Modelling of quantum well semiconductor lasers based on Green's functions

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Abstract

We formulated a Wigner function-based model for quantum well (QW) lasers. This model has benefits over other models as it is less phenomenological and can be generalized easily to incorporate additional effects. We start with standard non-equilibrium Green's functions and apply the Wigner transformations as well as some key techniques to get a complete system of equations. We include bias potential and electromagnetic interactions. We will also discuss some of the possible generalizations.

Keywords: Quantum well semiconductor lasers; Wigner functions; Quantum Boltzmann equation

1. Introduction

A challenge in modelling quantum well (QW) lasers is to find a model that is computationally practical but can still model complicated interactions. Without such a model, predictions and design of novel devices, especially those that rely heavily on quantum mechanical effects, are limited. In this paper, we present a model based on Wigner functions and the quantum Boltzmann equation (QBE).

There are two methods that we can use to arrive at the QBEs, depending on the nature of interactions under study and the detail desired. These are represented schematically in Fig. 1. For more complicated interactions such as general phonon and Coulombic scattering, it is most convenient to start with non-equilibrium Green's functions (starting point 1 in Fig. 1) and evolution described by Dyson's equations to arrive at stage *a* of Fig. 1. We then apply a Markovian approximation, the Kadanoff–Baym ansatz and the Wigner–Weyl transformation to arrive at the Wigner function formulation and the QBEs (stage *c* of Fig. 1). If the interactions are classical or of Boltzmann form, then we can describe the system with density matrix theory and the quantum Louiville equation (stage *b* of Fig. 1) by using Heisenberg's equation of motion. A Wigner–Weyl transformation is then applied to arrive at the Wigner functions and QBE. If we wished, we could go from stage *a* to stage *b* and then stage *c*, but it is more convenient to skip this intermediate step as far as the Green's functions are concerned. Finally, we perform various simplifying approximations to arrive at the final form of the QBE's to be solved (stage *d* of Fig. 1).

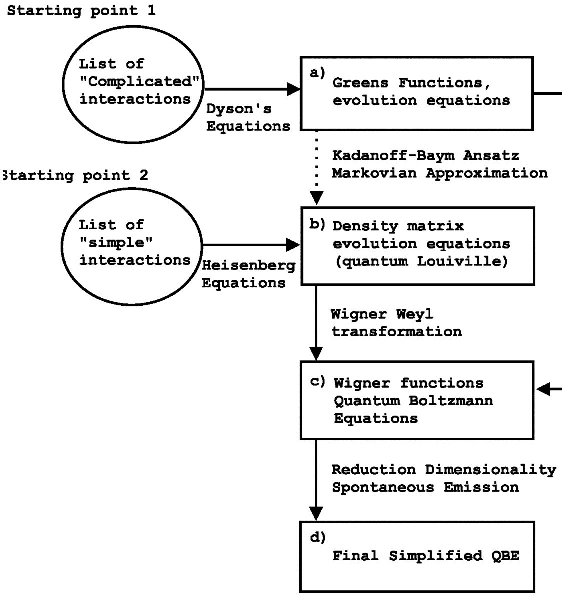

Fig. 1. Schematic relation between methods used in this paper.

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In the Green's function form, interactions are incorporated rigorously through the self-energies. In this paper, we discuss the applied bias potential and classical electromagnetic interactions. Phonon and Coulombic interactions can be incorporated but will be represented here only as a general scattering term and will be written as a Boltzmann term in the final set of equations for simplicity (therefore, in this work we could begin at starting point 2 instead of 1, but we choose the latter for demonstration purposes).

In relation to other work, the final QBEs are based on Wigner models for describing the electron and hole distributions in resonant tunnelling diodes [1] and QWs [2]. We extend that approach to the laser by incorporating the off-diagonal elements that will be coupled (to first order) via the electromagnetic interactions. The electric field will be related to the off-diagonal elements of the QBE, which essentially are the polarization functions.

