Optics: gain/absorption calculation

There are two different kind of gain/absorption calculations which is given by nextnano.NEGF:

- the semiclassical one, which uses the populations and the linewidths calculated from the NEGF steady-state solution to calculate the gain/absorption in a semiclassical way;
- the “self-consistent” one, fully calculated using the NEGF formalism . In this case, linear response theory to an a.c. incoming field is considered, and time-dependent Green's functions are used.

Semiclassical gain/absorption calculation

From the Green's functions calculated in steady-state, the populations are extracted in the Wannier-Stark basis. The linewidths are also calculated in this basis. The semiclassical gain/absorption spectrum is then calculated according to:

$$ g(\hbar \omega) = \sum_{i \neq j} (\rho_j - \rho_i) ~ d_{ij}^2 ~ \frac{\Gamma_{ij}}{(\hbar\omega-E_{ij})^2+\Gamma_{ij}^2/4} \frac{e^2 ~ E_{ij}} {\hbar ~ \epsilon_0 \sqrt{\epsilon_r} ~ c} $$

where

- ρ_i is the electron density in the state i. $\rho_i = p_i ~ n_{3D}$ where p_i is the normalized population in state i and n_{3D} the averaged 3D electron density.
- $E_{ij} = E_j - E_i$ is the transition energy between states i and j
- d_{ij} is the dipole of the transition. $d_{ij} = \int dz ~ \psi_j(z) ~ z ~ \psi_i(z)$.
- Γ_{ij} is the linewidth (full half at half maximum) of the transition calculated from the NEGF steady state
- ϵ_r is the relative permittivity
- ϵ_0 is the vacuum permittivity
- e is the elementary charge.

This semiclassical gain calculation has the following limitations:

- it depends on the choice of the basis (the Wannier-Stark basis is considered, but an other basis could be considered as well). Coherent terms are not considered, only populations.
- the linewidths are extracted at the Wannier-Stark energies, which might not be accurate as in the NEGF formalism they are energy dependent.
- the broadening is assumed to be Lorentzian, whereas in the NEGF treatment no assumption is made (non-Markovian treatment).

For the above reasons, the quantum treatment described below using perturbation theory is much more accurate.

Gain/absorption calculation from NEGF linear response theory

In this case the perturbation due to an a.c. electric field along z is considered. The perturbating

Hamiltonian reads in the Lorenz Gauge: $$ H_{ac} = e ~ z ~ \delta F ~ e^{-i\omega t} $$ where the amplitude δF of the electric field is small and can be considered as a perturbation. The response Green's function $\delta G^<(E,\omega)$ is calculated within linear response theory. As shown by Wacker (Phys. Rev. B 66, 085336 (2002)), the Green's function linear response reads: $$ \delta G^R(E,\omega) = G^R(E+\hbar\omega) (H_{ac}+\delta\Sigma^R(E,\omega))G^R(E) $$

$$ \delta G^<(E,\omega) = G^R(E+\hbar\omega) H_{ac} G^<(E) \\ + G^<(E+\hbar\omega) H_{ac} G^A(E) \\ + G^R(E+\hbar\omega) \delta\Sigma^R(E,\omega) G^<(E) \\ + G^R(E+\hbar\omega) \delta\Sigma^<(E,\omega) G^A(E) \\ + G^<(E+\hbar\omega) \delta\Sigma^A(E,\omega) G^A(E) $$

In the self-consistent gain calculation, the 3 last terms are accounted. Indeed, to account for them, the self-energies $\delta\Sigma (E,\omega)$ need to be calculated from $\delta G^<(E,\omega)$, requiring a self-consistent loop. This self-consistent Gain calculation is activated by the command

```
<Gain>
  <GainMethod>1</GainMethod>
  ...
</Gain>
```

in the input file. On the other hand, in the case of this command option 0 (not recommended in general though much faster), the 3 terms involving self-energies are neglected.

From this Green's function response, the a.c. conductivity is calculated: $$ \sigma(\omega) = \frac{\delta j(\omega)}{\delta F} $$ where the current a.c. response reads $$ \delta j(\omega) = Tr(\delta G^< J) $$

where J is the current operator.

Self-consistent gain at the boundaries

By default the self-consistent gain calculation is not performed at the boundaries between periods. Indeed, while the perturbating term H_{ac} in the Lorenz gauge is in principle not periodic, it is considered as periodic in the default case to speed up the simulation.

Hence, for periodic quantum cascade structures, it should be avoided that the boundary between periods is chosen at a place where an optical transition takes place in the energy range of interest. This can be easily checked in the position-resolved gain.

However, in the case of short period QCLs, this cannot be done. To restore the correct periodic boundary condition for the gain calculation, the following command should be used.

```
  <Gain>
    <GainMethod>1</GainMethod>
    ...
     <Self_consistent_boundary>yes</Self_consistent_boundary>
  </Gain>
```

Permittivity and gain/absorption

The bulk relative permittivity, or dielectric constant, is assumed to be given by the Lyddane–Sachs–Teller relation:

$$ \epsilon^{\text{bulk}}_{\text{r}}(\omega) = \epsilon_{\infty} + (\epsilon_{\infty}-\epsilon_{\text{static}}) \frac{\omega_{\text{TO}}}{\omega^2-\omega^2_{\text{TO}}}$$

In the self-consistent gain calculation, the quantity which is actually calculated is the a.c. conductivity $\sigma(\omega)$.

The complex relative permittivity which is output is then:

$$ \epsilon_{\text{r}}(\omega) = \epsilon^{\text{bulk}}_{\text{r}}(\omega) - i \frac{\sigma(\omega)}{\omega \epsilon_0} $$

Finally the gain reads

$$ g(\omega) = -\frac{\text{Re}(\sigma(\omega))}{\epsilon_{\text{r}}(\omega)} $$