Self-Consistent Theory of the Gain Linewidth for Quantum-Cascade Lasers

F. Banit, S.-C. Lee, and A. Knorr
Institut für Theoretische Physik, Technische Universität Berlin, D-10623 Berlin, Germany

A. Wacker
Fysiska Institutionen, Lunds Universitet, Box 118, 22100 Lund, Sweden

The linewidth in intersubband transitions can be significantly reduced below the sum of the lifetime broadening for the involved states, if the scattering environment is similar for both states. This is studied within a nonequilibrium Green function approach here. We find that the effect is of particular relevance for a recent, relatively low doped, THz quantum-cascade laser.

Material gain engineering in semiconductor quantum wells is a major topic in the physics of semiconductor laser emission [1]. In particular, the position of the peak gain and the linewidth of the active medium are of importance for applications in telecommunication or short pulse generation. Whereas the gain properties of semiconductor interband quantum well lasers are well understood [2], intersubband emitters, such as quantum-cascade lasers (QCLs) [3], are still a subject of intensive research. Major differences of QCLs in comparison to interband lasers result from the similar in-plane band curvature for the electronic transitions and the low energy collective excitations involved in the photon emission. Besides model calculations [1,4] for a standard QCL design [5], a detailed many-particle study of the gain linewidth of intersubband lasers for the broad variety of QCL structures available [4,6,7,8] is still missing. The purpose of this Letter is to evaluate a self-consistent theory for the influence of the electronic scattering mechanism on the gain linewidth of QCLs and to clarify its impact on the description of QCL structures ranging from the infrared to THz-regime.

For interband lasers the many-particle interactions are well described on the level of the second order Born approximation [2]. Due to the expansion of the scattering matrix in wavenumber space, the linewidth of the transitions is determined by diagonal (proportional to the inverse lifetime) and non-diagonal dephasing mechanisms [10,11]. The consistent description of the detailed interplay of diagonal and non-diagonal scattering mechanisms [2] results in a proper prediction of the gain shape. In particular spurious absorptions below the band gap could be eliminated from the theory [12]. Our aim is to evaluate similar information for the gain in the intersubband gain of QCL structures. So far, only simple two band intersubband emitters [13,14] have been investigated on this self-consistent level.

Here, we bridge the gap to real QCL devices, and explore the influence of a self-consistent description of the electron-phonon and electron-impurity scattering on the gain linewidth. Although excluded in the present study, electron-electron scattering can be treated on the same footing [14]. Our results are illustrated for two different samples: (A) the terahertz QCL reported in Ref. [2], (B) a midinfrared QCL reported in Ref. [6]. We demonstrate, that the different behavior can be understood by the impact of non-diagonal dephasing on the linewidth. Finally, we give general conditions, when non-diagonal dephasing is important and thus a full quantum theory of the gain is indispensable.

First, we evaluate the nonequilibrium electron occupations with nonequilibrium Green functions [15] using nominal sample parameters. Here, however, we extend the model in two ways: (i) Scattering at ionized impurities is treated microscopically using Debye screening by a fictitious homogeneous 3D electron gas matching the average doping density. (ii) We include the non-diagonal elements in the self-energies, so that Eqs. (6-8) of Ref. 4 take the form:

\[ \Sigma_{\alpha_1\alpha_2}^{\text{re,imp}}(\mathbf{k}, E) = \sum_{\beta_1, \beta_2, \mathbf{k}'} \langle v_{\alpha_1 \beta_1}^{\text{imp}}(\mathbf{k} - \mathbf{k}') | v_{\beta_2 \alpha_2}^{\text{imp}}(\mathbf{k'} - \mathbf{k}) \rangle G^{\text{re}}_{\beta_1 \beta_2}(\mathbf{k}', E), \]

and similarly for the electron-phonon scattering processes (\(A\) denotes the normalization area and \(m_e\) is the effective mass). The values of \(\gamma_{\alpha_1 \alpha_2 \beta_1 \beta_2}\) are taken for a typical fixed momenta \(|\mathbf{k}|, |\mathbf{k}'|\), while the integration over \(\mathbf{l}(\mathbf{k}, \mathbf{k}')\) is performed. The current voltage characteristic is evaluated along the lines of Ref. 2 and is shown in the inset of Fig. 1 for the THz-QCL A [16]. It agrees excellently with the data presented in Fig. 2 of Ref. 2.

