Numerical Methods for Quantum Hydrodynamics

Important quantum effects in semiconductor devices (resonant tunneling diodes, quantum field effect transistors, high electron mobility transistors, super-lattice devices etc.)—as well as in problems involving plasma physics, nuclear physics, superfluidity, and superconductivity—can be efficiently simulated by means of quantum hydrodynamics. The two most useful quantum hydrodynamical approximations are the original $O(\hbar^2)$ quantum hydrodynamic (QHD) model (see [1] and references therein) and the $O(V)$ smooth quantum hydrodynamic model [2], where $V$ is the classical potential energy.

The smooth QHD model [2] is an extension of the classical hydrodynamic model for semiconductor devices which can handle in a mathematically rigorous way the discontinuities in the classical potential energy which occur at heterojunction barriers in quantum semiconductor devices. Quantum transport effects including electron or hole tunneling through potential barriers and charge buildup in quantum wells are incorporated into the hydrodynamic description of charge propagation in semiconductor devices. Ref. [3] reviews the smooth QHD model emphasizing its derivation from a moment expansion of the Wigner-Boltzmann equation, using a quantum Maxwellian to close the moments.

VLSI (Very Large Scale Integrated) chips incorporate billions of semiconductor devices (transistors, diodes, optical devices, etc.). To predict the performance of the VLSI circuits, the current-voltage (IV) characteristics of the semiconductor devices are required. Semiconductor device simulation codes [4] provide a way of predicting IV curves as device parameters are varied, without having to fabricate the device first. (These parameters include semiconductor material, size, doping, and geometry.) Thus, many different designs for devices and circuits can be explored efficiently using computer simulations. Promising designs then can be selected for actual fabrication and testing.

Many devices including MOSFETs (metal oxide semiconductor field effect transistors) and MESFETs (metal semiconductor field effect transistors) can be modeled using a semiclassical approach [4]. That is, the charge transport of electrons and/or holes is described by the classical Boltzmann equation, or a classical hydrodynamic model with effective masses for electrons and holes input from quantum theory. The charge transport equations are then coupled to Poisson’s equation for the electrostatic potential. Quantum semiconductor devices like resonant tunneling diodes and transistors, HEMTs
(high electron mobility transistors), and super-lattice devices are increasingly being used in VLSI chips. These devices rely on quantum tunneling of charge carriers through potential barriers for their operation. Advanced microelectronic applications include multiple-state logic and memory devices, and high frequency oscillators and sensors. In addition, increasing miniaturization enhances unwanted quantum effects in standard MESFETs and MOSFETs (for instance, current leakage in the MOSFETs due to quantum tunneling through the oxide insulator between the gate and the channel). Both types of quantum effects must be simulated in order to design robust ultra-small semiconductor devices.

A fundamental approach to modeling quantum transport of electrons and holes in semiconductor devices is the Wigner-Boltzmann equation, the quantum generalization of the Boltzmann equation. The Wigner-Boltzmann equation differs from its classical counterpart principally in that particle transport couples to the potential energy in a non-local way; i.e., the values of the electrostatic potential energy integrated over a finite region in space determine the transport at a point in space.

Simulating the kinetic equations (the classical Boltzmann equation or the quantum Wigner-Boltzmann equation) is computationally expensive because the distribution function for the electrons or holes is a function of six variables (three space and three momentum) plus time for a three-dimensional device. Thus, a hydrodynamic approximation to the kinetic equations, where the density, velocity and temperature of a charge carrier are functions only of three spatial dimensions plus time, offers enormous computational speedups in simulating devices. This approach has worked well in modeling semiclassical devices using the classical hydrodynamic model (see Fig. 1, where the hyperbolic transport equations are solved using the Tadmor central scheme), and quantum devices using the quantum hydrodynamic model.

The classical hydrodynamic model has become a standard industrial simulation tool that incorporates important hot electron phenomena in submicron semiconductor devices. Hot electron effects are missing in the simpler drift-diffusion model, which assumes the electron gas is always at ambient temperature. The hydrodynamic model consists of nonlinear hyperbolic conservation laws for particle number, momentum, and energy (with a heat conduction term), coupled to Poisson’s equation for the electrostatic potential. In the momentum and energy conservation equations, charge carrier scattering by phonons is modeled by relaxation time approximations. The electric field appears as terms on the right-hand sides.
Figure 1: Hydrodynamic simulation of electron density in $10^{18}$ cm$^{-3}$ in a Si MESFET at 300 K by Anne Gelb (Dartmouth University) and the PI. $x$ and $y$ are in microns. S, G, and D label the source, gate, and drain, respectively.

