Chapter 6

Summary and Recommendations

Advanced heteroepitaxial growth techniques have made possible several novel device structures that exploit quantum mechanical tunneling of electrons across multi-barrier systems. In this thesis we have discussed quantum transport models for the study of such vertical transport heterostructure devices. In chapter 2 we presented a self-consistent Schrödinger-Poisson model, the simplest level at which transport across heterostructures can be understood. A new Hamiltonian for spatially varying parabolic energy bands, based on the Weyl correspondence rule, was finite-differenced to yield the effective-mass equation for a spatially varying tight-binding energy band. The quantum transmitting boundary method was used to define the open system boundary conditions. The model was also extended to include the entire , $-X$ 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. Since many useful quantum devices have significant regions in which transport is not phase coherent or dissipationless, the need for a model that comprehends both quantum interference and processes such as electron-phonon scattering was discussed. In chapter 3, it was shown that the Weyl transform and the associated Wigner function led to such a model. After showing how the Weyl transform casts the quantum transport problem into the familiar language of semiclassical theory, the Wigner function was applied to the study of heterostructure devices. An equation of motion was obtained that is consistent with the Weyl transform. It was shown that expanding the real bandstructure in terms of its Fourier components allows it to be consistently incorporated into the Wigner transport equation. In addition to allowing the incorporation of general energy bands into the transport equation, the approach also led to a more consistent discrete numerical model.

In chapter 4, numerical aspects of simulating the Wigner equation were discussed. It was shown that the standard upwind difference schemes for the drift term, 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 $Al_xGa_{1-x}As/GaAs$ heterostructure devices, improvements in the numerical treatment of the Wigner transport equation, necessary to extend its application to the study of the more important devices based on high conduction band offset $In_yAl_{1-y}As/In_xGa_{1-x}As$ heterojunctions, were discussed. The tradeoff between numerical stability and physical accuracy makes the simulation of the Wigner equation challenging. Much work remains to be done in this area. The problems in the numerical models become evident as the scope of the physical model is broadened. For example, in this work, inclusion of effective-mass variations demonstrated the caution necessary in developing a numerical model. In a related Appendix, the importance of proper numerical treatment was demonstrated by showing how the physically unreasonable results of (Tsuchiya et al., 1991) can be avoided. Available computational resources have limited our study to transport in a nearest-neighbor tight-binding energy band. Including other details of the bandstructure will also present challenges in the numerical treatment, and may lead to better numerical models.

The first step in understanding the similarities between quantum and classical phase-space, in the context of resonant-tunneling device simulation, has been taken by Jensen and Buot (1991), who have calculated quantum trajectories from the numerical solution for the Wigner function. However, methods such as the Monte Carlo and cellular-gas techniques, proven to be extremely useful in understanding semiclassical transport, have not yet been explored for application to the quantum transport problem. Such methods, if applicable, will be as important in quantum transport as they have been in semiclassical transport.

Chapter 5 described an intriguing memory switching phenomenon 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 can be understood by the existence of multiple self-consistent charge distributions in the device, even when no external bias is applied. The discovery of the phenomenon being recent, much work remains to be done. A rigorous treatment of collisions is necessary to obtain a deeper understanding of the switching dynamics. High and low temperature behavior of the memory switching phenomenon will provide information regarding the importance of effects such as electron-phonon collisions. Capacitance measurements at low bias, in conjunction with small signal calculations using the Wigner function, will yield information regarding the charge distributions in the different states. The device switching speed, and its response to periodic switching pulses, needs to be characterized. Further study will depend on the design of memory switching devices with low current densities. While in the present two-terminal form the memory switching effect is difficult to characterize and use, further study might reveal more useful structures in which to observe memory switching.