THE QUANTUM HYDRODYNAMIC MODEL FOR SEMICONDUCTOR DEVICES*

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Abstract. The classical hydrodynamic equations can be extended to include quantum effects by incorporating the first quantum corrections. These quantum corrections are $O(\hbar^2)$.

The full three-dimensional quantum hydrodynamic (QHD) model is derived for the first time by a moment expansion of the Wigner–Boltzmann equation. The QHD conservation laws have the same form as the classical hydrodynamic equations, but the energy density and stress tensor have additional quantum terms. These quantum terms allow particles to tunnel through potential barriers and to build up in potential wells.

The three-dimensional QHD transport equations are mathematically classified as having two Schrödinger modes, two hyperbolic modes, and one parabolic mode. The one-dimensional steady-state QHD equations are discretized in conservation form using the second upwind method.

Simulations of a resonant tunneling diode are presented that show charge buildup in the quantum well and negative differential resistance (NDR) in the current-voltage curve. These are the first simulations of the full QHD equations to show NDR in the resonant tunneling diode. The computed current-voltage curve agrees quantitatively with experimental measurements. NDR is interpreted in terms of the time spent by electrons in the quantum well.

Key words. quantum hydrodynamics, nonlinear PDEs, conservation laws, semiconductor device simulation

AMS subject classifications. 76M20, 76W05, 76Y05

1. Introduction. The behavior of a quantum fluid near thermal equilibrium and in the high temperature limit can be approximated by adding $O(\hbar^2)$ corrections to the classical fluid dynamical equations. The $O(\hbar^2)$ terms allow particle tunneling through potential barriers and particle buildup in potential wells.

The primary application of various quantum hydrodynamic (QHD) equations to date has been in analyzing the flow of electrons in quantum semiconductor devices. The QHD equations, however, are quite general and may find applications in other areas of physics, e.g., fluid models of the nucleus, superconductivity, and superfluidity.

In this investigation, we derive the QHD equations from a moment expansion of the Wigner–Boltzmann equation [31] and solve the QHD equations numerically to simulate electron flow in the resonant tunneling diode.

The QHD model is introduced in §2, and the first derivation of the full three-dimensional (3D) QHD equations from a moment expansion of the Wigner–Boltzmann equation is presented in §3. The QHD transport equations are expressed in terms of conservation laws for particles, momentum, and energy. The quantum correction to the stress tensor appearing in the QHD equations was derived by Ancona, Iafrate, and Tiersten [1], [2]. In the one-dimensional (1D) case, the 3D QHD equations reduce to the QHD model of Grubin and Kreskovsky [14].

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A different set of 3D QHD equations was proposed in [34]. However, this QHD model does not agree with the QHD equations derived here from the $O(\hbar^2)$ thermal equilibrium Wigner distribution function, that, we believe, must give the leading behavior of the quantum corrections.

In §4 the 3D QHD equations are classified as having two Schrödinger modes, two hyperbolic modes, one parabolic mode, and one elliptic mode, and well-posed boundary conditions are specified for the 1D resonant tunneling diode. The second upwind discretization of the 1D QHD equations is presented in §5.

Numerical simulations of a resonant tunneling diode were presented in [14] and [32] using the 1D QHD model. The simulations in [14] show negative differential resistance (NDR) for a resonant tunneling diode at 77 K using only the first two moments (1) and (2) plus Poisson's equation. (Reference [32] applies the full 1D QHD model in simulating a resonant tunneling diode at 300 K, but fails to find NDR.) In §6 the first simulations of the full 1D QHD equations are presented that show NDR in the resonant tunneling diode. An analysis of electron behavior in the diode is given in terms of the fluid dynamical quantities density, velocity, and temperature. The computed current-voltage curve for the resonant tunneling diode agrees quantitatively with experimental measurements. Finally, NDR is interpreted in terms of the time spent by electrons in the quantum well (see [14]).

2. The QHD model. The QHD conservation laws have the same form as the classical hydrodynamic equations (for simplicity, we treat the flow of electrons in an electric field)

$$(1) \quad \frac{\partial n}{\partial t} + \frac{1}{m} \frac{\partial \Pi_i}{\partial x_i} = 0,$$

$$(2) \quad \frac{\partial \Pi_j}{\partial t} + \frac{\partial}{\partial x_i} (u_i \Pi_j - P_{ij}) = -n \frac{\partial V}{\partial x_j} - \frac{\Pi_j}{\tau_p},$$

$$(3) \quad \frac{\partial W}{\partial t} + \frac{\partial}{\partial x_i} (u_i W - u_j P_{ij} + q_i) = -\frac{\Pi_i}{m} \frac{\partial V}{\partial x_i} - \frac{(W - \frac{3}{2} n T_0)}{\tau_w},$$

