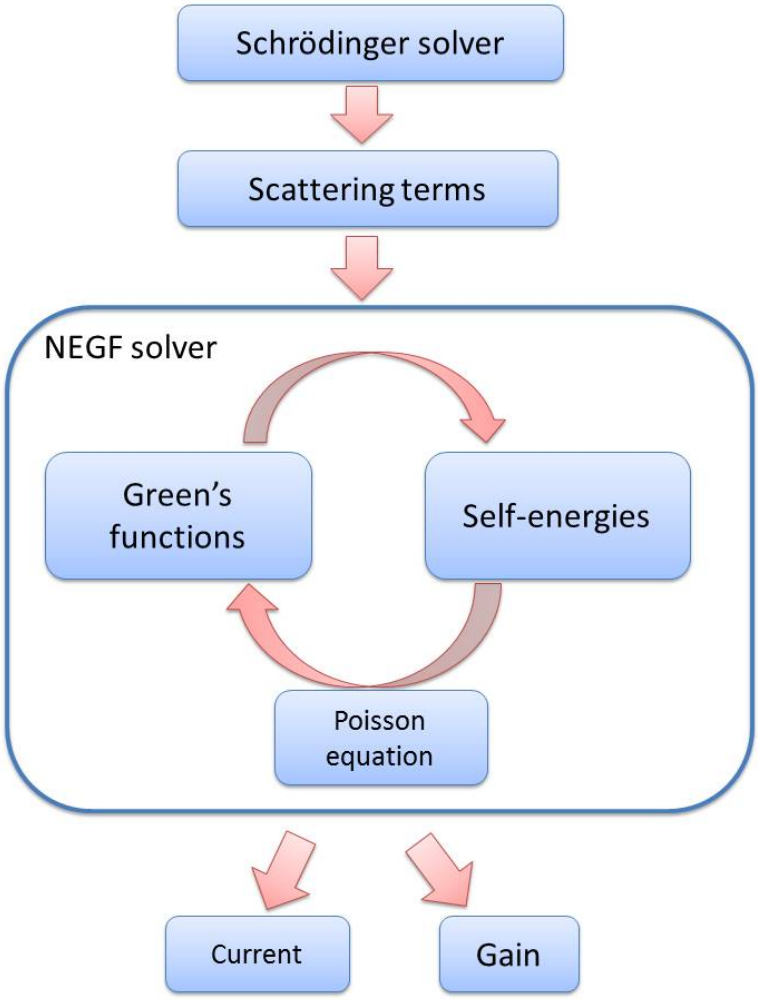
Working principle

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



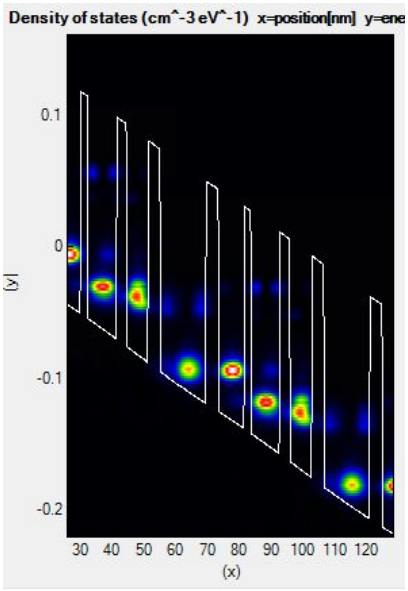
In the beginning of the calculation, the single-band effective mass Schrödinger equation is solved in real space. The energy levels (i.e. minibands) are selected up to an energy cut-off which is specified

in the input file by

```
<Energy_Range_Axial unit="meV">150</Energy_Range_Axial>
```

The minibands are transformed into a localized basis of modes which we name “Reduced Real Space” basis. These wave functions are then used as a basis in the NEGF algorithm.

As a second step, the scattering coupling terms are calculated for each of the accounted mechanism (optical and acoustic phonons, charged impurities, interface roughness, alloy disorder, electron-electron scattering).



Then, the main part of the calculation consists in the self-consistent NEGF solver. Starting from an initial guess of the Green's functions, the self-energies are calculated. The Green's functions are then calculated iteratively. Simultaneously, the mean-field electrostatic potential is calculted self-consistenly (Poisson's equation). Such iterations are made until convergence is reached for the Green's functions as well as for the calculated current.

From the Green's functions solution, the current density is directly calculated, as well as as the carrier density. To gain more insights into analysis, the populations, the density matrix, the oscillator strengths are displayed in different basis.

The gain is then calculated if requested in the input file. To this purpose, for each photon energy specified in the input file, an ac electromagnetic perturbation is considered. An additional self-consistent routine is used is to calculate the linear response of the Green's functions to this perturbation. The gain (or absorption) spectrum is then obtained from this linear response.