Next, we evaluate the gain according to Ref. 17. The material gain coefficient \(g(\Omega)\) reads as a function of the frequency \(\Omega\) [2]:

\[ g(\Omega) = -\Re \left\{ \frac{\delta J}{\delta F(\Omega)e^{\epsilon_\tau\Omega}} \right\}, \]

where \(\epsilon_\tau = 13\) is the dielectric constant. The change in the current density \(\delta J\) for a perturbative electric field \(\delta F(t) = \delta F(\Omega)e^{-\epsilon_\tau\Omega}e^{i\Omega t}\) is given by [17]:

\[ \delta J = \frac{e}{\hbar} \int \frac{dE}{2\pi A} \sum_{\mathbf{k}} \sum_{i,j} z_{ji}(E_j - E_i) \delta G_{ij}^{<}(\mathbf{k}, E) \]

*Electronic address: Andreas.Wacker@fysik.lu.se*
functions approach (4). For this purpose we assume that the Green mechanisms which cause the failure of the simple approach do not correctly describe the gain spectrum for all QCLs. This shows that the simple (Lifetime) approach does exhibit a far too large width of the gain peak for sample A. This justifies Eq. (4) by inserting into Eqs. (2,3). Thus the simple approach can be related to the neglect of non-diagonal dephasing, see also [14, 15]. Impurity scattering contributes with approximately $\gamma_{i j i}^{\text{imp}}$ to the full broadening $\Gamma_i$ of the states $i$. Therefore it is crucial to compare $\gamma_{i j i}^{\text{imp}}$ with $\gamma_{i i i}^{\text{imp}}$ and

$$
\delta G_{i j}^{<}(E) \approx \delta G_{i j}^{<0}(E, k) + \tilde{G}_{i}^{\text{adv}}(k, E + h\Omega)\delta_{G_{i j}}^{<}(k, E) \tilde{G}_{j}^{\text{adv}}(k, E) \quad (7)
$$

which justifies Eq. (4) by inserting into Eqs. (2,3). Thus the simple approach does not correctly describe the gain spectrum for all QCLs.

For $i \neq j$, the dominant contribution $2\pi$ to $\delta\Sigma_{i j}^{<, \text{imp}}$ takes the form

$$
\delta \Sigma_{i j}^{<, \text{imp}}(E) = \frac{i\gamma_{i j i}^{\text{imp}}}{\pi} 2\pi \int_{0}^{\infty} dE_{k} \delta G_{i j}^{<}(k', E), \quad (10)
$$

which gives the non-diagonal dephasing as a $k'$ integral similar to density matrix theory. We immediately see, that the width of the gain peak is reduced. This relates to the line narrowing due to non-diagonal elements in the self-energies (or non-diagonal dephasing, see also [14, 15]). Impurity scattering contributes with approximately $\gamma_{i i i}^{\text{imp}}$ to the full broadening $\Gamma_i$ of the states $i$. Therefore it is crucial to compare $\gamma_{i i i}^{\text{imp}}$ with $\gamma_{i i i}^{\text{imp}}$ and

$$
\delta G_{i j}^{<}(E) \approx 2\pi i \frac{-e\delta F(\Omega) z_{i j} [f_{j}(E) - f_{i}(E)]}{E_{j} + h\Omega - E_{i} + i \left(\Gamma_{i} + \Gamma_{j} - 2\gamma_{i i i}^{\text{imp}}\right)/2}, \quad (11)
$$

where the states $\Psi_{i}(z)$ are the eigenstates of the heterostructure potential including the self-consistent Hartree field, $z_{i j}$ is the dipole matrix element, and $d$ is the period of the structure. The field-induced changes $\delta G_{i j}^{<}$ of the Green functions are evaluated self-consistently including the non-diagonal elements of the self-energies in the $\delta \Sigma$ terms (full theory). The results are given in Figs. 1-2 (crosses) for the two samples considered here. For comparison, we have evaluated the gain by the simple approach (using lifetime broadening):

$$
g_{\text{simple}}(\Omega) = \sum_{i,j} \frac{e^2|z_{i j}|^2(E_{i} - E_{j})(n_{i} - n_{j})}{2\hbar c \epsilon_{i} \epsilon_{j}} \frac{\Gamma_{i} + \Gamma_{j}}{(E_{i} - E_{j} - h\Omega)^2 + (\Gamma_{i} + \Gamma_{j})^2/4} \quad (4)
$$

