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 E 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 $$ \delta j(\omega) = Tr(G^< J) $$

where J is the current operator.

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

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

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