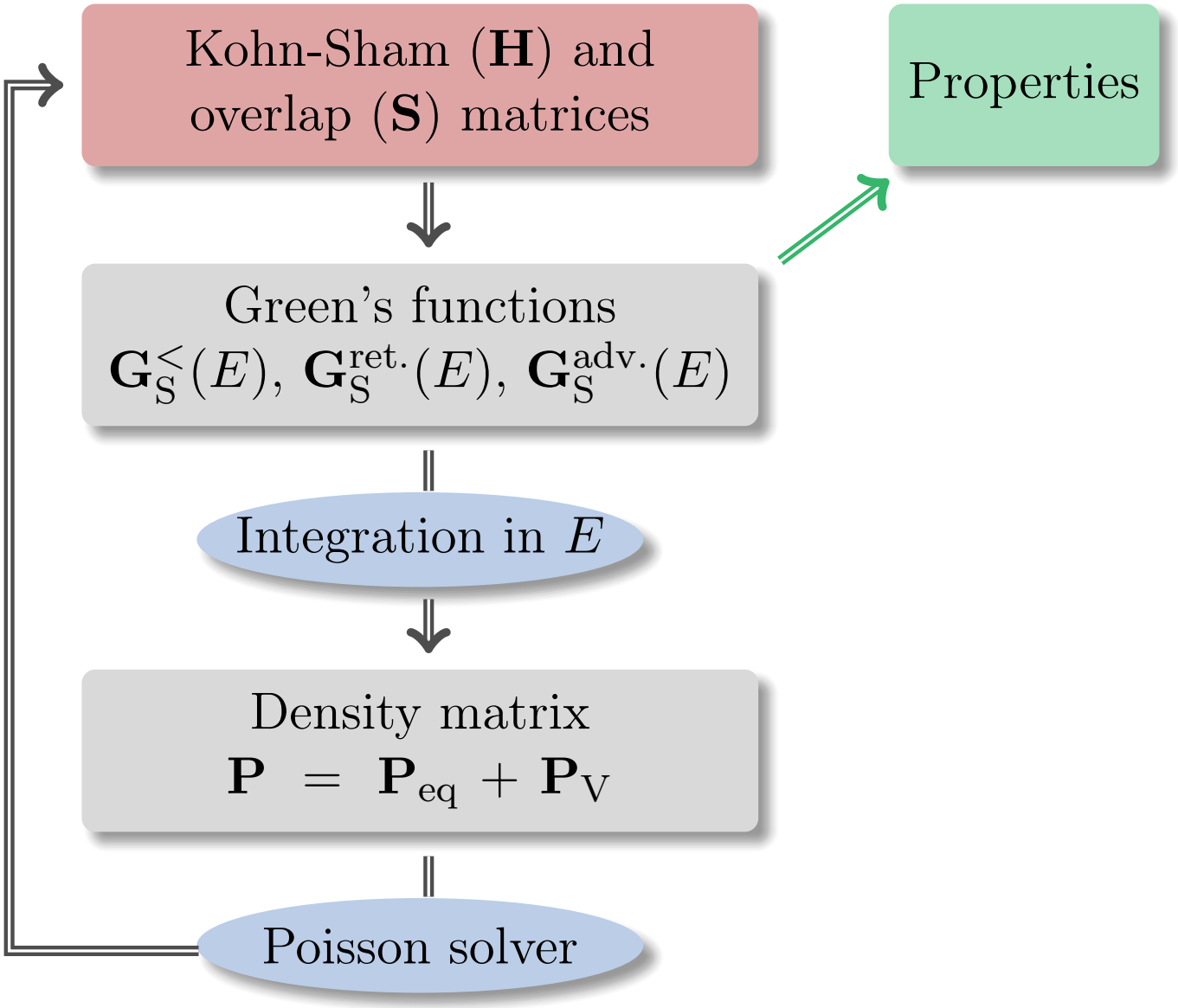
Assumption: Nearest-neighbour interaction



