Simulation output

For each simulation run, a new output folder is created in the simulation output folder. The created folder has the name of the input file.

In addition, date-time can be added to the folder name by the nextnanomat setting (Tools → Options → Expert settings before Aug 2021, Tools → Options → View/Output since Aug 2021). For nextnanomat before Aug 2021, this option is recommended in order to avoid overwriting existing output data. For nextnanomat after Aug 2021, simulation output is per default not overwritten and instead enumerated unless you manually check the option “Overwrite existing simulation…”.

The created output folder contains:

- the **input file** (.xml) and the **material database** (.xml).
- a folder '**Input**' which contains material parameters used in the calculation.
- a folder **Strain** (only if the strain option is activated).
- a folder **Polarization** if pyroelectric and/or piezoelectric effects are considered.
- a folder '**Init_Electron_Modes**' for the results of the initial Schrödinger solution.
- a **folder for each parameter step**. In particular, in case of voltage sweep, the name of the folder is the potential drop per period.
- Several files related to the sweep made. For a voltage sweep, it contains plots of physical quantities (current, gain,…) as a function of the applied voltage.
- a **log file** is created at the end of the simulation, containing all the information displayed during the simulation.

'Input' folder

The folder `Input/` contains all the simulation input such as material parameters as a function of position.

- `AlloyContent.dat`
  alloy concentration x vs. position for ternary materials such as `Al(x)Ga(1-x)As`
- `AlloyScatteringTerm.dat`
  alloy scattering term (in unit of [eV^2]) vs. position for ternary materials
- `BandEdges.dat`
  conduction band edge $E_{\rm c}$ and valence band edge $E_{\rm v}$ vs. position in units of [eV]
- `BandGap.dat`
  energy band gap $E_{\rm gap}$ vs. position in units of [eV]
- `Conduction_BandEdge.dat`
  conduction band edge $E_{\rm c}$ including shift due to strain vs. position in units of [eV]
- `DeformationPotential_ConductionBand.dat`
  conduction band deformation potential vs. position
- `DeformationPotential_ValenceBand.dat`
  valence band deformation potential vs. position
- `DeformationPotential_ValenceBand_Uniaxial.dat`
  valence band uniaxial deformation potential vs. position
- `DopingDensity.dat`

Doping density [cm^{-3}] vs. position

- `E_p(Kane energy).dat`
  Kane energy [eV] (material-dependent k.p parameter) vs. position
- `EffectiveMass.dat`
  effective conduction band mass $m_{\rm c}$ vs. position in units of [m0]. This input is not used for a k.p calculation.
- `ElasticConstants.dat`
  elastic constants c_{ij} vs. position in units of [GPa]
- `EpsOptic.dat`
  optical dielectric constant $\epsilon(\infty)$ vs. position
- `EpsStatic.dat`
  static dielectric constants $\epsilon(0)$ vs. position
- `L (Dresselhaus parameter L).dat`
  Dresselhaus parameter (material-dependent k.p parameter) vs. position. Default is -1.
- `LatticeConstants.dat`
  lattice constants a vs. position in units of [nm]
- `MaterialDensity.dat`
  material density vs. position in units of [kg/m^3]
- `PhononEnergy_LO.dat`
  longitudinal optical (LO) phonon energy in units of [eV]
- `PiezoConstants.dat`
  piezoelectric constants e_{ij} in units of [C/m^2]
- `PyroConstants.dat`
  pyroelectric polarization P_z (spontaneous polarization) in units of [C/m^2] (wurtzite only)
- `S (remote band parameter).dat`
  remote band parameter (material-dependent k.p parameter) vs. position
- `VelocityOfSound.dat`
  sound velocity in units of [m/s]

Strain

If the strain option is activated, a folder `Strain/` is created.

- `Strain_CrystalSystem.dat`
  (dimensionless) strain tensor components with respect to the crystal coordinate system.
- `Strain_Simulation.dat`
  (dimensionless) strain tensor components with respect to the simulation coordinate system.

If the crystal has not been rotated, above files contain identical values.

- `Strain_trace.dat`
  trace of the strain tensor

Piezo and pyroelectric polarization

The folder `Polarization/` contains the piezoelectric and pyroelectric polarization if these options are activated.