The nonlinear hyperbolic modes support shock waves or “velocity overshoot” in the parlance of semiconductor device physicists. The hydrodynamic model can be extended to include quantum tunneling effects by adding quantum corrections.

To accurately compute solutions including the sharp resolution of waves, a conservative hyperbolic method from gas dynamics can be employed. Hyperbolic methods like the WENO (weighted essentially non-oscillatory) scheme are well suited for simulating the transient classical and quantum hydrodynamic models. Steady-state solutions may be obtained as the asymptotic large time limit; i.e., the time-dependent equations are simulated to a large value of the time at which the solution remains steady.

Feynman introduced into quantum statistical mechanics a smoothing of the classical potential as a way of partly accounting for the long range effects of quantum mechanics. However, as he noted, his smoothed potential “fails in its present form when the (classical) potential has a very large derivative as in the case of hard-sphere interatomic potential” or heterojunction potential barriers in semiconductor devices.

The smooth QHD model involves a smoothing of the classical potential
over both space and inverse temperature. The double integration provides sufficient smoothing so that the leading singularity in the smooth potential cancels the leading singularity in the classical potential at a barrier (see Fig. 2). This cancellation leaves a residual smooth effective potential with a lower potential height in the barrier region. The lower barrier height, along with the smoothing, makes the barriers partially transparent to the particle flow and provides the mechanism for particle tunneling in the QHD model. Note that the effective barrier height approaches zero as the ambient temperature T goes to zero. This effect explains why particle tunneling is enhanced at low temperatures. As T goes to infinity, the effective potential approaches the classical double barrier potential and quantum effects in the QHD model are suppressed.

The original $O(\hbar^2)$ QHD model succeeded in simulating the effects of electron tunneling through potential barriers including single [1] and multiple regions [5] of negative differential resistance (a region of the current-voltage curve where the current decreases as the voltage is increased) and hysteresis [6] in the current-voltage curves of resonant tunneling diodes.

Smooth QHD model simulations of the resonant tunneling diode were presented in [7] which exhibit enhanced negative differential resistance (NDR).
when compared to simulations using the original $O(h^2)$ QHD model. At both 300 K and 77 K, the smooth QHD simulations correctly predict significant NDR even when the original QHD model simulations predict no NDR. The smooth QHD model was shown in [8] to give excellent qualitative agreement with the current-voltage curves for the resonant tunneling diode predicted by the industrial simulator NEMO, which is based on solving the full mixed-state quantum mechanics based on a nonequilibrium Green function technique.

Smooth QHD simulations of a GaAs resonant tunneling diode with Al-GaAs (aluminum gallium arsenide) double barriers at 300 K are presented in Figs. 3–5. The barrier height is equal to 280 meV. The diode consists of n+ source (at the left) and drain (at the right) regions, and an n channel. The channel is 200 Angstroms long, the barriers are 25 Angstroms wide, and the quantum well between the barriers is 50 Angstroms wide. There are 50 Angstrom spacers between the barriers and the contacts. Figure 3 displays the experimental signal of quantum resonance—negative differential resistance. The resonant peak of the current-voltage curve occurs as the electrons tunneling through the first barrier come into resonance with the energy levels of the quantum well (see Fig. 4 showing enhanced charge in the quan-

Figure 3: Current in MA/cm$^2$ vs. applied voltage in volts for the resonant tunneling diode at 300 K.
Figure 4: Electron density in $10^{18} \text{ cm}^{-3}$ vs. $x$ in 0.1 microns in the resonant tunneling diode at 300 K and $V_{bias} = 0.1$ volt.

Figure 5: Electron temperature for the resonant tunneling diode at $T_0 = 300$ K and $V_{bias} = 0.1$ volt vs. $x$ in 0.1 microns.
tum well). The resonant peak occurs at 100 millivolts. As the voltage bias \( V_{\text{bias}} \) increases above 100 millivolts, the resonance effect rapidly decreases because the right barrier height is progressively reduced. As a result, electrons tunnel out of the well through the thin portion of the effective parabolic well.