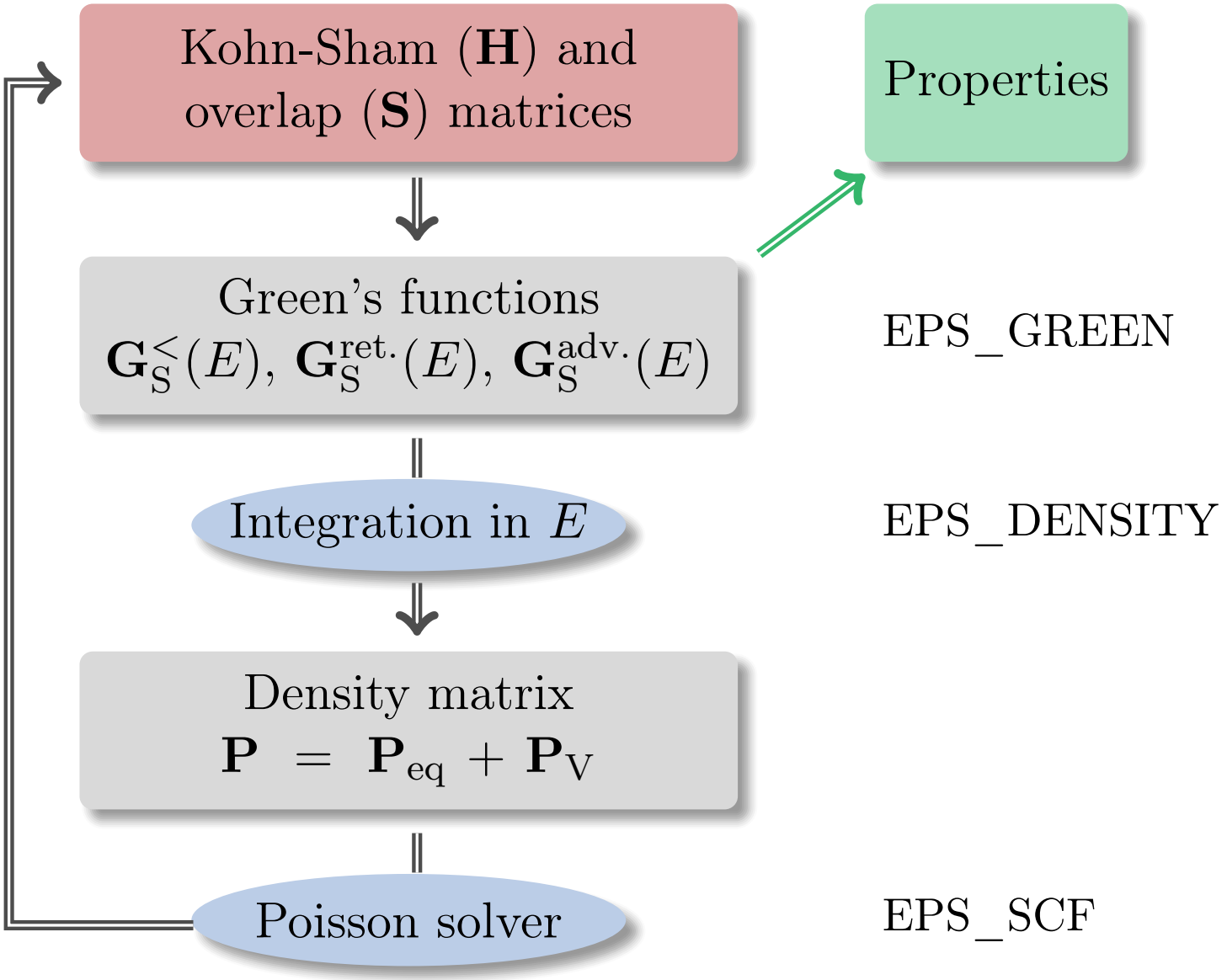
The same is also true for semi-infinite electrodes:

$$\mathbf{H}_{\mathrm{L(R)}} = \begin{pmatrix} \mathrm{h} & \mathrm{t} & 0 & 0 \\ \mathrm{t}^{\dagger} & \mathrm{h} & \mathrm{t} & 0 \\ 0 & \mathrm{t}^{\dagger} & \mathrm{h} & \ddots \\ 0 & 0 & \ddots & \ddots \end{pmatrix}$$

