A NEW QUANTUM HYDRODYNAMIC MODEL FOR SEMICONDUCTOR DEVICES

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Abstract

A new quantum hydrodynamic (QHD) model for semiconductor devices is presented. The quantum hydrodynamic conservation laws have the same form as the classical hydrodynamic model, but the electron potential energy and average energy have additional quantum terms. These quantum terms allow particles to tunnel through potential barriers. Simulations of a resonant tunneling diode are presented which show charge enhancement in the quantum well and negative differential resistance (NDR). These are the first simulations of the full QHD equations to show NDR in the resonant tunneling diode.

1 The Quantum Hydrodynamic Model

The hydrodynamic model for semiconductor devices can be extended to include quantum tunneling effects by adding the first quantum corrections [1]. These quantum corrections are $O(\hbar^2)$. In this presentation I propose a new set of quantum hydrodynamic (QHD) equations as a set of nonlinear conservation laws based on the quantum potential of Bohm and a quantum kinetic energy term due to Wigner:

$$\frac{\partial n}{\partial t} + \nabla\cdot(n\mathbf{v}) = 0 \tag{1}$$

$$\frac{\partial \mathbf{p}}{\partial t} + \mathbf{v}\nabla\cdot\mathbf{p} + \mathbf{p}\cdot\nabla\mathbf{v} = -n\nabla U - \nabla(nT) - \frac{\mathbf{p}}{\tau_p} \tag{2}$$

$$\frac{\partial W}{\partial t} + \nabla\cdot(\mathbf{v}W) = -n\mathbf{v}\cdot\nabla U - \nabla\cdot(\mathbf{v}nT) + \nabla\cdot(\kappa\nabla T) - \frac{\left(W - \frac{3}{2}nT_0\right)}{\tau_w} \tag{3}$$

$$\nabla\cdot(\epsilon\nabla\phi) = -e(N_D - N_A - n) \tag{4}$$

where n is the electron density, $\mathbf{v}$ is the velocity, $\mathbf{p} = mn\mathbf{v}$ is the momentum density, m is the effective electron mass, T is the temperature in energy units, κ is the thermal

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conductivity, ϵ is the dielectric constant, ϕ is the electric potential, N_D is the density of donors, and N_A is the density of acceptors. Eq. (1) expresses conservation of electron number, Eq. (2) expresses conservation of momentum, Eq. (3) expresses conservation of energy, and Eq. (4) is Poisson's equation for the electric potential. Here $U = -e\phi + Q$ is the effective potential, Q is the quantum potential of Bohm

$$Q = -\frac{\hbar^2}{2m}\frac{1}{\sqrt{n}}\nabla^2\sqrt{n}\ , \tag{5}$$

and the energy density W now includes a quantum term (first proposed by Wigner)

$$W = \frac{3}{2}nT + \frac{1}{2}mnv^2 - \frac{\hbar^2 n}{24m}\nabla\cdot\left(\frac{1}{n}\nabla n\right)\ . \tag{6}$$

The collision terms have been treated classically through momentum and energy relaxation times τ_p and τ_w.

These quantum hydrodynamic conservation laws have the same form as the classical hydrodynamic model, but the electron potential energy and average energy have additional quantum terms. These quantum terms allow particles to tunnel through potential barriers.

A different set of equations was first derived by Grubin and Kreskovsky [1] based on the moment method of Stroscio [2] for the quantum Liouville equation. Numerical simulations of a resonant tunneling diode were presented in Refs. [1] and [3] using this set of equations. The simulations in Ref. [1] show NDR for a resonant tunneling diode at 77 K using only the first two moments Eqs. (1) and (2) plus Poisson's equation.