### Smooth QHD Model Equations

The smooth QHD equations have the same form as the classical hydrodynamic equations:

1. \[
\frac{\partial n}{\partial t} + \frac{\partial}{\partial x_i} (n u_i) = 0
\]
2. \[
\frac{\partial}{\partial t} (m n u_j) + \frac{\partial}{\partial x_i} (m n u_i u_j - P_{ij}) = -n \frac{\partial V}{\partial x_j} - \frac{m n u_j}{\tau_p}
\]
3. \[
\frac{\partial W}{\partial t} + \frac{\partial}{\partial x_i} (u_i W - u_j P_{ij} + q_i) = -n u_i \frac{\partial V}{\partial x_i} - \left( W - \frac{3}{2} n T_0 \right) \frac{1}{\tau_w}
\]

where \( n \) is the electron density, \( u_i \) is the velocity, \( m \) is the effective electron mass, \( P_{ij} \) is the stress tensor, \( V \) is the potential energy, \( W \) is the energy density, and \( q_i \) is the generalized heat flux. Boltzmann’s constant \( k_B \) is set equal to 1. Indices \( i, j \) equal 1, 2, 3, and repeated indices are summed over. Electron scattering is modeled by the standard relaxation time approximation, with momentum and energy relaxation times \( \tau_p \) and \( \tau_w \).

The stress tensor and energy density are

4. \[
P_{ij} = -n T \delta_{ij} - \frac{\hbar^2 n}{4 m T_0} \frac{\partial^2 V}{\partial x_i \partial x_j}
\]
5. \[
W = \frac{3}{2} n T + \frac{1}{2} m n u^2 + \frac{\hbar^2 n}{8 m T_0} \nabla^2 V
\]

where \( T \) is the temperature of the electron gas and the “quantum potential” \( \mathbf{V} \) is given by (\( \beta = 1/T_0 \))

\[
\mathbf{V}(\beta, \mathbf{x}) = \int_0^\beta d\beta' \left( \frac{\beta'}{\beta} \right)^2 \int d^3 x' \left( \frac{2 m \beta}{\pi (\beta - \beta')(\beta + \beta') \hbar^2} \right)^{3/2} \exp \left\{ -\frac{2 m \beta}{(\beta - \beta')(\beta + \beta') \hbar^2} (\mathbf{x}' - \mathbf{x})^2 \right\} V(\mathbf{x}')
\]
The generalized heat flux

\[ q = -\kappa \nabla T - \frac{\hbar^2 n}{8m} \nabla^2 u \]  

includes both classical and quantum effects incorporates important effects of the higher moments of the Wigner-Boltzmann transport equation which are omitted in the fluid dynamical approximation.

We model the relaxation times \( \tau_p \) and \( \tau_w \) in the contacts by modified Baccarani-Wordeman models

\[ \tau_p = m \mu_{n0} \frac{T_0}{T}, \quad \tau_w = \frac{\tau_p}{2} \left( 1 + \frac{3T}{2m v_s^2} \right) \]  

and the coefficient \( \kappa \) by

\[ \kappa = \kappa_0 \mu_{n0} \bar{n} T_0 \]  

where \( \mu_{n0} \) is the low-field electron mobility, \( v_s \) is the electron saturation velocity, and \( \kappa_0 > 0 \) is a phenomenological constant.

The transport equations (1)–(3) are coupled to Poisson’s equation for the electrostatic potential energy

\[ \nabla \cdot (\epsilon \nabla V_P) = e^2 (N - n) \]  

where \( \epsilon \) is the dielectric constant, \( e > 0 \) is the electronic charge, and \( N \) is the density of donors. The total potential energy \( V \) consists of two parts, one from Poisson’s equation \( V_P \) and the other from the potential barriers \( V_B \):

\[ V = V_B + V_P. \]  

\( V_B \) has a step function discontinuity at potential barriers.

Fig. 3 displays the experimental signal of quantum resonance—negative differential resistance—for the smooth QHD model applied to the resonant tunneling diode at 300 K.

**Numerical Methods**

The main prediction needed by semiconductor device modelers is the steady-state current-voltage curve of a particular device (classical or quantum diode or transistor). With the QHD model, a steady-state solution and output current are computed for each (constant) voltage configuration.
The smooth QHD equations (1)–(6) plus (10) can be solved in steady-state by using either a steady-state Newton solver or by simulating the time-dependent equations to steady state. In 1D, solving the steady-state equations is efficient and robust, but in 2D and 3D the cost of the linear solves within the Newton method becomes prohibitive. The most efficient technique then in 2D and 3D is to solve the time-dependent equations to steady state.

For each timestep $\Delta t$,

- Solve the gas dynamical part of the smooth QHD equations using WENO
- Treat the quantum mechanical terms as source terms
- Add in the effects of heat conduction using TRBDF2

Then

- Solve Poisson’s equation using Chebyshev SOR

References