- `InterfaceCharges\PiezoCharges.dat`
  piezoelectric charge density due to strain. If the strain is zero, the piezoelectric charge density is zero.
- `InterfaceCharges\PyroCharges.dat`
  pyroelectric charge density due to spontaneous polarization in wurtzite crystals.
- `PiezoPolarization.dat`
  z-component of the piezoelectric polarization vector
- `PyroPolarization.dat`
  z-component of the pyroelectric polarization vector

Initial electronic states

The folder `Init_Electr_Modes\` contains 3 different folders corresponding to 3 different sets of basis states. They are calculated at the first step of the calculation, before the NEGF calculation. These 3 sets of states are basis of the reduced Hilbert space obtained after applying the energy cut-off <Energy_Range_Axial>.

These states are displayed for a default voltage of <Energy_Range_Axial>/2. This voltage at which the states are visualized can be modified by the input file command:

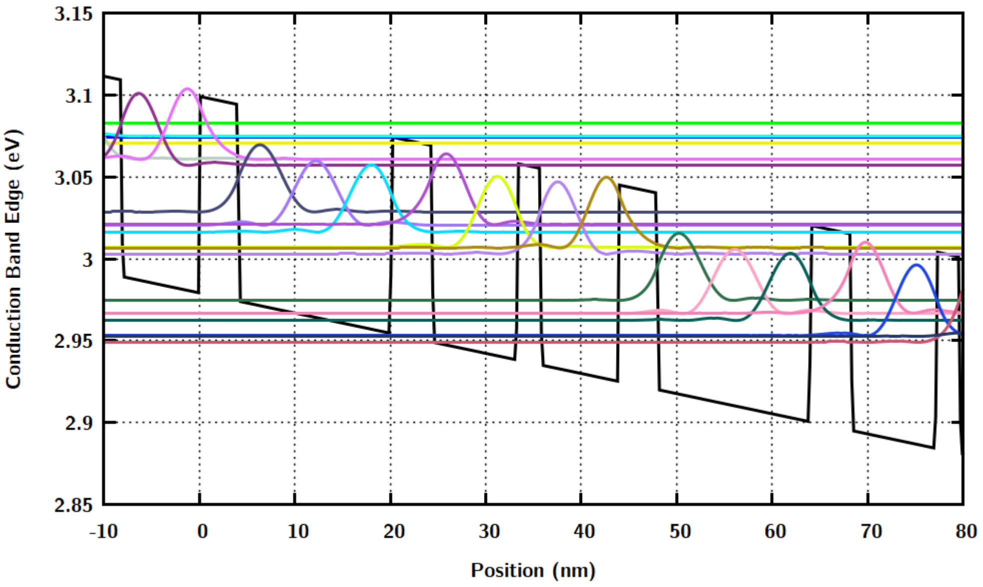
```
<Simulation_Parameter>
  ...
  <Bias_for_initial_Electronic_Modes
unit="meV">54</Bias_for_initial_Electronic_Modes>
  ...
</Simulation_Parameter>
```

'Reduced Real Space' modes

The 'reduced real space' modes are eigenstates of the position operator in the reduced Hilbert space (i.e. after the energy cut-off). Because of the energy cut-off, these states are spatially extended instead of being δ functions. This basis set is the one which is used in the NEGF calculation. It does not depend on the applied voltage. However, this basis has generally little use in terms of physical interpretation.

The folder `Init_Electr_Modes\ReducedRealSpace\` contains:

- `ReducedRealSpaceModes.dat`
  Conduction band edge and square of the wave functions (shifted in energy) vs. the heterostructure coordinate position.
  3 periods are displayed. 'per.0' 'per.1' 'per.2' in the wavefunction names refer to the left, middle and right period shown. The numbers of states displayed is equal to 3 times the number of states per period, that is the number of selected minibands.