where n is the electron density, $\mathbf{u}$ is the velocity, Π_i is the momentum density, P_{ij} is the stress tensor, $V = -e\phi$ is the potential energy, ϕ is the electric potential, $e > 0$ is the electronic charge, W is the energy density, $\mathbf{q}$ is the heat flux, and T_0 is the temperature of the semiconductor lattice in energy units (k_B is set equal to 1). Indices i, j, k, l equal 1, 2, 3, and repeated indices are summed over using the Einstein convention. Equation (1) expresses conservation of electron number, (2) expresses conservation of momentum, and (3) expresses conservation of energy. The last terms in (2) and (3) represent electron scattering,¹ which is modeled by the standard relaxation time approximation with momentum and energy relaxation times τ_p and τ_w .

The classical hydrodynamic equations can be derived from physical arguments or from a moment expansion of the Boltzmann equation.² The quantum conservation laws have the same form as their classical counterparts. However, to close the

¹The collision terms may include the effects of electron-phonon and electron-impurity collisions, intervalley and interband scattering, etc.

²Whitham [30] gives a clear account of the physical arguments leading to the classical hydrodynamic equations. For a derivation of the hydrodynamic model for semiconductor devices from the Boltzmann equation, see [25].

moment expansion at three moments, we must define, for example, Π_i , P_{ij} , W , and $\mathbf{q}$ in terms of n , $\mathbf{u}$, and T , where T is the electron temperature.

We assume that the heat flux is specified by the Fourier law $\mathbf{q} = -\kappa \nabla T$. Section 3 shows that, for the $O(\hbar^2)$ “momentum-shifted” thermal equilibrium Wigner distribution function, the momentum density $\Pi_i = mnu_i$, where m is the effective electron mass, the stress tensor³ is given by

$$(4) \quad P_{ij} = -nT\delta_{ij} + \frac{\hbar^2 n}{12m} \frac{\partial^2}{\partial x_i \partial x_j} \log(n) + O(\hbar^4),$$

and the energy density is given by

$$(5) \quad W = \frac{3}{2}nT + \frac{1}{2}mnu^2 - \frac{\hbar^2 n}{24m} \nabla^2 \log(n) + O(\hbar^4).$$

The quantum correction to the energy density was first derived by Wigner [31]. The quantum correction to the stress tensor was proposed by Ancona and Tiersten [2] on general thermodynamical grounds and derived by Ancona and Iafrate [1] in the Wigner formalism. The stress tensor is related to the quantum potential of Bohm [22]

$$(6) \quad Q = -\frac{\hbar^2}{2m} \frac{1}{\sqrt{n}} \nabla^2 \sqrt{n}$$

through the formula

$$(7) \quad -\frac{\partial}{\partial x_i} P_{ij} = \frac{\partial}{\partial x_j} (nT) + \frac{n}{3} \frac{\partial Q}{\partial x_j}.$$

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

$$(8) \quad \nabla \cdot (\epsilon \nabla V) = e^2 (N_D - N_A - n),$$

where ϵ is the dielectric constant, N_D is the density of donors, and N_A is the density of acceptors.

3. Moment expansion of the Wigner–Boltzmann equation. In this section, the QHD equations are derived as a set of nonlinear conservation laws by a moment expansion of the Wigner–Boltzmann equation [31] and an expansion of the thermal equilibrium Wigner distribution function to $O(\hbar^2)$.

To derive the QHD equations, we assume that the electron flow can be approximated by a single-particle effective mass Schrödinger equation with a self-consistent many-body field,

$$(9) \quad i\hbar \frac{\partial \psi_\lambda}{\partial t} = E_\lambda \psi_\lambda = -\frac{\hbar^2}{2m} \nabla^2 \psi_\lambda + V\psi_\lambda,$$

where the wavefunctions $\psi_\lambda(\mathbf{x}, t)$ ($\lambda = 1, 2, \dots$) have energies E_λ and where $V(\mathbf{x})$ is the self-consistent potential energy. The effective mass approximation states that Schrödinger’s equation with the free electron mass and the total potential energy, which includes the periodic potential energy of the semiconductor lattice plus V , can

³The stress tensor is symmetric due to conservation of angular momentum.

be rewritten with the total potential energy replaced by V and the electron mass replaced by the effective electron mass (see, e.g., [19, Chap. 2]). Many-body electron correlation effects are neglected in this theory. Also neglected are the effects of Fermi–Dirac statistics, although these effects can be included. These approximations are valid in semiconductors in the low density ($\leq 10^{19} \text{ cm}^{-3}$) and high temperature ($\geq 77 \text{ K}$) limit. We also assume that the fluid dynamical state variables n , $\mathbf{u}$, and T are slowly varying functions of $\mathbf{x}$ and t .