2 QHD Simulations of the Resonant Tunneling Diode

The QHD model allows for efficient simulation of the behavior of quantum devices that depend on quantum tunneling. I will present simulations of a GaAs resonant tunneling diode with 0.3 eV double $Al_xGa_{1-x}As$ barriers. The diode consists of n^+ source and drain regions with the doping density $N = 10^{17}$ cm^{-3}, and an n channel with $N = 5\times10^{14}$ cm^{-3}. The channel is 250 Å long (indicated by the dark gray lines at $x = 0$ and $x = 0.25$ in Figs. 2 and 3), and the barriers are 25 Å wide (indicated by the light gray bands).

Current-voltage curves for the resonant tunneling diode are plotted in Fig. 1 for three different values of heat conduction κ_0 in $\kappa = \kappa_0\mu_{n0}nT_0/e$. The physically relevant value of κ_0 is approximately 0.075 for this device. These are the first simulations of the full QHD equations to show NDR in the resonant tunneling diode. For $\kappa_0 \lesssim 0.05$ there is too little heat conduction to allow for NDR, while for $\kappa_0 \gtrsim 0.1$ there is too much heat conduction (allowing for multiple regions of NDR).

With $\kappa_0 = 0.075$ the current-voltage curve displays a single region of NDR. The peak (near $V = 0.074$ volts) to valley (near $V = 0.14$ volts) current ratio of 1.5 is too small as compared to experiment, but this may be due to the presence of the collision terms in the QHD model [1]. Fig. 2 shows charge enhancement in the quantum well between the barriers for applied voltages of $V = 0.05$, 0.1, 0.15, and 0.2 volts. Note the

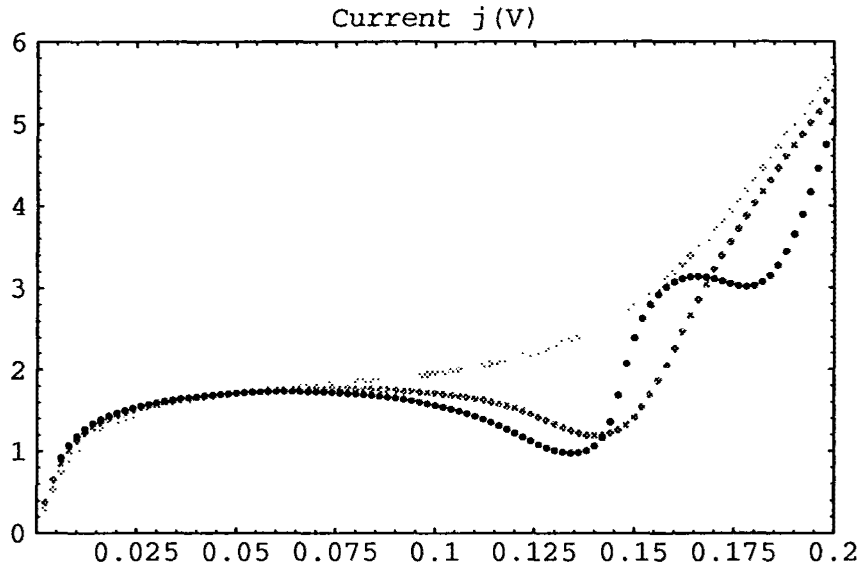

Figure 1: Current in kiloamps/cm^2 vs. voltage for the resonant tunneling diode at 77 K. $\kappa_0 = 0.05, 0.075$, and 0.1 from light gray to black.