Here, we evaluate the level energies $E_{i}$ and their respective widths $\Gamma_{i}$ (FWHM) from the spectral functions $-2\Im\{G_{i i}^{<}(k = 0, E)\}$ and the densities are given by $n_{i} = \sum_{k} \int d E \delta(G_{i i}^{<}(k, E))/|\pi A|$. Eq. (4) can be derived restricting to diagonal dephasing, see, e.g., Ref. [16], where effects due to different effective masses were studied, which are neglected here. It has also been used in Ref. [4] except for the replacement $E_{i} - E_{j} = h\Omega$ in the first line and the neglect of counter-rotating terms with $E_{i} < E_{j}$. Figs. 1-2 show, that the simple approach is in good agreement with the full theory for sample B, but exhibits a far too large width of the gain peak for sample A. This shows that the simple (Lifetime) approach does not correctly describe the gain spectrum for all QCLs.

In the following we want to shed light into the physical mechanisms which cause the failure of the simple approach. For this purpose we assume that the Green functions $\tilde{G}_{i j}$ of the stationary state are diagonal in our basis of eigenstates and given by their generic forms

\[
\tilde{G}_{i j}^{\text{ret/adv}}(k, E) = \frac{1}{E - E_{i} - E_{k} \pm i\Gamma_{i}/2} \quad (5)
\]

\[
\tilde{G}_{i}^{<}(k, E) = i f_{i}(E) \frac{\Gamma_{i}}{(E - E_{i} - E_{k})^2 + \Gamma_{i}^2/4} \quad (6)
\]

Figure 1: Calculated gain at an operating bias of 11.5 V for sample A (Ref. [6]). The inset shows the current-voltage characteristic where the bias equals 177 times the bias drop per period $Fd$ and the current is evaluated for an area of 54000 $\mu$m$^2$.

Figure 2: Calculated gain for sample B (Ref. [6]).
main levels.

Figure 3: Band diagrams for samples A and B together with the dominating 4-5 transition (see Fig. 3) for sample A.

...ing in a narrowing of the gain feature. Indeed we find for the transitions are less affected by the scattering, resulting in the strong narrowing in the gain visible in Fig. 1. In contrast the main gain peak at $eF_d = 260 \text{meV}$ in sample B can be attributed to the 7-8 transition with $\gamma_7^{\text{imp}} = 2 \text{meV}$, $\gamma_8^{\text{imp}} = 2.7 \text{meV}$, and $\gamma_{5555}^{\text{imp}} = 2.2 \text{meV}$. This means both scattering environments are highly correlated, resulting in the strong narrowing in the gain feature. Indeed we find for the dominating 4-5 transition (see Fig. 3) for sample A $\gamma_{4545}^{\text{imp}} = 2.2 \text{meV}$, $\gamma_{4444}^{\text{imp}} = 2.7 \text{meV}$, and $\gamma_{5555}^{\text{imp}} = 2.2 \text{meV}$. This means both scattering environments are highly correlated, resulting in the strong narrowing in the gain visible in Fig. 3. In contrast the main gain peak at $eF_d = 65 \text{meV}$ in sample B. Thus the scattering potential is much more local for sample B causing significant differences in the scattering environment for both levels. This effect is strengthened by the fact that interface roughness (with $\delta$-function potentials) is also of relevance for sample B.

Note that the analytical motivation given above reproduces the right trend, but cannot be used for quantitative analysis because: (i) Phonon scattering shows also some line narrowing due to correlations in the potentials, which is contained in the full theory. (ii) The influence of $\delta \Sigma_{ij}^{\text{ret/adv}}(E)$ has been neglected. (iii) Significant non-diagonal elements in $G_{ij}(E)$ are present even in the basis of energy eigenstates.

In conclusion we have shown that the simple approach for QCL gain is not reliable if the states involved in the lasing transition are exposed to the same scattering environment. Non-diagonal dephasing then becomes important and narrows the linewidth below the sum of the individual widths of the levels (lifetime broadening). This requires a full quantum kinetic description of the gain in QCLs.

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