Density matrix description of transport and gain in quantum cascade lasers in a magnetic field

Ivana Savić*, Nenad Vukmirović*, Zoran Ikonić*, Dragan Indjin* , Robert W. Kelsall*, Paul Harrison*, and Vitomir Milanović†

* School of Electronic and Electrical Engineering, University of Leeds, Leeds LS2 9JT, United Kingdom

†Faculty of Electrical Engineering, University of Belgrade, 11120 Belgrade, Serbia

Email: I.Savic@leeds.ac.uk

***Abstract*—A density matrix theory of electron transport and optical gain in quantum cascade lasers in an external magnetic field is formulated. Starting from a general quantum kinetic treatment, we describe the intra- and inter-period electron dynamics at the non-Markovian, Markovian and Boltzmann approximation levels. Interactions of electrons with longitudinal optical phonons and classical light fields are included in the present description. The non-Markovian calculation for a prototype structure reveals a significantly different gain spectra in terms of linewidth and additional polaronic features in comparison to the Markovian and Boltzmann ones. Despite strongly controversial interpretations of the origin of the transport processes in the non-Markovian or Markovian and the Boltzmann approaches, they yield comparable values of the current densities.**

I. Introduction

Experimental interest in the quantum cascade laser (QCL) performance in a magnetic field has stimulated theoretical efforts to describe the influence of a magnetic field on the physical processes involved. The majority of theoretical studies have been focused on the modeling of various scattering rates (electron-phonon, electron-electron, interface roughness) between the Landau levels (LLs) stemming from the upper and lower laser levels [1], [2], [3]. Also, a semiclassical model of the electron transport in a magnetic field based on the Boltzmann equation has been proposed [4]. Currently, no experimental or theoretical data on coherent phenomena in QCLs in a magnetic field are available. Since the energy spectra in such structures is discrete, it is reasonable to expect that coherent effects are more significant than for QCLs without magnetic field. The aim of this work is to present a quantum-mechanical theory of transport and gain properties of QCLs in an external magnetic field, which takes into account both phase coherence and incoherent scattering processes. A comprehensive analysis is performed for an example GaAs/$Al_{0.3}Ga_{0.7}As$ QCL and nonequilibrium steady state results obtained from quantum kinetic, Markovian and Boltzmann approaches are compared.

II. Theoretical Considerations

We derived quantum kinetics equations for QC structures in a magnetic field, based on the density matrix formalism [5], which include interaction of electrons with longitudinal optical (LO) phonons and optical field [6]. The quantum-kinetic dynamics is essentially non-Markovian, since the time evolution of the density matrix elements depends on their values at earlier times i.e. on the memory of the system. Furthermore, we obtained the corresponding equations in the Markovian approximation, from which the semiclassical Boltzmann transport equations can be recovered. The periodicity of the QCL structure was accounted for. The current density in the non-Markovian and Markovian treatment may be estimated from the expectation value of the carrier drift velocity [7]. The gain spectra may be estimated from the linear response of nonequilibrium stationary populations and polarizations to a small optical perturbation [8].

III. Numerical results and discussion

As a prototypical system, we consider a QCL design which comprises a three-level scheme, and employs LO-phonon depopulation of the lower laser level to the ground state. No injector region is present and efficient injection into the upper laser level is enabled by its alignment with the ground level of the preceding period. The QCL period consists of two QWs (see Fig. 1), one of which confines the ground and lower laser levels, whose energy difference is set to be approximately one LO phonon energy (36.9 meV). The upper laser level is localized in the other well. The transition energy between the upper and lower laser levels is 15.2 meV, and the energy difference between the ground state and the upper laser level of the following period is 2.6 meV.

For discrete energy spectra in QCLs in a magnetic field, broadening of LLs needs to be taken into account. Its self-consistent calculation in the non-Markovian approach for complex structures like QCLs would result in a computationally inaccessible task. Therefore, we have to resort to a phenomenological description of broadening in all three approaches used. In the non-Markovian treatment, a damping parameter $\hbar\gamma_{ph}$ describing collisional broadening appears, while in the Markovian and Boltzmann description, a Lorentzian with the full width at half maximum (FWHM) γ is accounted for. In order to give a fair comparison between the different models presented here, we restrict our further analysis to a choice of the pairs of phenomenological parameters for which the populations are almost identical ($\gamma = 2$ meV and $\hbar\gamma_{ph} = 1$ meV; $\gamma = 4$ meV and $\hbar\gamma_{ph} = 2$ meV), and then we compare the results for other physical quantities.

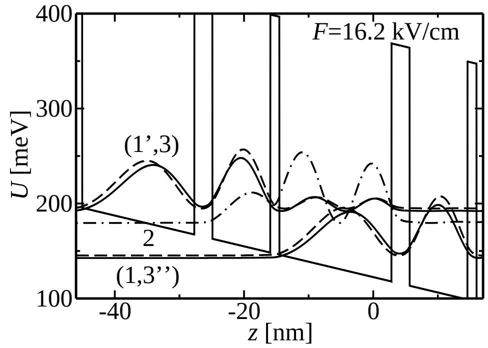

Fig. 1. A schematic diagram of the conduction band profile, size-quantized energy levels from which Landau levels originate and squared wave functions for one full period and parts of adjacent periods of the GaAs/AlGaAs QCL for zero magnetic field and an electric field of 16.2 kV/cm. States 1 and $1'$ (solid line), 2 (dash-dotted line), 3 and $3''$ (dashed line) denote the ground, lower laser and upper laser levels, respectively. State $1'$ belongs to the preceding period, while state $3''$ belongs to the following period.