For a pure quantum mechanical state described by a wavefunction $\psi(\mathbf{x}, t)$, the Wigner distribution function is defined as

$$(10) \quad f_w(\mathbf{x}, \mathbf{p}) = (\pi \hbar)^{-3} \int d^3 y \psi^*(\mathbf{x} + \mathbf{y}) \psi(\mathbf{x} - \mathbf{y}) e^{2i\mathbf{p} \cdot \mathbf{y} / \hbar},$$

where $\mathbf{p}$ is the molecular momentum. (The time dependence in ψ , f_w , etc., will be left implicit except when needed for clarity. All integrals are from $-\infty$ to $+\infty$.)

For a mixed quantum mechanical state described by wavefunctions $\psi_\lambda(\mathbf{x}, t)$ with occupation numbers a_λ , the Wigner distribution function is defined as

$$(11) \quad f_w(\mathbf{x}, \mathbf{p}) = (\pi \hbar)^{-3} \sum_\lambda a_\lambda \int d^3 y \psi_\lambda^*(\mathbf{x} + \mathbf{y}) \psi_\lambda(\mathbf{x} - \mathbf{y}) e^{2i\mathbf{p} \cdot \mathbf{y} / \hbar}.$$

Here $\sum_\lambda a_\lambda = M$, where M is the total number of electrons in the system. We assume that the a_λ 's vary slowly with $\mathbf{x}$ and t . For a mixed state in thermal equilibrium with a heat bath at temperature $T \equiv 1/\beta$, $a_\lambda \propto e^{-\beta E_\lambda}$. Equations (10) and (11) are the Fourier transforms of the quantum mechanical density matrices for pure and mixed states, respectively. “Global” expectation values of observables A are given in the Wigner formalism by

$$(12) \quad \langle A \rangle_{\text{global}} = \int d^3 x d^3 p A(\mathbf{x}, \mathbf{p}) f_w(\mathbf{x}, \mathbf{p}).$$

When $A(\mathbf{x}, \mathbf{p})$ is the sum of a function of $\mathbf{p}$ and a function of $\mathbf{x}$ (all physically important operators including the Hamiltonian are of this form), (12) is equivalent to

$$(13) \quad \langle A \rangle_{\text{global}} = \int d^3 x \psi^* A\left(\mathbf{x}, \frac{\hbar}{i} \nabla\right) \psi$$

for a pure state and

$$(14) \quad \langle A \rangle_{\text{global}} = \sum_\lambda a_\lambda \int d^3 x \psi_\lambda^* A\left(\mathbf{x}, \frac{\hbar}{i} \nabla\right) \psi_\lambda$$

for a mixed state, where the wavefunctions are normalized so that $\int d^3 x \psi^* \psi = 1$ and $\int d^3 x \psi_\lambda^* \psi_\lambda = 1$.

Thus f_w plays a role in quantum mechanics analogous to that of the Boltzmann distribution function in classical mechanics. However, the Wigner distribution function cannot be interpreted as a classical probability since it can take on negative values. “Local” average values of A are here defined in the Wigner formalism as

$$(15) \quad \langle A(x) \rangle = \int d^3 p A(\mathbf{x}, \mathbf{p}) f_w(\mathbf{x}, \mathbf{p}).$$

The Wigner distribution function obeys an equation similar to the classical Boltzmann equation

$$(16) \quad \frac{\partial f_W}{\partial t} + \frac{\mathbf{p}}{m} \cdot \nabla f_W - \sum_{\lambda_1, \lambda_2, \lambda_3=0}^{\infty} \frac{(\hbar/2i)^{\lambda_1+\lambda_2+\lambda_3-1}}{\lambda_1! \lambda_2! \lambda_3!} \frac{\partial^{\lambda_1+\lambda_2+\lambda_3} V}{\partial x_1^{\lambda_1} \partial x_2^{\lambda_2} \partial x_3^{\lambda_3}} \frac{\partial^{\lambda_1+\lambda_2+\lambda_3} f_W}{\partial p_1^{\lambda_1} \partial p_2^{\lambda_2} \partial p_3^{\lambda_3}} = 0,$$

with $\lambda_1 + \lambda_2 + \lambda_3$ an odd integer, or in compact form

$$(17) \quad \frac{\partial f_W}{\partial t} + \frac{\mathbf{p}}{m} \cdot \nabla f_W - \frac{2}{\hbar} \sin\left(\frac{\hbar}{2} \mathbf{V}_x^V \cdot \nabla_p\right) V(\mathbf{x}) f_W(\mathbf{x}, \mathbf{p}) = 0,$$

where ∇_x^V acts only on V . (We assume that the potential energy V has a Taylor series expansion. If V does not have a Taylor series expansion, the integrodifferential form [31] of the Wigner–Boltzmann equation can be used.) Equation (16) is known as the Wigner–Boltzmann equation. In the limit $\hbar \rightarrow 0$, (16) reduces to the classical collisionless Boltzmann equation. The Wigner–Boltzmann equation follows directly from Schrödinger’s equation and represents an exact reformulation of quantum mechanics (in its $6M$ -dimensional form, with the full potential energy and the free electron mass).