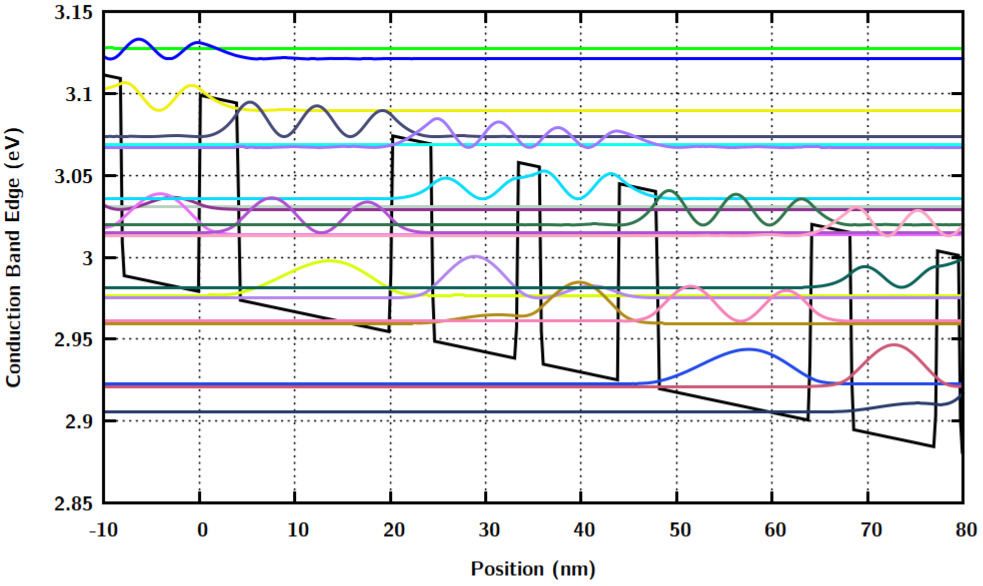


- `ReducedRealSpaceModesOn.dat`
  Same as in `ReducedRealSpaceModes.dat` but the vanishing parts of the wavefunctions are not shown (plot not supported by nextnanomat).
- `H0ReducedRealSpace_nobias.mat`
  Expression of the Hamiltonian in this basis when no external bias voltage is applied.
- `H0ReducedRealSpace_nobias.mat`
  Expression of the Hamiltonian in this basis with an applied external voltage.
- Single-band case: `Wavefunction.dat`
  Envelope function of the wavefunction $\Psi_i(z)$
- Multiband-case: `Wavefunction_ConductionBand.dat`, `Wavefunction_LHBand.dat`, and `Wavefunction_SOBand.dat`
  Different component of the envelope wavefuntions

$$\Psi_i(z) = f^{\text{c}}_i(z)u_{\text{c}}(z) + f^{\text{LH}}_i(z)u_{\text{LH}}(z) + f^{\text{SO}}_i(z)u_{\text{SO}}(z)$$

'Tight-binding' states

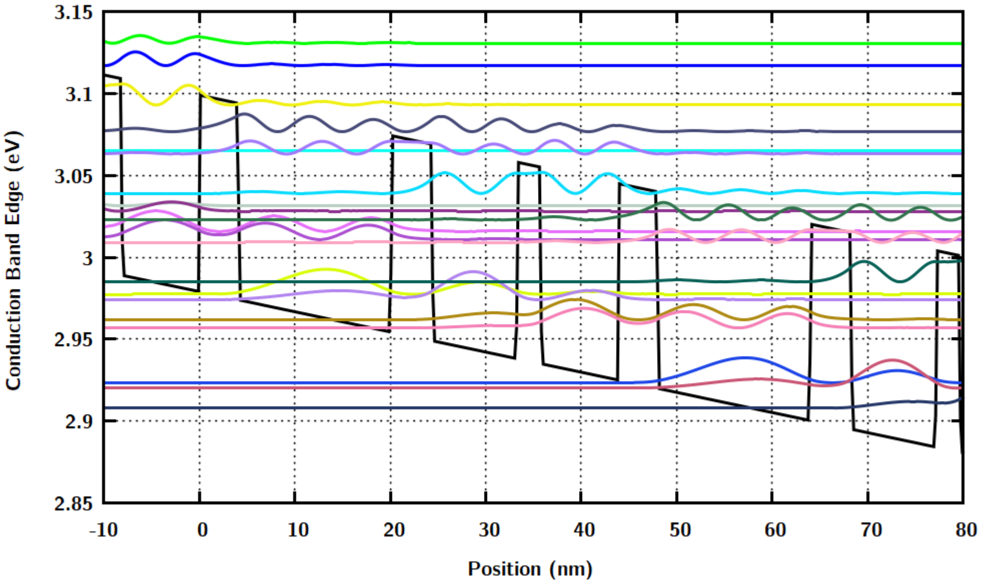
The `Tight-binding\` folder contains data only if one or several `<Analysis_Separator>` are defined in the input file. The tight-binding basis corresponds to piecewise solution of the Schrödinger equation between these separators.



