Transport Simulations for Quantum Well Heterostructures and Lasers

Matt Grupen and Karl Hess

Beckman Institute for Advanced Science and Technology,
University of Illinois,
Urbana, IL 61801

Abstract
A review of the simulation of electronic transport at and over quantum well heterostructures is given. A large number of experimental results relating to thermionic emission, phonon-bottlenecks, electron-electron interaction, tunneling, as well as spontaneous and stimulated emission will be reviewed in the presentation, while this short note will concentrate on effects pertinent to quantum well lasers.

I. Introduction

Transport over a quantum well and recombination of electrons (holes) in the well form, in principle, a formidable problem. Obviously the transport in the immediate vicinity of the well can only be treated by quantum methods, while in the remainder of the structure (laser) the transport is well described in a semiclassical way using drift-diffusion theory and extended versions of it.[1, 2] To bring classical and quantum transport regions together requires sophisticated theories such as the Bardeen Transfer Hamiltonian approach[3] or the Landauer-Büttiker theory[4, 5] extended to include inelastic processes. Under ordinary circumstances a rate equation approach and rates such as those used by Brum and Bastard[6] may be sufficient. However, subtleties with the Pauli Priciple and the ranges and normalizations of classical and quantum regions present problems.[7]

In the presentation related to this paper, a number of cases of generation-recombination and transport near quantum wells is going to be discussed. In this paper, however, we discuss only a few facts relevant to the development of complete tools for semiconductor laser simulation. It is in the modulation response of lasers that the subtleties of quantum well transport most obviously manifest themselves. The model we propose is not to be viewed as a final version but as a starting point for a complete numerical approach.

II. The Multiscale Problem

As mentioned, transport in heterostructures such as a quantum well laser poses a difficult problem. The quantum well must be treated appropriately because it is the region of positive gain, and, therefore, it is the most critical determinate of optical output. However, the regions surrounding the quantum well also play important roles in the device characteristics. For example, the current blocking regions significantly influence the effective quantum efficiency of the device. Also, the transport in the separate confinement regions can lead to low frequency roll-off in the modulation response[8] and gain saturation.[9, 10]

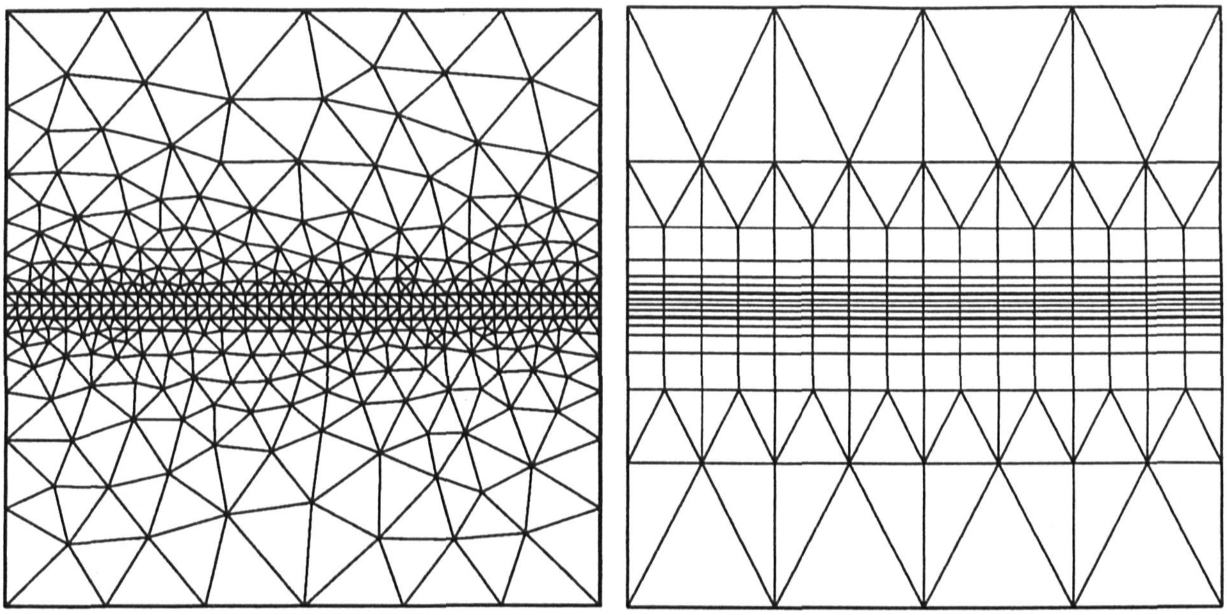

Figure 1: Triangular tesselation of a quantum well device is inappropriate due to a small aspect ratio. A combination of rectangles and triangles produces a mesh consistent with the quasi-one-dimensional nature of quantum wells.