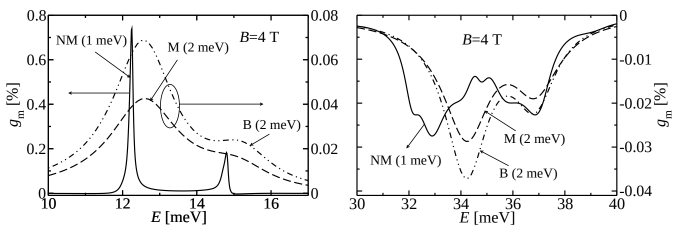

Fig. 2. Optical gain vs energy for a magnetic field of 4 T. Solid, dashed and dash-double dotted lines represent non-Markovian (NM) ($\hbar\gamma_{ph} = 1$ meV), Markovian (M) ($\gamma = 2$ meV) and Boltzmann (B) ($\gamma = 2$ meV) results, respectively. Left: The energy range is in the vicinity of the optical transition energies. Right: The energy range is in the vicinity of one longitudinal optical phonon energy.

The gain spectra for a magnetic field of 4 T in the energy range close to the optical transition energies and one LO phonon energy, are shown in Fig. 2. The gain was calculated for the non-Markovian ($\hbar\gamma_{ph} = 1$ meV), Markovian and Boltzmann ($\gamma = 2$ meV) dynamics. The modal gain obtained from the Boltzmann theory, has identical major features as the one predicted from the Markovian approach, for the same value of FWHM. Disregarding nondiagonal scattering and dephasing processes in the Boltzmann model, which affect the gain linewidth, results only in a quantitative modification of the Markovian prediction. In the case of the non-Markovian dynamics, the gain linewidth is significantly decreased for optical transition energies in comparison to the corresponding Markovian and Boltzmann estimates (≈ 10 times). This result might seem somewhat unexpected because scattering and dephasing are increased compared to the Markovian treatment by including the memory of the interaction process. However, it is due to the fact that in the non-Markovian approach, the broadening caused by the scattering terms is energy dependent.

In the Markovian limit, energy renormalizations, describing

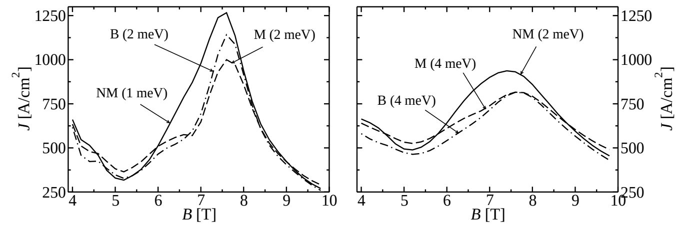

Fig. 3. Left: Current density vs magnetic field dependence. Left: Solid, dashed and dash-dotted lines represent non-Markovian (NM) ($\hbar\gamma_{ph} = 1$ meV), Markovian (M) ($\gamma = 2$ meV) and Boltzmann (B) ($\gamma = 2$ meV) results, respectively. Right: Solid, dashed and dash-dotted lines represent non-Markovian ($\hbar\gamma_{ph} = 2$ meV), Markovian ($\gamma = 4$ meV) and Boltzmann ($\gamma = 4$ meV) results, respectively.

the polaron corrections to the band structure, are ignored. However, the polaron shift is always included in the quantum-kinetic treatment. It is more prominent for the energy transitions close to one LO phonon energy (~ 1 meV), but it is also present for the optical transition energies (~ 0.4 meV).

The current densities as functions of magnetic field, calculated using the non-Markovian ($\hbar\gamma_{ph} = 1$ meV and $\hbar\gamma_{ph} = 2$ meV), Markovian and Boltzmann description ($\gamma = 2$ meV and $\gamma = 4$ meV), are shown in Fig. 3. In the Markovian and non-Markovian approach, diagonal density matrix elements do not contribute to the total current [7], [9]. Therefore, the electron transport is entirely due to nondiagonal density matrix contributions i.e. scattering induced phase coherences between the laser states. This quantum-mechanical picture of completely coherent current is in a stark contrast with the semiclassical picture of transport through scattering transitions. However, both descriptions give similar results, see Fig. 3. Here, the nondiagonal density matrix element are considerably smaller in comparison to the diagonal ones, which results in comparable values of the current density [9].

REFERENCES

[1] C. Becker, A. Vasanelli, C. Sirtori, and G. Bastard, Phys. Rev. B **69**, 115328 (2004).

[2] K. Kempa, Y. Zhou, J. R. Engelbrecht, P. Bakshi, H. I. Ha, J. Moser, M. J. Naughton, J. Ulrich, G. Strasser, E. Gornik, and K. Unterrainer, Phys. Rev. Lett. **88**, 226803 (2002).

[3] A. Leuliet, A. Vasanelli, A. Wade, G. Fedorov, D. Smirnov, G. Bastard, and C. Sirtori, Phys. Rev. B **73**, 085311 (2006).

[4] I. Savić, Z. Ikonić, V. Milanović, N. Vukmirović ,V. D. Jovanović, D. Indjin, and P. Harrison, Phys. Rev. B **73**, 075321 (2006).

[5] T. Kuhn, and F. Rossi, Rev. Mod. Phys. **74**, 895 (2002).

[6] I. Savić, N. Vukmirović, Z. Ikonić, D. Indjin, R. W. Kelsall, P. Harrison, and V. Milanović, cond-mat/0702508, to be submitted to Phys. Rev. B.

[7] R. C. Iotti, E. Ciancio, and F. Rossi, Phys. Rev. B **72**, 125347 (2005).

[8] S. C. Lee, and A. Wacker, Phys. Rev. B **66**, 245314 (2002).

[9] S. C. Lee, F. Banit, M. Woerner, and A. Wacker, Phys. Rev. B **73**, 245320 (2006).