HETEROSTRUCTURE DEVICE SIMULATION USING THE WIGNER FUNCTION

APPROVED BY
DISSERTATION COMMITTEE:

Supervisor: ______________________

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To my parents

HETEROSTRUCTURE DEVICE SIMULATION USING THE WIGNER FUNCTION

by

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DISSERTATION

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In the past decade, advanced heteroepitaxial technology has allowed the exploration of a wide variety of semiconductor heterostructures in which the electronic properties can be varied significantly over atomic length scales. Semiclassical models of electron transport are not useful for the analysis of such structures. Perhaps the most dramatic phenomenon illustrating the need for advanced quantum transport models is resonant-tunneling across a double barrier quantum well structure. Since the early work on resonant-tunneling, many devices have been proposed that incorporate double barrier quantum wells, the motivation being the increased functionality per device. Because significant regions in these devices can still be described by semiclassical equations, it is highly desirable that the quantum transport equation have the structure of the semiclassical Boltzmann equation, and reduce to it when appropriate. Such a model is afforded by the Weyl transform and the associated Wigner function. In this work, a quantum transport model based on the Wigner function is developed for the analysis of heterostructure devices. Past work on the use of the Wigner function has assumed that the effective-mass is spatially uniform, clearly not the case in heterostructure devices. In this work, the spatially

varying effective-mass has been correctly incorporated in the Wigner transport equation. While past work using the Wigner function has been restricted to relatively unimportant $Al_xGa_{1-x}As/GaAs$ heterostructure devices, this work presents improvements in the numerical treatment of the Wigner transport equation that are necessary to extend its application to the study of the more important devices based on $In_yAl_{1-y}As/In_xGa_{1-x}As$ heterojunctions.

With the aid of the quantum transport models developed during this work, an intriguing memory switching phenomena was discovered in double barrier resonant-tunneling diodes that contain $N^- - N^+ - N^-$ spacers. Experimentally, the devices can be reversibly switched between two conduction curves. They retain memory of the curve last switched to, even after removal of the external bias. Within the scope of the quantum transport models, the phenomenon is explained by the existence of two self-consistent charge distributions in the device, even when no external bias is applied.

Table of Contents

List of Figures

Chapter 1

Introduction

During the past few years, advanced heteroepitaxial technology has allowed the exploration of a wide variety of semiconductor heterostructures in which the electronic properties change significantly over atomic length scales. The semiclassical limit cannot be taken in modeling electron transport in such heterostructures, and fully quantum mechanical models are necessary. Perhaps the most dramatic evidence of quantum phenomenon in semiconductor devices motivating the need for advanced quantum transport models is the negative differential resistance exhibited by resonant-tunneling diodes. Since the proposal (Iogansen, 1964; Tsu & Esaki, 1973) and observation of resonant-tunneling (Chang et al., 1974), it has been the focus of much attention during the last 20 years. Resonant-tunneling diodes have been studied for their potential in high-frequency oscillators (Brown et al., 1991), pulse forming and trigger circuits (Özbay et al., 1991), and for multivalued memory and logic (Seabaugh et al., 1992; Micheel & Paulus, 1990). More recently, neural networks based on vertically integrated resonant-tunneling diodes have also been demonstrated (Levy & McGill, 1993).

Resonant-tunneling has also been the basis of more ambitious proposals aimed at the needs of a post-VLSI era. Resonant tunneling transistors have been proposed to extend the downscaling of electronic devices, and increase the functional density of an integrated circuit (Reed et al., 1990; Seabaugh et al., 1991; Yang et al., 1989; Bonnefoi et al., 1985; Beltram et al., 1988). The basic idea is to control the resonant levels and hence the current across an emitter-collector multi-barrier quantum well structure. Such transistor action is feasible if the resonant levels associated with the emitter-collector heterostructure are well separated from the energy levels into which charge is injected by the base. The energy levels associated with the base can then be used to independently control the positions of resonant levels available for emitter-collector conduction. The transfer characteristics of such resonant tunneling transistors enable the implementation of complex logic functions that would normally require several transistors (Maezawa et al., 1993; Seabaugh et al., 1993).

The operation of heterostructure tunneling devices is most easily and usefully understood in terms of the resonant states they support. In Chapter 2, a self-consistent model based on the effective-mass Schrödinger and Poisson equations is presented for the evaluation of transport across heterojunctions. In this work, we obtain the effective-mass equation by exploiting the connection of the tight-binding approach to the finite-difference formulation. A new Hamiltonian for spatially varying parabolic energy bands, based on the Weyl correspondence rule, is finite-differenced to yield the effective-mass equation for a spatially varying tight-binding energy band. The treatment of the boundary conditions is based on the work of Frensley (1991) and Lent and Kirkner (1990). Finally the model is extended to include the full , $-X$ conduction band edge in the position representation.