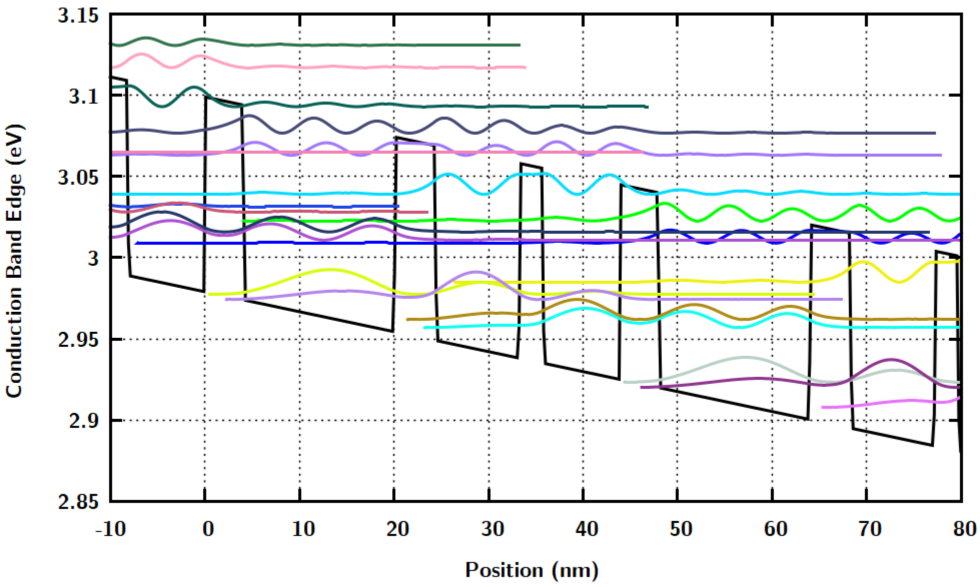
Wannier-Stark states

The Wannier-Stark states correspond to the eigenstates of the Schrödinger equation without accounting for Poisson equation (i.e. electrostatic mean-field).
It contains:

- `Wannier-Stark_States.dat` shows the conduction band edge and the probability densities of the eigenstates of the Schrödinger equation (the Wannier-Stark states).



- `Wannier-Stark_levelsOn.dat`. Same as `Wannier-Stark_States.dat` except that the points with almost zero probability density are omitted.



- `Dipoles.mat` gives the dipole matrix elements (i.e. matrix elements of the position operator)

The expression in the single-band case is: $$ d_{ij} = \int dz f_i(z) ~ z ~ f_j(z) $$ In the multiband case: $$ d_{ij} = \sum_{\mu} \int dz f^{(\mu)}_i(z) ~ z ~ f^{(\mu)}_j(z) $$

- `EffectiveMasses.dat` gives the position and energy-dependent effective mass
- `H0_WannierStark.mat` gives the Hamiltonian in the Wannier-Stark basis.
- `Oscillator_Strength.mat` gives the oscillator strengths.

In-plane discretization

The file `Lateral_spectrum.dat` gives the energy discretization for the states used to describe the 2-Dimensional (2D) motion in the directions (x,y) perpendicular to the heterostructure. The lateral motion is discretized using cylindrical boundary conditions, and the corresponding eigenstates are Bessel funcitons.
x axis: `Lateral state index`
y axis: `order of Bessel (zero index)-1 of Bessel` `Relative Energy (meV)`.

Simulation output for each voltage/temperature step

For each voltage or temperature step, the following files are produced as a result of the NEGF calculation:

- `CarrierDensity.dat`
  Electron density in [cm^{-3}] as a function of position [nm].

- `Conduction_BandEdge.dat`
  Calculated heterostructure conduction band edge profile $E_{\rm c}^\prime$ as a function of position in units of [eV]. It includes the mean field electrostatic potential ϕ [V] as $E_{\rm c}^\prime = E_{\rm c} - e \phi$.

- `Convergence.txt`
  This file contains values for
    - Convergence factor
      convergence factor for the lesser Green's function $\mathbf{G}^<$, which corresponds to the relative variation between the last two consecutive Green's functions. Should be as close as possible to 0.
    - Current convergence factor
      convergence factor for the current density, which corresponds to the relative variation of the last two consecutive current density values. Should be as close as possible to 0.
    - Number of iterations
    - Normalization of lesser Green's function $\mathbf{G}^<$
      Should be as close as possible to 1.
    - Sum normalised spectral function
      Should be as close as possible to 1. If not, it usually means that the energy grid spacing is too large.
- `NO-CONVERGENCE.txt`
  This file is generated instead if the calculation did not converge.