To derive (16) from Schrödinger’s equation (9), first differentiate (11) with respect to t as follows:

$$(18) \quad i\hbar \frac{\partial f_W}{\partial t} = \sum_{\lambda} a_{\lambda} \int \frac{d^3 y}{(\pi \hbar)^3} e^{2i\mathbf{p} \cdot \mathbf{y}/\hbar} \left\{ \frac{\hbar^2}{2m} [\{\nabla_x^2 \psi_{\lambda}^*(\mathbf{x} + \mathbf{y})\} \psi_{\lambda}(\mathbf{x} - \mathbf{y}) - \psi_{\lambda}^*(\mathbf{x} + \mathbf{y}) \nabla_x^2 \psi_{\lambda}(\mathbf{x} - \mathbf{y})] - [V(\mathbf{x} + \mathbf{y}) - V(\mathbf{x} - \mathbf{y})] \psi_{\lambda}^*(\mathbf{x} + \mathbf{y}) \psi_{\lambda}(\mathbf{x} - \mathbf{y}) \right\},$$

where a_{λ} is considered constant for the derivation. Then, by replacing ∇_x with ∇_y and integrating the first two terms on the right-hand side of (18) by parts, we obtain

$$(19) \quad \frac{\partial f_W}{\partial t} = \sum_{\lambda} a_{\lambda} \int \frac{d^3 y}{(\pi \hbar)^3} e^{2i\mathbf{p} \cdot \mathbf{y}/\hbar} \left\{ \frac{\mathbf{p}}{m} \cdot [-\{\nabla_y \psi_{\lambda}^*(\mathbf{x} + \mathbf{y})\} \psi_{\lambda}(\mathbf{x} - \mathbf{y}) + \psi_{\lambda}^*(\mathbf{x} + \mathbf{y}) \nabla_y \psi_{\lambda}(\mathbf{x} - \mathbf{y})] + \frac{2i}{\hbar} \sum_{\lambda_1, \lambda_2, \lambda_3} \frac{y_1^{\lambda_1} y_2^{\lambda_2} y_3^{\lambda_3}}{\lambda_1! \lambda_2! \lambda_3!} \frac{\partial^{\lambda_1+\lambda_2+\lambda_3} V}{\partial x_1^{\lambda_1} \partial x_2^{\lambda_2} \partial x_3^{\lambda_3}} \psi_{\lambda}^*(\mathbf{x} + \mathbf{y}) \psi_{\lambda}(\mathbf{x} - \mathbf{y}) \right\}$$

with $\lambda_1 + \lambda_2 + \lambda_3$ an odd integer and where $V(\mathbf{x} \pm \mathbf{y})$ has been expanded in a Taylor series. Replacing ∇_y with ∇_x leads to the Wigner–Boltzmann equation (16).

The moment expansion of the Wigner–Boltzmann equation involves integrating powers of p_j against $f_W(\mathbf{x}, \mathbf{p})$ in (16) to obtain conservation laws for particle number, momentum, and energy [15], [27]. Integrating a function $\chi(\mathbf{p})$ with respect to $\mathbf{p}$ against

the Wigner–Boltzmann equation, we obtain

$$(20) \quad \frac{\partial \langle \chi \rangle}{\partial t} + \nabla \cdot \left\langle \frac{\mathbf{p}}{m} \chi \right\rangle + \sum_{\lambda_1, \lambda_2, \lambda_3} \frac{(\hbar/2i)^{\lambda_1 + \lambda_2 + \lambda_3 - 1}}{\lambda_1! \lambda_2! \lambda_3!} \frac{\partial^{\lambda_1 + \lambda_2 + \lambda_3} V}{\partial x_1^{\lambda_1} \partial x_2^{\lambda_2} \partial x_3^{\lambda_3}} \left\langle \frac{\partial^{\lambda_1 + \lambda_2 + \lambda_3} \chi}{\partial p_1^{\lambda_1} \partial p_2^{\lambda_2} \partial p_3^{\lambda_3}} \right\rangle = 0$$

with $\lambda_1 + \lambda_2 + \lambda_3$ an odd integer.