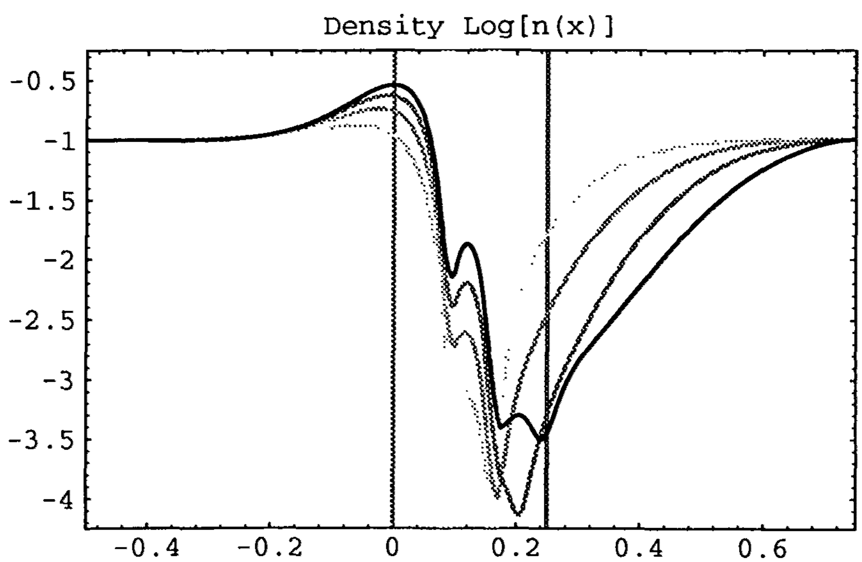

Figure 2: Log[Density/10^{18} cm^{-3}]. The curves are for $V = 0.05, 0.1, 0.15$, and 0.2 volts from light gray to black. x is in 0.1 microns.

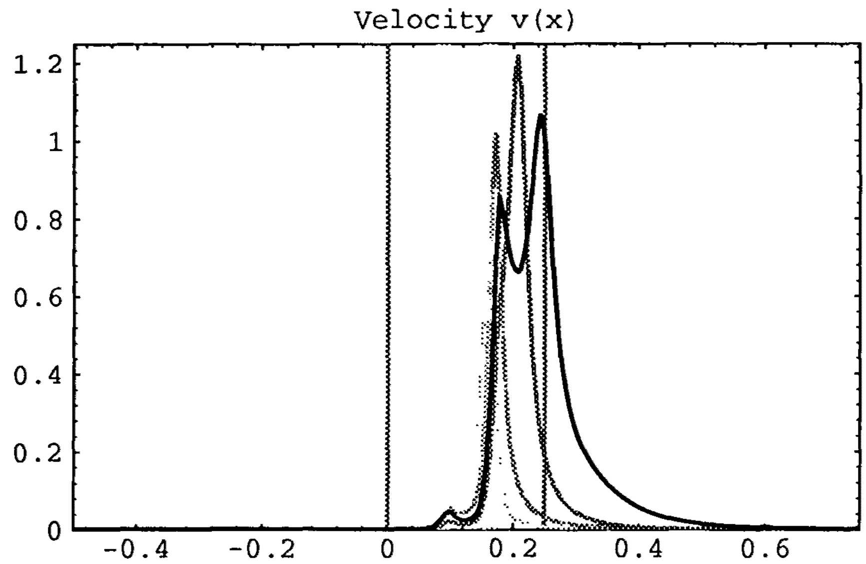

Figure 3: Velocity in 10^8 cm/sec. The curves are for $V = 0.05, 0.1, 0.15$, and 0.2 volts from light gray to black.

accumulation of electrons at the source-channel junction, and the depletion of electrons around the channel-drain junction. Fig. 3 presents the electron velocities for the same set of applied voltages. The electrons spend significantly more time in the quantum well (where the velocity is low) than in the barriers (where the velocity is high). Of special note is the fact that the *lowest* velocity in the well occurs at the current-voltage valley.

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References

[1] H. L. Grubin and J. P. Kreskovsky, "Quantum moment balance equations and resonant tunnelling structures," *Solid-State Electronics*, vol. 32, pp. 1071–1075, 1989.

[2] M. A. Stroscio, "Moment-equation representation of the dissipative quantum Liouville equation," *Superlattices and Microstructures*, vol. 2, pp. 83–87, 1986.

[3] D. L. Woolard, M. A. Stroscio, M. A. Littlejohn, R. J. Trew, and H. L. Grubin, "A new nonparabolic hydrodynamic model with quantum corrections," in *Computational Electronics: Semiconductor Transport and Device Simulation*, Boston: Kluwer Academic Publishers, 1991.