- `CurrentDensity.dat`
  Current density in [A/cm^2] as a function of position [nm].

- `Current-miscellaneous.txt`
  General information on the simulation.
    - Current density in [A/cm^2]
    - Average electron velocity in [nm/ps]
    - Time for one electron to travel through one period in [ps]
    - Electric field in [kV/cm]
    - Doping sheet density per period in [cm^{-2}]
    - 3D doping density averaged over one period in [cm^{-3}]
    - Effective electronic temperature in [Kelvin]. This is only an effective temperature as electrons are not in thermal equilibrium, which is obtained by averaging the kinetic energy for the in-plane motion. This effective temperature is given by the following formula:

$$ T_{\text{eff}} = \sum_{i} ~ p_{i} ~ E_{\parallel}(i) ~ / ~ k_b $$ where p_{i} is the fraction (i.e. population normalized to 1) of occupation in the in-plane state i, $E_{\parallel}(i)$ is the in-plane energy for the in-plane state i, and k_b the Boltzmann constant.

- `Electrostatic-Potential.dat`
  Mean field electrostatic potential ϕ [V] as a function of position. The electrostatic potential ϕ is the solution of the Poisson equation and has been calculated self-consistently.

Output in basis sets (ReducedRealSpace, WannierStark, TightBinding)

3 folders are created to output physical quantities in the 3 different basis sets (`Reduced Real Space`, `Wannier-Stark`, and `Tight-Binding`).

For each basis set, the folder contains:

- the probability density $\vert \Psi_i(z) \vert^2$ for the each state Ψ_i. Each level is shifted accordingly to its energy.

- the wavefunction $\Psi_i(z)$ in the file `Wavefunctions.dat`
- `CarrierDistribution_Energy.dat` shows the energy-resolved populations in each state.
- `DensityMatrix.txt` and `DensityMatrix_elements.txt` display the density matrix in a text file.
- `DensityMatrix_Real.mat` displays the real part of the density matrix. The labeling is made accordingly to the one of the wavefunctions $\Psi_i(z)$, so that the matrix element (i,j) corresponds to the real part of $\langle \Psi_i \vert \rho \vert \Psi_j \rangle$, where ρ is the density matrix. Note that the diagonal element (i,i) is equal to the population of the level Ψ_i.
- `DensityMatrix_Imaginary.mat` displays the imaginary part of the density matrix.
- `Dipoles.mat` gives the dipole matrix elements (see above for definition)
- `EffectiveMasses.dat` gives the position and energy-dependent effective mass
- `Populations.text` indicates the population (i.e. the probability of occupation) in each level Ψ_i (normalized to 1 for one period of the structure).
- `SpectralFunctions.dat` shows the diagonal part of the spectral function, i.e. the energy-resolved density of states (DOS).
- `Subband_KineticEnergy.txt` contains the averaged kinetic energy for each level/subband i. Its calculation is given by:

$$ \langle E_i \rangle = \frac{ \sum_{k} ~ p_{i,k} ~ E_{\parallel}(k)}{\sum_{k} ~ p_{i,k}}, $$ where $E_{\parallel}(k)$ is the in-plane kinetic energy.

- `Subband_Temperature.txt` gives the effective temperature of each level/subband i, according to

$$ T^{\text{eff}}_i = \langle E_i \rangle / ~ k_b $$

2D plots

The folder `2D_plots\` contains 2D color maps as a function of **position [nm]** (horizontal axis) and **energy [eV]** (vertical axis). Note that these 2D plots show 2 QCL periods although only 1 period is simulated.

- `DOS_energy_resolved.vtr` / `*.plt` / `*.fld`
  Energy-resolved local density of states (LDOS) in units of [eV^{-1} nm^{-1}]. The LDOS is related to the spectral function. It shows the available states for the electrons at $k_\parallel = 0$.
- `CarrierDensity_energy_resolved.vtr` / `*.plt` / `*.fld`
  Energy-resolved electron density $n(z,E)$ [cm^{-3} eV^{-1}]. It is related to the lesser Green's function $\mathbf{G}^<$.
- `CurrentDensity_energy_resolved.vtr` / `*.plt` / `*.fld`
  Energy-resolved current density $j(z,E)$ [A cm^{-2} eV^{-1}].