Setting χ equal to 1, p_j , and $p^2/2m$ yields the first three moment equations

$$(21) \quad \frac{\partial n}{\partial t} + \frac{1}{m} \frac{\partial \langle p_i \rangle}{\partial x_i} = 0,$$

$$(22) \quad \frac{\partial \langle p_j \rangle}{\partial t} + \frac{\partial}{\partial x_i} \left\langle \frac{p_i p_j}{m} \right\rangle = -n \frac{\partial V}{\partial x_j},$$

$$(23) \quad \frac{\partial}{\partial t} \left\langle \frac{p^2}{2m} \right\rangle + \frac{\partial}{\partial x_i} \left\langle \frac{p_i p^2}{2m^2} \right\rangle = -\frac{1}{m} \langle p_i \rangle \frac{\partial V}{\partial x_i}.$$

The quantum conservation laws have the same form as their classical counterparts. Explicit factors of $\hbar$ enter only at the fourth ($\chi = \langle p_j p^2/2m^2 \rangle$) and higher moments due to the structure of the average value in the third term on the left-hand side of (20).

To calculate the average values in the first three moment equations, we use the “momentum-shifted” version of the $O(\hbar^2)$ solution [31] to (16)

$$(24) \quad f_W^{(2)}(\mathbf{x}, \mathbf{p}) = \mathcal{A} \frac{e^{-\beta E}}{(2\pi\hbar)^3} \times \left[1 + \hbar^2 \left\{ -\frac{\beta^2}{8m} \frac{\partial^2 V}{\partial x_k^2} + \frac{\beta^3}{24m} \left(\frac{\partial V}{\partial x_k} \right)^2 + \frac{\beta^3 p'_k p'_l}{24m^2} \frac{\partial^2 V}{\partial x_k \partial x_l} \right\} + O(\hbar^4) \right],$$

where $\mathcal{A}$ is a slowly varying function of $\mathbf{x}$ and t , the classical nonrelativistic energy $E = p'^2/2m + V$, and the macroscopic fluid velocity $\mathbf{u}$ is related to the molecular momentum $\mathbf{p}$ by

$$(25) \quad \mathbf{p} = m\mathbf{u} + \mathbf{p}'.$$

The actual expansion parameter in the asymptotic series (24) is $\hbar^2/8mTl^2$, where l is a characteristic length scale of the problem [1], [26].

The leading term in $f_W^{(2)}$ as $\hbar \rightarrow 0$ is the classical Maxwell–Boltzmann distribution function. With $\mathbf{u} = 0$, $f_W^{(2)}$ is the thermal equilibrium solution to the Wigner–Boltzmann equation to $O(\hbar^2)$. We then assume that the momentum-shifted $f_W^{(2)}$ approximates the actual Wigner distribution function closely enough for the average values in (21)–(23) to be close to the actual values.

Equation (24) for the Wigner distribution function has five free parameters $\mathcal{A}$ (which is proportional to n), $\mathbf{u}$, and $1/\beta = T$, which correspond to the five unknowns in the hydrodynamic transport equations (1)–(3).

The integral of f_W with respect to $\mathbf{p}$ is the particle density $n(\mathbf{x}, t)$ (which equals $\psi^*\psi$ for a pure state and $\sum_\lambda a_\lambda \psi_\lambda^* \psi_\lambda$ for a mixed state)

$$(26) \quad \begin{aligned} n(\mathbf{x}, t) &= \int d^3p f_W(\mathbf{x}, \mathbf{p}) \approx \int d^3p' f_W^{(2)}(\mathbf{x}, \mathbf{p}) \\ &= C e^{-\beta V} \left[1 + \hbar^2 \left\{ -\frac{\beta^2}{12m} \frac{\partial^2 V}{\partial x_k^2} + \frac{\beta^3}{24m} \left(\frac{\partial V}{\partial x_k} \right)^2 \right\} + O(\hbar^4) \right], \end{aligned}$$

where $C = (m/2\pi\beta\hbar^2)^{3/2} \mathcal{A}$.