While adequate for describing the resonant states in a heterostructure, the Schrödinger model cannot comprehend important processes such as electron-phonon scattering. This is a serious limitation of the model, especially since many quantum devices have significant regions where transport is not phase coherent or dissipationless. Difficulties also arise when a time-dependent description is required. Although time-irreversible, non-Markovian boundary conditions for the time-dependent Schrödinger equation have been recently formulated (Hellums & Frensley, 1994), application of the time-dependent equation to the description of an entire system is impractical. Since the device potential changes with time, the resonant states also change. Since the evolution of the system is not known apriori, for a proper treatment, the initial state of the device must be evaluated with an infinite basis of wave functions. Clearly, descriptions based on individual wavefunctions must be abandoned for a more appropriate kinetic theory of transport. To describe transport in general, it is necessary to develop a model that comprehends both quantum interference and processes such as electron-phonon scattering. It is also highly desirable that a quantum transport equation have the structure of the semiclassical Boltzmann equation, and reduce to it when appropriate.

Such a model is afforded by the Weyl transform and the associated Wigner function. In Chapter 3, a quantum transport model based on the Wigner function is developed for the analysis of heterostructure diodes. After showing how the Weyl transform casts the quantum transport problem into the familiar language of semiclassical theory, the Wigner function is applied to the study of heterostructure devices. Much of the past work on the Wigner transport equation (Buot & Jensen, 1990; Frensley, 1990; Klukshdahl, Kriman, Ferry, & Ringhofer, 1989; Mains & Haddad, 1988) has assumed that the effective-mass is spatially uniform, clearly not the case in heterostructures. Only recently have there been attempts to incorporate position-dependent energy bands into the Wigner transport simulation of heterostructure devices (Miller & Neikirk, 1991; Tsuchiya et al., 1991). It is shown that the equation derived by Tsuchiya et al. (1991) for transport in a position-dependent parabolic energy band is inconsistent with the Weyl transform (see Appendix A for a discussion and critique of the work of Tsuchiya *et al.*). While the approach of Miller and Neikirk (1991) is based on the discrete Weyl transform, and leads directly to a discrete equation, it does not satisfy current continuity. In this work, an equation of motion has been derived that is consistent with the Weyl transform and also satisfies current continuity.

A second issue addressed in Chapter 3 is that the band structure in real semiconductors is far from being a parabola that extends to infinite energy. It is shown that expanding the real bandstructure in terms of its Fourier components allows it to be elegantly incorporated into the Wigner transport equation. Beyond allowing the incorporation of general energy bands into the transport equation, the approach also leads to a more consistent discrete numerical model (Gullapalli & Neikirk, 1994), resolving for example, the confusion concerning the periodicity of the Wigner function (Miller, 1994).

To obtain any useful information, an accurate numerical model of the Wigner transport equation must be developed. In the past, the issue of numerical stability has been considered the most important, fidelity to the physical model receiving much less attention. In Chapter 4, it is shown that conventional upwind schemes, chosen from stability concerns, are completely inadequate for the description of AlAs/GaAs devices. While past work using the Wigner function has been restricted to relatively unimportant low aluminum mole-fraction $\mathrm{Al}_x\mathrm{Ga}_{1-x}\mathrm{As/GaAs}$ heterostructure devices, this work presents improvements in the numerical treatment of the Wigner transport equation that are necessary to extend its application to the study of the more important devices based on high conduction band offset $\mathrm{In}_y\mathrm{Al}_{1-y}\mathrm{As/In}_x\mathrm{Ga}_{1-x}\mathrm{As}$ heterojunctions (Gullapalli & Neikirk, 1994). For the first time, we present the proper numerical treatment of the Wigner transport equation in the presence of spatially varying bandstructure.

Chapter 5 describes an intriguing memory switching phenomena in double barrier resonant-tunneling diodes that contain $\mathrm{N}^- - \mathrm{N}^+ - \mathrm{N}^-$ spacers (Gullapalli, Tsao, & Neikirk, 1992). Discovered during a theoretical study of the impact of the cathode side spacer on the tunneling characteristics, devices with such spacers can be reversibly switched between two conduction curves. They retain memory of the curve last switched to, even after removal of the external bias. Within the scope of the quantum transport models, the phenomenon is explained by the existence of two self-consistent charge distributions in the device, even when no external bias is applied. Chapter 6 concludes this dissertation with a summary and recommendations for future work.