For different extensions of 2D outputs, please also see advanced settings in the input file.

Gain

The folder `Gain\` contains one- and two-dimensional plots of the intensity gain simulated. A negative value of gain corresponds to absorption.

2D color maps show the gain $G(z,E_{\rm ph})$ [cm^{-1} nm^{-1}], where the horizontal axis is **position** z [nm] and the vertical axis is photon energy $E_\rm{ph}$ in units of either **energy** [meV] or **frequency** [THz]. Note that the units of gain in the nextnano.MSB code are [eV^{-1} cm^{-1}]. Also note that these 2D plots show 2 QCL periods although only 1 period is simulated.

- `Energy-Resolved_Gain_Simple-Approximation.fld` / `*.coord` / `*.dat`
- `Gain_vs_Position_and_Energy_SelfConsistent.vtr`
- `Gain_vs_Position_and_Frequency_SelfConsistent.vtr`

1D plots show the gain $G(E_\rm{ph})$ [cm^{-1}] against photon **energy** [meV], **frequency** [THz], and **wavelength** [micron].

- `Gain_Simple-Approximation.dat` Intensity gain obtained without the self-consistent calculation.
- `GainSemiClassical_vs_Energy.dat`
- `GainSemiClassical_vs_Frequency.dat`
- `GainSemiClassical_vs_Wavelength.dat`
- `Gain_SelfConsistent_vs_Energy.dat`
- `Gain_SelfConsistent_vs_Frequency.dat`
- `Gain_SelfConsistent_vs_Wavelength.dat`

Note that the gain output is only done for the voltages specified in the input file.

```
<!-- Calculate gain only between the following values of
     potential drop per period in order to save CPU time -->
     <Vmin unit="mV"> 160 </Vmin>
     <Vmax unit="mV"> 400 </Vmax>
```

Green's functions

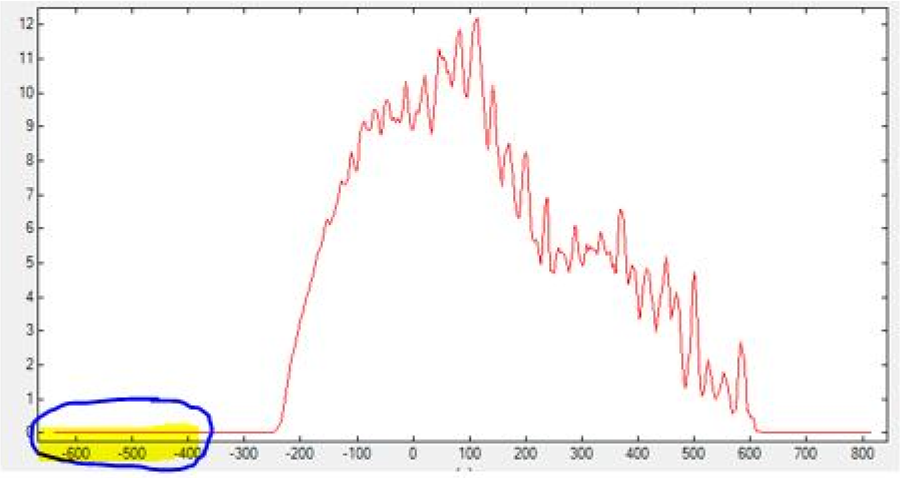
The folder `GreenFunctions/` contains information on the Green's functions.

The **electron density** $n(x,E_x)$ is related to the lesser Green's function $\mathbf{G}^<$ (“G lesser”): $$n(x,E_x) = - \frac{{\rm i}}{2\pi} \mathbf{G}(x,x^\prime=x,E_x)$$

- `GreenLesser_All.dat`
  lesser Green's function $\mathbf{G}^<$
  This file contains the sum over **<u>all</u>** the diagonal (i.e. $x=x^\prime$) lesser Green's functions (sum over one period) as a function of energy E_x.
- `GreenLesser_Z.dat`
  lesser Green's function $\mathbf{G}^<$
  This file contains the lesser Green's function $\mathbf{G}^<$ (i.e. density $n(E)$) for each mode space used in the calculation.