2. Brief description of Green's functions-based model

Our approach is based on the standard non-equilibrium single-particle Green's functions: the advanced G^a, retarded G^r, time-ordered G^t, anti-time-ordered $G^{\bar{t}}$ and $G^<$, $G^>$. These have standard definitions and we write them in Craig's matrix form ($\tilde{G}$) [3,4]. Expanding into a Bloch function basis, we can write the Green's functions as

$$\tilde{G}(x_1,x_2) = \sum_{i,j} u_i(\mathbf{r}_1)\, u_j^*(\mathbf{r}_2)\tilde{G}_{i,j}(x_1,x_2) \tag{1}$$

where $x = (\mathbf{r}, t)$ and u_i $(\mathbf{r})$ are functions for each band periodic in the unit cell. The evolution of the Green's functions is governed by Dyson's equations [4] and can be shown to be

$$\left[i\hbar\left(\frac{\partial}{\partial t_1}+\frac{\partial}{\partial t_2}\right) - (H_{io}(\mathbf{r}_1) - H_{jo}(\mathbf{r}_2))\right]\tilde{G}_{i,j}(x_1,x_2) = \hbar\int dx_3 \sum_{j'} \begin{bmatrix} \tilde{\sum}_{i,j'}(x_1,x_3)\tilde{G}_{j',j}(x_3,x_2) \\ -\tilde{G}_{i,j'}(x_1,x_3)\tilde{\sum}_{j',j}(x_3,x_2) \end{bmatrix} \tag{2}$$

The self-energies $\tilde{\Sigma}$ are defined in a similar fashion to the Green's functions. $H_{io}(\mathbf{r})$ is the unperturbed Hamiltonian $-\frac{\hbar^2}{2m_i^*}\nabla_r^2 + V_i(r)$, while m_i^* and $V_i(\mathbf{r})$ are the effective mass and heterostructure potential of this band.

The self-energies considered explicitly here are the slowly varying applied bias V^{app} and classical electromagnetic field **E**. The self-energy for a classical interaction has a standard form [3,4].

Next, we transform from the Green's functions and Eq. (2) to the Wigner functions and the QBE (stages *a–c* in Fig. 1). We perform the following transformations:

1. Change to the centre-of-mass variables and perform the Wigner–Weyl transformation [1].
2. Perform the generalized Kadanoff–Baym ansatz [5].
3. Apply the Markovian approximation, which in this format is an integration over the variable ω. Additionally, we have used the rotating wave approximation and a two-band model (*c*, conduction; *v*, valence). The electric field is separated into slow and fast (at optical frequency Ω_{op}) varying components and we use a rotating wave approximation and Boltzmann scattering.

For a self-consistent formulation, we have to find expressions for the electric fields. The relations between macroscopic polarization and the off-diagonal Wigner functions are known [6].

The electric field is related to the macroscopic polarization by Maxwell's equations. Therefore, after some manipulations, we can write the electric field in terms of the off-diagonal Wigner functions.

Finally, because we started with a classical interaction approximation to the electric field, we need to add in spontaneous emission by hand in order to start the lasing process. We use a quantum Langevin approximation [7] in which we add a random Langevin force to the QBE of the off-diagonal Wigner function to model the spontaneous emission.

Additionally, in order to speed up the calculations, we perform a number of simplifying approximations:
1. Transform to electron-hole representation.
2. Integrate over space directions.
3. Integrate over momentum directions.
4. Use an off-diagonal correlation function.

After these mathematical manipulations, we arrive at our equations in the final form.

3. Results and discussion

We applied the present formalism with a relaxation time approximation for a structure consisting of five layers, two barrier layers of length 15 nm and $In_{0.72}Ga_{0.28}As_{0.61}P_{0.39}$ composition and a 7-nm well with composition $In_{0.53}Ga_{0.47}$ As. The outer cladding and substrate were taken to be 20-μm InP layers. Our results for this structure at steady state are presented in Figs 2–4. In Fig. 2, we show the heterostructure plus applied bias and electrostatic effects for three applied biases. Figs 2 and 3 show the electron and hole concentrations in the structure for two different applied biases with and without electromagnetic interactions included. From Figs 3 and 4, we see that the electromagnetic interaction reduces carrier densities within the well region. The density reduction is a result of recombination of the electrons and holes to produce laser light output.