As a result, the simulation of such structures is also a multiscale problem.

The first difficulty with such a multiscale problem involves the tesselation of the device. It is standard practice to use triangles to discretize a complicated device structure because they conform well to nonrectangular features, such as contoured current blocking regions. However, in the case of quantum well structures, triangles have a serious drawback. A well formed triangle usually has an aspect ratio on the order of one. If a ridge waveguide laser structure with a 10 μm wide and 100 Å thick quantum well is being simulated, then the use of triangles leads to an explosion in the number of mesh points. Rectangles, on the other hand, lend themselves very well to the quasi-one-dimensional nature of quantum wells. As a result, the use of rectangles and triangles produces the most convenient tesselation for a quantum well device. Figure 1 shows two meshes generated for a simple quantum well structure. The more flexible aspect ratio of the rectangles produces a much more appropriate mesh.

III. Coupling the Classical and Quantum Regions

In addition to optimizing the number of mesh points, the use of rectangles in and near the quantum well is crucial to the treatment of transport in these regions. Rectangles allow the quantum well to be divided up into transverse cross-sections. The mesh points in each cross-section can then be used to solve a one-dimensional Schrödinger's Equation, giving the eigenenergies and wavefunctions for the bound states in the well. Transport in and around the well can then be treated in a special way. Figure 2 is a schematic represention

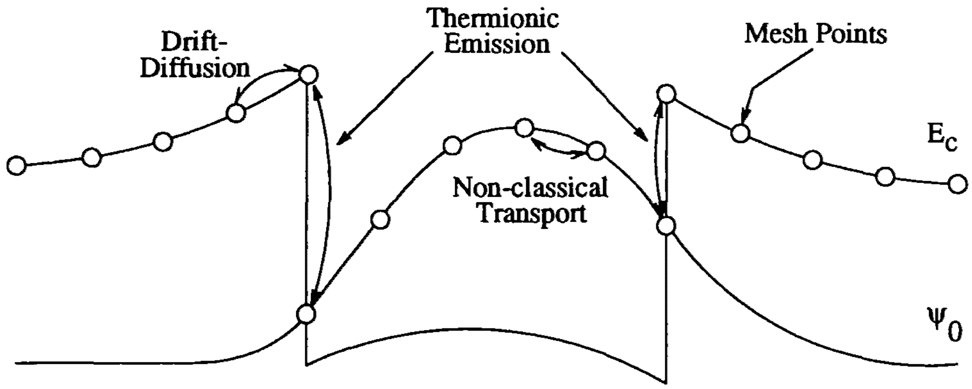

Figure 2: The schematic diagram shows a transverse cross-section of the quantum well. The classical and quantum mechanisms that determine the carrier distributions are labelled where they apply. Note that the circles represents mesh points in the discretization, not charge carriers.

of this treatment. The figure shows the conduction band edge and the ground state wavefunction for one of the transverse cross-sections of the well. Drift-diffusion theory describes the transport up to the quantum well. The particle fluxes are expressed in the following form.

$$\vec{j}_n = -\mu_n N_c \mathcal{F}_0(\eta_n)(T\nabla\eta_n + \nabla E_c)$$
$$\vec{j}_p = -\mu_p N_v \mathcal{F}_0(\eta_p)(T\nabla\eta_p - \nabla E_v)$$

where,

$$\eta_n = (F_n - E_C)/T, \eta_p = (E_V - F_P)/T$$
$$\mathcal{F}_j = \frac{1}{j!}\int_0^\infty dx \frac{x^j}{1 + e^{x-\eta}}$$

In each of the flux equations, the first term in parentheses is the diffusion term and the second is the drift term, where the gradient in the band edge determines the field. Thermionic emission theory then determines the flux of carriers into or out of the well according to the following expression.

$$j = A_2^* T^2 \frac{2m_1 m_2}{m_1 + m_2}\left\{exp\left(\frac{E_{Fn2} - E_{C2}}{kT}\right) - exp\left(\frac{E_{Fn1} - E_{C1} - E_B}{kT}\right)\right\}$$

where, A_2^* = the Richardson constant.

Inside the quantum well, classical transport is not valid in the transverse direction; it is the form of the wavefunctions that determines the distribution of carriers inside the well. When carriers are injected into the well, they conform to the distribution established by the wavefunctions almost instantaneously. Classical transport is eliminated by requiring that the quasi-Fermi levels inside the well are constant in the transverse direction. Their absolute positions are determined by the carrier fluxes into or out of the well. Consequently, it is the self-consistent agreement between drift-diffusion and thermionic emission transport that ultimately determines the filling of the well and, thus, the gain of the laser. Inclusion of quantum reflections and resonances represents a straight forward extension of this treatment.

