

Optics: gain/absorption calculation

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

- the semiclassical one 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:

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

where

- ρ_i is the electron density in the state i . $\rho_i = p_i \sim n_{3D}$ 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. $d_{ij} = \int dz \sim \psi_j(z) \sim z \sim \psi_i(z)$.
- 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 linear response theory

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

Hamiltonian reads in the Lorenz Gauge: $H_{ac} = e \cdot z \cdot \delta F \sim e^{-i\omega t}$ 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), 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 $\delta j(\omega) = \text{Tr}(G^< J)$

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](#):

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

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:

$$\epsilon_r(\omega) = \epsilon^{\text{bulk}}_r(\omega) - i \frac{\sigma(\omega)}{\omega \epsilon_0}$$

Finally the gain reads

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

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