Using the shifted Wigner distribution function (24) and expanding $\mathbf{p}$ according to (25), we obtain

$$(27) \quad \langle p_i \rangle \equiv \Pi_i = m n u_i,$$

$$(28) \quad \left\langle \frac{p_i p_j}{m} \right\rangle = u_i \Pi_j - P_{ij}, \quad P_{ij} \equiv - \left\langle \frac{p'_i p'_j}{m} \right\rangle,$$

$$(29) \quad \left\langle \frac{p^2}{2m} \right\rangle \equiv W, \quad W = \frac{1}{2} m n u^2 + \left\langle \frac{p'^2}{2m} \right\rangle,$$

$$(30) \quad \left\langle \frac{p_i p^2}{2m^2} \right\rangle = u_i W - u_j P_{ij} + q_i, \quad q_i \equiv \left\langle \frac{p'_i p'^2}{2m^2} \right\rangle.$$

We used the fact that odd powers of p'_i against $f_W^{(2)}$ integrate to zero, except that a heat flux term $\mathbf{q}$ is allowed, since heat conduction plays an important role in both the classical and QHD models. (The heat conduction term, in its Fourier form $\mathbf{q} = -\kappa \nabla T$, is believed to incorporate the most important effects of non-Maxwellian distributions. Extended models for $\mathbf{q}$ can also represent important effects of higher moments; see [33].) Note that $\Pi_i = m n u_i$ is exact to all orders in $\hbar$ for the Wigner distribution function given by (24). The definitions in (27)–(30) in terms of the Wigner distribution function have the same form as the classical definitions (see [30]) in terms of the Boltzmann distribution function. Substituting the expressions (27)–(30) into the moment equations (21)–(23), we derive the collisionless QHD model ((1)–(3) with $\tau_p, \tau_w \rightarrow \infty$).

Finally, to calculate P_{ij} and W , first observe that

$$(31) \quad \begin{aligned} &\int d^3p' \frac{p'_i p'_j}{m} f_W^{(2)}(\mathbf{x}, \mathbf{p}) \\ &= \frac{C}{\beta} e^{-\beta V} \left[\delta_{ij} + \hbar^2 \left\{ \delta_{ij} \left(-\frac{\beta^2}{12m} \frac{\partial^2 V}{\partial x_k^2} + \frac{\beta^3}{24m} \left(\frac{\partial V}{\partial x_k} \right)^2 \right) \right. \right. \\ &\quad \left. \left. + \frac{\beta^2}{12m} \frac{\partial^2 V}{\partial x_i \partial x_j} \right\} + O(\hbar^4) \right]. \end{aligned}$$

Substituting for $C e^{-\beta V}$ to $O(\hbar^2)$ from (26), we find that

$$(32) \quad P_{ij} = - \left\langle \frac{p'_i p'_j}{m} \right\rangle = -nT \delta_{ij} - \frac{\hbar^2 n}{12mT} \frac{\partial^2 V}{\partial x_i \partial x_j} + O(\hbar^4).$$

By setting $i = j$ in (32) and summing, we obtain

$$(33) \quad W = \frac{1}{2} m n u^2 + \left\langle \frac{p'^2}{2m} \right\rangle = \frac{3}{2} nT + \frac{1}{2} m n u^2 + \frac{\hbar^2 n}{24mT} \nabla^2 V + O(\hbar^4).$$

At this point, the stress tensor and energy density involve quantum corrections proportional to the second derivatives of the potential energy, and the QHD equations can be formulated in this way. However, Ancona and Tiersten [2] argued on general thermodynamical grounds that the equation of state for a quantum gas near thermal equilibrium should depend on the density gradient (rather than ∇V) as well as the density of the gas. In addition, to apply to neutral quantum fluids, e.g., superfluids, the QHD equations should be available in a form valid when the electrostatic potential energy in Poisson's equation is set equal to zero.

In this spirit, we can approximate

$$(34) \quad \frac{\partial}{\partial x_i} \log(n) \approx -\beta \frac{\partial V}{\partial x_i} + O(\hbar^2)$$

from (26) if

$$(35) \quad \left| \frac{1}{\mathcal{A}} \frac{\partial \mathcal{A}}{\partial x_i} \right|, \left| \frac{1}{\beta} \frac{\partial \beta}{\partial x_i} \right|, \left| V \frac{\partial \beta}{\partial x_i} \right| \ll \beta \left| \frac{\partial V}{\partial x_i} \right|.$$

Equation (34) is, to leading order in $\hbar^2$, equivalent to the classical thermal equilibrium expression $n \propto \exp(-\beta V)$ and should be approximately valid for slowly varying n , $\mathbf{u}$, and T . Assuming that $\mathcal{A}$ and T are slowly varying according to (35), we can write the stress tensor as

$$(36) \quad P_{ij} = -nT\delta_{ij} + \frac{\hbar^2 n}{12m} \frac{\partial^2}{\partial x_i \partial x_j} \log(n) + O(\hbar^4)$$

and the energy density as

$$(37) \quad W = \frac{3}{2}nT + \frac{1}{2}mnu^2 - \frac{\hbar^2 n}{24m} \nabla^2 \log(n) + O(\hbar^4).$$

We use (36) and (37) in this investigation.