The model presented lays the foundation for later

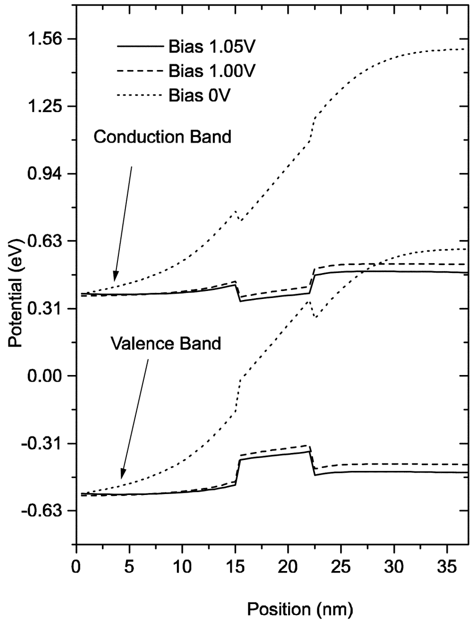

Fig. 2. The total potential experienced by the carriers for different applied biases.

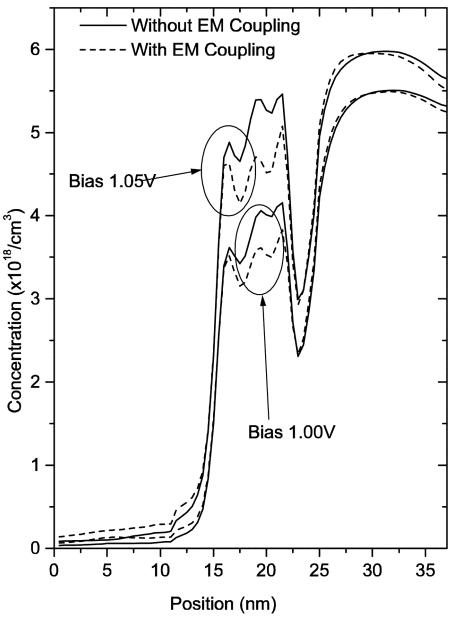

Fig. 4. The hole concentration for two biases with and without electromagnetic interactions.

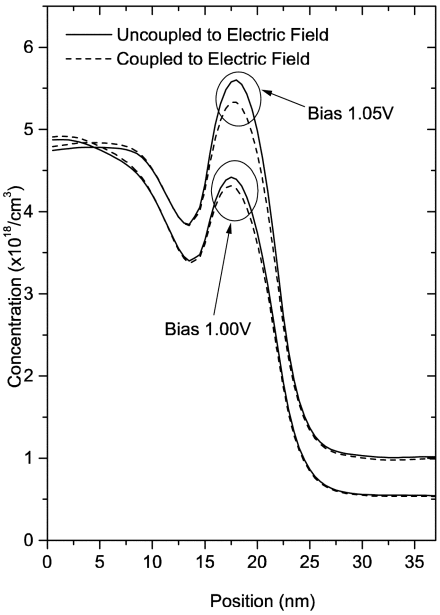

Fig. 3. The electron concentration for two biases with and without electromagnetic interactions.

work analysing QW lasers in detail. It will be useful in modelling novel devices such as the tunnelling injection laser [8,9], in which the carrier injection is hypothesized to occur via phonon-assisted tunnelling. Further in the future, it will be useful to incorporate more detailed bandstructures by adding in more self-energy terms to describe the interband spin-orbit coupling.

We have formulated a Wigner function model for the QW laser. We approximated scattering processes in the Boltzmann form. However, this formulation is ideally suited for incorporating of explicit phonon and Coulombic interactions, which we intend to incorporate in the future to investigate devices such as the tunnelling injection laser. We have used a two-band model above, but this can be generalized to multiple and non-parabolic bands [5], which is more computer-intensive. More details can be found in Wartak and Weetman [10].

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