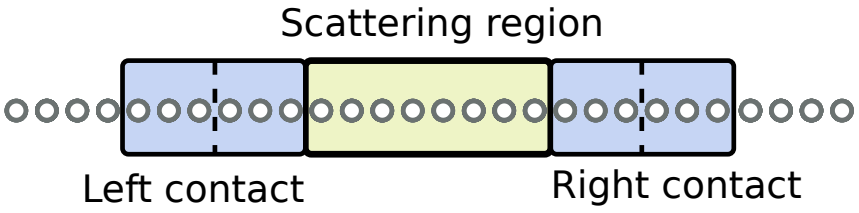
Iterative algorithm



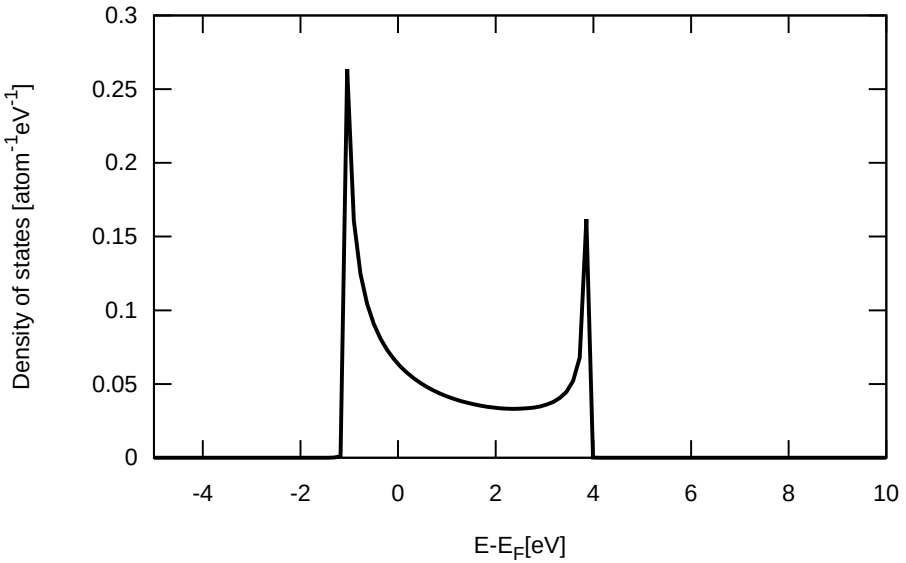
Iterative algorithm

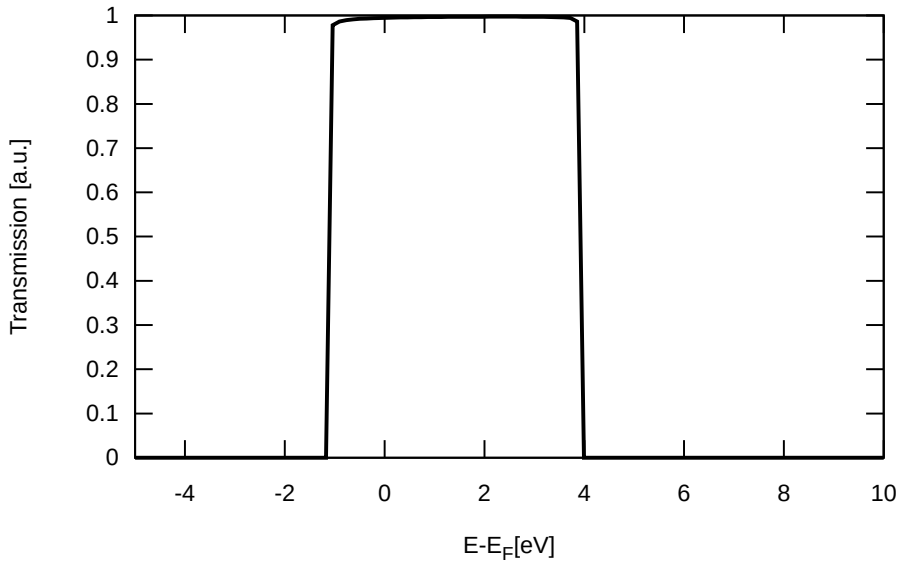


Example: Lithium chain



- ✓ 8 atoms in contact unit cell;
- ✓ 16 atoms in scattering region;
- ✓ 100 atoms in total;
- ✓ $20 \times 20 \times 300$ Å^3 unit cell;
- ✓ PBE / SZV-MOLOPT / GTH





Example input file: Lithium chain

```
 &GLOBAL
   PROJECT Li
   RUN_TYPE negf
 &END

 &NEGF
   &CONTACT
      &BULK_REGION
         MOLNAME L1 L2
      &END

      ELECTRIC_POTENTIAL [eV] 0.0
#     FERMI_LEVEL        -0.10677
      FORCE_EVAL_SECTION  1
   &END

   ... second contact ...

   &SCATTERING_REGION
      LIST 43..58
   &END SCATTERING_REGION
   TEMPERATURE            293

   &PRINT
      &DOS
         FILENAME dos
      &END
      &TRANSMISSION
         FILENAME transm
      &END
   &END
 &END
```

```
# [FORCE_EVAL 0] : entire system
&FORCE_EVAL
   METHOD Quickstep

   ... DFT parameters ...

   &SUBSYS
      &COORD
         ... all atoms go here ...
      &END
   &END
&END

# [FORCE_EVAL 1] : the first contact
&FORCE_EVAL
   METHOD Quickstep
   &DFT
     ...
     &KPOINTS
        SCHEME  MONKHORST-PACK 4 4 4
     &END
   &END

   &SUBSYS
      &COORD
Li      0.00    0.00   99.00 L1
Li      0.00    0.00  102.00 L1
...
Li      0.00    0.00  117.00 L1
Li      0.00    0.00  120.00 L1
      &END
   &END
&END
```

Example output log: Lithium chain

```
COMPUTE FERMI LEVEL OF CONTACT 1 AT 293.000 KELVIN

Electronic density of the isolated contact unit cell:           -24.0000000000