Classical transport is, however, permitted in the lateral direction. And again, the rectangular tesselation enables this to be treated correctly. The lateral transport is treated with drift-diffusion theory. The divergence in the carrier flux is calculated for each point in a transverse cross-section of the well, but these divergences are added together to determine the continuity equation for the wavefunction as a whole. The result is the propagation along the quantum well of entire wavefunctions that represent the carrier distribution, and maintaining the shape of the wavefunctions as carriers propagate is necessary for the correct simulation of quantum systems.

The importance of coupling the classical and quantum regions correctly is evident in figure 3. This figure shows the modulation responses for two different lasers. Each laser has 5000 Å *AlGaAs* separate confinement regions on each side of a 100 Å *GaAs* quantum well. However, for the device in the top figure, the optical confining region was ungraded, whereas for the bottom device, it was linearly graded. The ungraded device shows low frequency roll-off and increased saturation of the resonant peaks when compared to the graded device. The roll-off is due to slow carrier drift in the separate confinement region, and the gain saturation is the result of diffusive diode current. Even though the active regions are identical in the two devices, the optical output characteristics are very different due to transport in the surrounding bulk regions. Consequently, it is critical that the classical regions are properly coupled to the quantum region in order to accurately calculate the device performance.

IV. Accounting for Carrier Capture

Although the method described above is an effective way of coupling the classical regions of a laser with the quantized active region, there is an element missing that may affect the measured characteristics of the device. We discussed the way in which thermionic emission theory is used to determine the filling of the well. Thermionic emission theory assumes that the carriers on one side of a heterojunction are in thermal equilibrium with themselves but not with carriers on the other side of the junction. This is valid, but it also assumes that once a carrier passes to the other side of the junction it immediately relaxes and is in thermal equilibrium with carriers on that side. It does not consider the finite time it takes for the hot injected carrier to lose its excess energy. This time is typically on the order of a picosecond or less. However, due to the self-consistent agreement of the thermionic emission current injected into the well and the drift-diffusion current in the surrounding regions, any finite hot carrier concentration in the well can lead to increased carrier densities in the separate confinement regions.[7] This increase in carrier density will produce a diffusive barrier to transport and increase gain saturation, thereby affecting the laser characteristics.

The coupling of the classical and quantum regions described above can be extended to account for the relaxation of hot quantum carriers into bound states. Figure 4 schematically represents this extension. As before, the conduction band edge and the ground