The **local density of states** $\rho(x,E_x)$ is related to the spectral function $\mathbf{A}$: $$\rho(x,E_x) = \frac{1}{2\pi} \mathbf{A}(x,x^\prime=x,E_x)$$ $\mathbf{A}$ is defined as $\mathbf{A} = {\rm i} (\mathbf{G}^{\rm R} - \mathbf{G}^{{\rm R}\dagger}) = - 2 {\rm Im}(\mathbf{G}^{\rm R})$. $\mathbf{G}^{\rm R}$ is the retarded Green's function.

- `GreenSpectral_All.dat`
  This file contains the sum over all the spectral functions (sum over one period) as a function of energy E_x.
  Example: In the figure below, for instance, one can see that <`Emin_shift unit="meV"`> can be increased (by 200 meV) to reduce the calculation time. Essentially, the energy range of the Green's functions is altered by adjusting <`Emin_shift unit=meV`> and <`Emax_shift unit=meV`>.



- `GreenSpectral_Z.dat`
  This file contains the spectral function for each mode space used in the calculation.

Density matrix

The folder `DensityMatrix/` contains the density matrix ρ which is a complex quantity and it is dimensionless. The trace of the density matrix equals 1. In our case, the trace is 1 if we sum over one period. The state labels (state i, period j) are specified in the complex density matrix. $$\rho(i,j) = \rho({\rm state},{\rm period})$$

- `DensityMatrix_complex.mat`
  This file contains the density matrix.
  The x axis contains real and imaginary value.
  The y axis is number of periods.
- `DensityMatrix_RealPart_AbsoluteValue.mat`
  This file contains the absolute value of the real part of the density matrix.
  The x axis contains absolute value of the imaginary part.
  The y axis is number of periods.
- `DensityMatrix_ImaginaryPart_AbsoluteValue.mat`
  This file contains the absolute value of the imaginary part of the density matrix.
  The x axis contains absolute value of the real part.
  The y axis is number of periods.

Output files for voltage sweep

If you sweep voltage, the following files are generated.

- `Energy_WannierStarkStates.dat`
  Energy levels of the Wannier-Stark states (“E_1 = Energy of level 1”, “E_2 = Energy of level 2”,…) as a function of voltage, i.e. potential drop per period in units of [mV].
- `Energy_TightBinding.dat`
  Energy levels of the tight-binding states.
- `Gain_vs_Voltage.dat` and `Gain_vs_EField.dat`
  Intensity gain [cm^{-1}] and the photon energy at maximum gain [meV] (or photon frequency in [THz]) as a function of **voltage** (potential drop per period [mV]) or **electric field** [kV/cm].
- `Current_vs_Voltage.dat` and `Current_vs_EField.dat`
  Current-voltage characteristics, i.e. the current density in units of [A/cm^2] as a function of **voltage** (potential drop per period [mV]) or **electric field** [kV/cm]. The current is the average of the file `Current-Density.dat`.

Combined temperature-voltage sweep

a combined temperature-voltage sweep can be done using the keyword `Temperature-Voltage` in the field <SweepType> of `<SweepParameters>` (see the example of code below). In this case, the simulation can be parallelized. `<Threads>` defines the number of parallel threads. Its optimal value should be the number of CPU cores available (if the available memory is sufficient). Within each parallel temperature sweep, a serial voltage sweep is performed.

```
<SweepParameters>
    <SweepType>Temperature-Voltage</SweepType>
    <MinV> 50</MinV>
    <MaxV> 60</MaxV>
    <DeltaV> 2</DeltaV>

    <MinT> 25</MinT>
    <MaxT> 300</MaxT>
    <DeltaT> 25</DeltaT>

    <Threads>12</Threads> <!-- Parallelization for Temperature-Voltage sweep
-->
</SweepParameters>
```

Note that for such voltage-temperature sweep, `<Maximum_Number_of_Threads>` in `<Simulation_Parameter>` should be set to 1. (A combined parallelization will result in lower performances.)

```
<Simulation_Parameter>
  ...
  <Maximum_Number_of_Threads>1</Maximum_Number_of_Threads>
</Simulation_Parameter>
```

At the end of the simulation, current and gain maps can be displayed. `Gain_map.fld` gives the maximum gain at each (voltage,temperature) point. `Max_Gain_frequency.fld` gives the map of the corresponding photon energy for which the gain is maximum.

Folder view:

Gain map (V,T):

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