 Step     Integration method      Time      Fermi level   Convergence (density)
 ------------------------------------------------------------------------------
    1     CC 98     2.74E-06       0.1      -0.08488095            3.27524E+00
    2     CC 98     2.73E-06       0.1      -0.07963757            3.94160E+00
    3     CC 98     3.09E-06       0.1      -0.11065280           -6.94556E-01
    4     CC 98     2.97E-06       0.1      -0.10614376            1.07967E-01
    5     CC 98     2.98E-06       0.1      -0.10686857           -1.71633E-02
    6     CC 98     2.98E-06       0.1      -0.10676915            8.37216E-05
    7     CC 98     2.98E-06       0.1      -0.10676963           -4.08547E-07

NEGF| Contact No. 1
NEGF|    Fermi level at 293.000 Kelvin (a.u.):                     -0.10676963
NEGF|    Electric potential (V):                                    0.00000000

NEGF| Contact No. 2
NEGF|    Fermi level at 293.000 Kelvin (a.u.):                     -0.10676963
NEGF|    Electric potential (V):                                    0.00000000

NEGF SELF-CONSISTENT PROCEDURE

Initial electronic density of the scattering region:       -47.70439078463643

 Step     Integration method      Time     Electronic density      Convergence
 ------------------------------------------------------------------------------
    1     CC 98     2.98E-06       0.1           -47.70429406      9.67289E-05

           *** NEGF run converged in 1 iteration(s) ***
```

Acknowledgements

CP2K community

ARCHER
EPSRC