Note that both forms for the stress tensor and energy density display the “nonlocal” character of solutions to Schrödinger’s equation. In (32) and (33), P_{ij} and W depend on the potential energy not only at $\mathbf{x}$, but in a neighborhood of $\mathbf{x}$, while, in (36) and (37), P_{ij} and W depend on the electron density in a neighborhood of $\mathbf{x}$, as in the quantum potential (6) of Bohm.

The classical equations of compressible fluid dynamics are derived for dilute gases from a moment expansion of the Boltzmann equation by assuming that the distribution function of the gas particles is locally a velocity-shifted Maxwellian and that n , $\mathbf{u}$, and T vary slowly with $\mathbf{x}$ and t . However, the resulting conservation laws of compressible fluid dynamics are much more generally valid. Similarly, we expect the QHD equations to be more generally valid than the conditions under which they were derived and to apply to electron flow that is not near thermal equilibrium. In addition to the assumption that the electron flow is near thermal equilibrium, the QHD transport equations were derived assuming that V is sufficiently smooth to have a Taylor series expansion. The potential energy of the resonant tunneling diode, however, has abrupt “jumps” at the GaAs/Al_xGa_{1-x}As heterojunctions (see Fig. 7). We believe that the QHD equations are valid for this type of potential, as comparison of the current-voltage results of §6 with experiment demonstrates. One reason for the extended validity of the QHD equations may be due to the fact that the $\log(n)$ forms (36) and (37) for P_{ij} and W are better able to handle jumps in the potential energy

than the V forms (32) and (33). The V forms for P_{ij} and W introduce *third* derivatives of the potential energy into the hydrodynamic transport equations—thus the computed solutions in this case will be extremely sensitive to the exact shape of the computational heterojunction.

The potential energy V for problems like the resonant tunneling diode may be decomposed into a smooth part and a discontinuous part with a finite set of jumps. Odeh and Steinrueck [26] developed an asymptotic, thermal equilibrium solution to the Wigner–Boltzmann equation, treating the discontinuous part of the potential energy separately to obtain a boundary layer solution near the jumps. Future work will apply this approach to deriving quantum fluid dynamical equations that treat the discontinuities in V more rigorously.

As noted above, the thermal equilibrium Wigner distribution function is actually expanded in powers of $\hbar^2/8mTl^2$. Thus the QHD equations approximate the full Wigner–Boltzmann equation when the electron gas is not too far from equilibrium (so that the moment expansion of the Wigner–Boltzmann equation is valid) and in the high temperature limit (in which the expansion of the Wigner distribution function is valid).

For the resonant tunneling diode simulations in §6 with $T \approx T_0 = 77$ K and $l = 100$ Å, the expansion parameter ≈ 0.23 .

4. Classification of the QHD equations. To classify the QHD equations, we first rewrite (1)–(3) and (8) (with $\tau_p, \tau_w \rightarrow \infty$) as

$$(38) \quad \frac{\partial n}{\partial t} + \frac{\partial}{\partial x_i} (nu_i) = 0,$$

$$(39) \quad \frac{\partial u_j}{\partial t} + u_i \frac{\partial u_j}{\partial x_i} + \frac{1}{mn} \frac{\partial}{\partial x_j} (nT) - \frac{\hbar^2}{12m^2n} \frac{\partial}{\partial x_i} \left(n \frac{\partial^2}{\partial x_i \partial x_j} \log(n) \right) + \frac{1}{m} \frac{\partial V}{\partial x_j} = 0,$$

$$(40) \quad \frac{\partial T}{\partial t} + u_i \frac{\partial T}{\partial x_i} + \frac{2}{3} T \frac{\partial u_i}{\partial x_i} - \frac{2}{3n} \frac{\partial}{\partial x_i} \left(\kappa \frac{\partial T}{\partial x_i} \right) + \frac{\hbar^2}{36mn} \frac{\partial}{\partial x_i} (n \nabla^2 u_i) = 0,$$

$$(41) \quad -\nabla \cdot (\epsilon \nabla V) + e^2 (N_D - N_A - n) = 0.$$

Next, we perturb a solution of the QHD equations with a Fourier mode, linearize the partial differential equations (PDEs) (38)–(41) with respect to the perturbation, and freeze coefficients. Set

$$(42) \quad \begin{bmatrix} n \\ u_i \\ T \\ V \end{bmatrix} = \begin{bmatrix} \bar{n} \\ \bar{u}_i \\ \bar{T} \\ \bar{V} \end{bmatrix} + e^{-\sigma t + i\mathbf{k} \cdot \mathbf{x}} \begin{bmatrix} \delta n \\ \delta u_i \\ \delta T \\ \delta V \end{bmatrix},$$

where $[\bar{n}, \bar{u}_i, \bar{T}, \bar{V}]$ is a solution of the QHD equations. We write the linearized QHD equations as

$$(43) \quad -\text{diag}\{\sigma, \sigma, \sigma, \sigma, \sigma, 0\} [\delta n, \delta u_i, \delta T, \delta V] + \mathcal{L} [\delta n, \delta u_i, \delta T, \delta V] = 0,$$

where $\mathcal{S}$ is the symbol of the linearized PDE system (38)–(41). Asymptotically as $|\mathbf{k}| \rightarrow \infty$, $\mathcal{S} = \text{diag}\{\sigma, \sigma\delta_{ij}, \sigma, 0\}$ has the form

