nextnano.QCL - Software documentation

General remarks

nextnano.QCL is a console application that is run from within the nextnanomat software (GUI). Alternatively, it can be executed from the command line. The input file specifies the device that shall be simulated.

nextnanomat

nextnanomat is a convenient graphical user interface for nextnano.QCL. It can be downloaded from here. It can visualize 1D, 2D and 3D simulations results.

Input file

The input file specifies all properties of the device, such as geometry, material composition, temperature, grid,… Furthermore, it sets all parameters that are needed to define the program flow of nextnano.QCL. The keywords that can be used for this purpose are defined in the syntax of the input file.

Output

nextnano.QCL exports its results to a directory. The output files are documented here.

Examples

The nextnano.QCL installation provides some example tutorials that can be run with nextnanomat, to get familiar with the program.

Database

All material properties that are needed for simulation are described here.

Download

The software can be obtained from here.

If you have further questions, see the FAQ or contact support@nextnano.com.

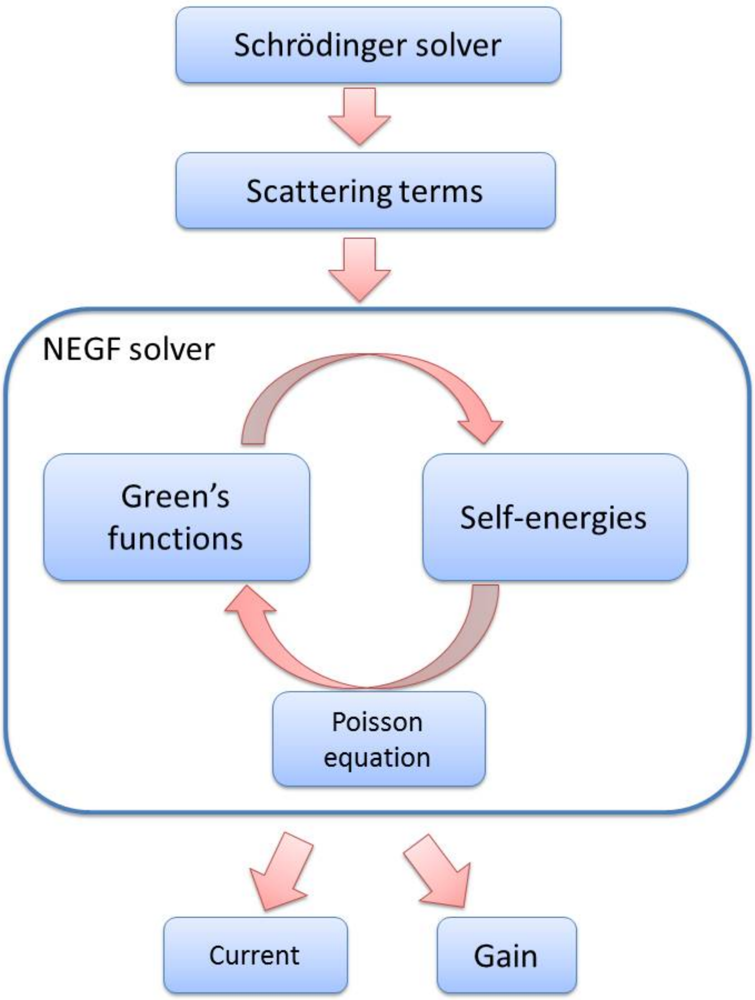
Working principle

The code is based on the non-equilibrium Green's functions (NEGF) formalism (also known as the Keldysh, or Kadanoff-Baym formalism). This formalism allows to account for both quantum transport effects (i.e. coherent transport effects, such as resonant tunneling), as well as scattering mechanisms.

In the NEGF formalism, scattering processes are described in terms of self-energies. Self-energies and Green's functions are calculated in a self-consistent way, as both elastic and inelastic scattering processes are accounted within the the self-consistent Born approximation.

The code uses **field-periodic boundary condition**. In this way the simulation accounts for an infinite periodic structure, with a periodic electric field. Coherent transport between periods is accounted on a length set by <Coherence_length_in_Periods>.

Program flow



In the beginning of the calculation, the single-band effective mass Schrödinger equation is solved in real space. The calculated energy levels and wave functions are then used as input to the NEGF algorithm. The wave functions are termed **modes** and the NEGF algorithm is written in terms of **mode space** and not **real space** to make it computationally more efficient. The number of QCL periods that are input to this Schrödinger equation are specified in <Number_of_lateral_periods_for_band_structure>. In general, the core of the NEGF algorithm should be rather independent of this number, e.g.

```
<Number_of_lateral_periods_for_band_structure> 4
</Number_of_lateral_periods_for_band_structure>
```

should lead to very similar results compared to a value of 5 but the numerical values might differ slightly.