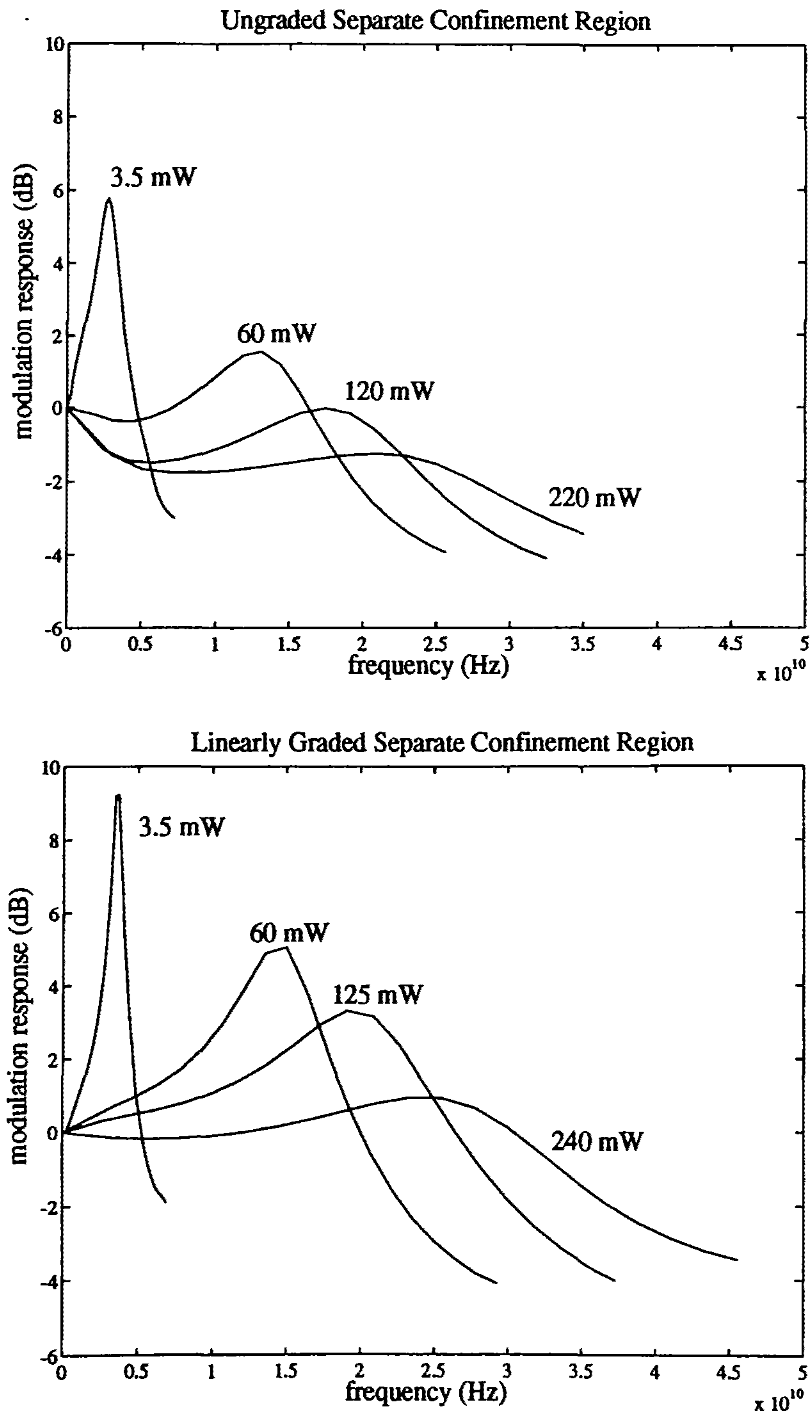

Figure 3: The modulation responses for two different 100 Å *GaAs* quantum well lasers. Each device has 5000 Å *AlGaAs* separate confinement regions on each side of the quantum well. However, the optical confinement region for the top device is ungraded while the confinement region for the bottom device is linearly graded.

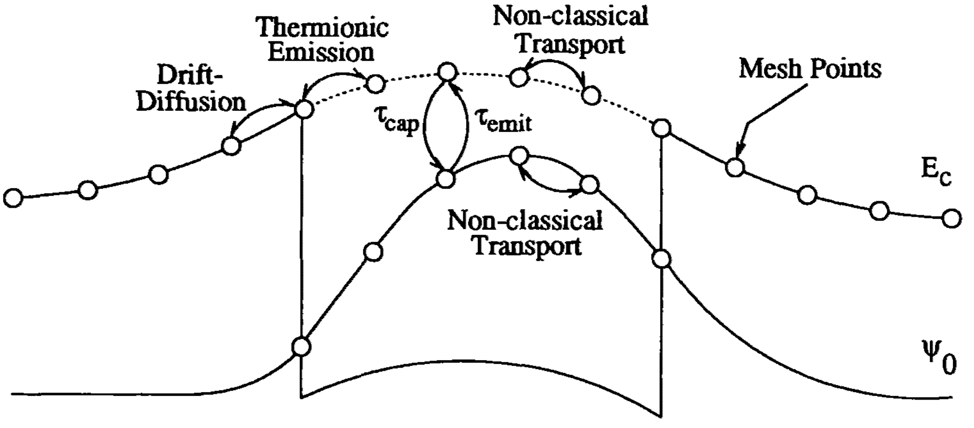

Figure 4: The schematic diagram shows a transverse cross-section of the quantum well. The classical and quantum mechanisms that determine the carrier distributions are labelled along with the scattering between quasi-bound and bound quantum states.

state wavefunction for a transverse cross-section of the quantum well is shown. Like the previous method, drift-diffusion theory is used to determine carrier transport up to the well, and thermionic emission theory is used to determine injection into the well region. However, now carriers are not injected into bound states but rather into higher energy, quasi-bound states. This is achieved by simply using thermionic emission with zero barrier height. The quasi-bound states are not assumed to be in thermal equilibrium with the bound states in the quantum well. They have a separate quasi-Fermi level to determine their occupancy. The quasi-bound states exchange carriers with the bound states through a scattering lifetime, e.g. as calculated in [6]. The result will be a finite hot quantum carrier concentration, the consequence of which can only be determined by the self-consistent solution of the transport equation throughout the rest of the device.

V. Conclusion

The characteristics of quantum well devices are most critically dependent on the properties of the well, which can be accurately treated only with quantum mechanical methods. However, the device performance can also depend strongly on transport in the remainder of the device, as we have shown with the modulation response of semiconductor lasers. Transport in these other regions is most tractable when treated with classical theories, but this leads to the problem of coupling the quantum treatment of the active region with the classical treatment of the surrounding regions. To do this correctly requires complex mesoscopic theories which are not easily implemented in computer simulation. In this paper, we have presented a model which serves as a starting point for the numerical solution of this difficult problem.

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