(44)

$$j \downarrow \begin{bmatrix} i\mathbf{k} \cdot \mathbf{u} - \sigma & ik_in & 0 & 0 \\ ik_j \frac{T}{mn} + ik_j k^2 \frac{\hbar^2}{12m^2 n} & (i\mathbf{k} \cdot \mathbf{u} - \sigma)\delta_{ij} & i \frac{k_j}{m} & i \frac{k_j}{m} \\ ik_i \frac{\hbar^2}{36mn} \nabla^2 u_i & \frac{2}{3} ik_i T - ik_i k^2 \frac{\hbar^2}{36m} & i\mathbf{k} \cdot \mathbf{u} + \frac{2}{3} k^2 \frac{\kappa}{n} - \sigma & 0 \\ 0 & 0 & 0 & k^2 \epsilon \end{bmatrix}, \quad i \rightarrow$$

where i labels columns in the velocity perturbation δu_i and j labels rows in the velocity equation (39). The bar over the solution has been dropped for clarity of notation, and the leading terms in $\mathbf{k}$ for the limits $\hbar \rightarrow 0$ and $\kappa \rightarrow 0$ have been separately kept.

The asymptotic eigenvalues σ of the symbol as $|\mathbf{k}| \rightarrow \infty$ determine the mathematical type of the PDE system. The eigenvalues to leading order in $\mathbf{k}$ can most easily be deduced from the trace and determinant of the symbol. In fact, we need only consider the upper 5×5 block $\mathcal{S}_5$ of the symbol, since the coupling of the transport equations (38)–(40) to Poisson's equation (41) only introduces the elliptic Poisson mode and does not affect the modes of the transport equations.

There are three physically interesting cases to consider.

Case 1. $\hbar = 0$, $\kappa = 0$ (electrostatics). $\text{Tr } \mathcal{S}_5 = 5i\mathbf{k} \cdot \mathbf{u}$ and $\det \mathcal{S}_5 = -i(\mathbf{k} \cdot \mathbf{u})^3(k^2 c^2 - (\mathbf{k} \cdot \mathbf{u})^2)$, where $c = \sqrt{5T/3m}$. The eigenvalues of the symbol $\mathcal{S}_5$ and corresponding modes are

$$(45) \quad \begin{array}{ll} i(\mathbf{k} \cdot \mathbf{u} \pm kc) & \text{hyperbolic,} \\ i\mathbf{k} \cdot \mathbf{u} & \text{hyperbolic, multiplicity 3.} \end{array}$$

There are five nonlinear waves in classical electrostatics corresponding to the five hyperbolic modes: two shock waves with characteristic speeds $u_n \pm c$, where u_n is the velocity normal to the wave, and three contact waves with characteristic speed u_n . Two contact waves can be labeled by a jump in the tangential velocity $\mathbf{u}_t$ across the wave, and one contact wave by a jump in the temperature T .

Case 2. $\hbar = 0$, $\kappa > 0$ (hydrodynamic model or electrostatics with heat conduction). $\text{Tr } \mathcal{S}_5 = \frac{2}{3} k^2 \kappa / n + 5i\mathbf{k} \cdot \mathbf{u}$ and $\det \mathcal{S}_5 = -\frac{2}{3} k^2 (\kappa / n)(\mathbf{k} \cdot \mathbf{u})^2(k^2 c^2 - (\mathbf{k} \cdot \mathbf{u})^2) - i(\mathbf{k} \cdot \mathbf{u})^2(k^2 c^2 - (\mathbf{k} \cdot \mathbf{u})^2)$, where $c = \sqrt{T/m}$. The eigenvalues of the symbol $\mathcal{S}_5$ and corresponding modes are

$$(46) \quad \begin{array}{ll} i(\mathbf{k} \cdot \mathbf{u} \pm kc) & \text{hyperbolic,} \\ i\mathbf{k} \cdot \mathbf{u} & \text{hyperbolic, multiplicity 2,} \\ \frac{2}{3} k^2 \kappa / n + i\mathbf{k} \cdot \mathbf{u} & \text{parabolic.} \end{array}$$

With heat conduction, there are four nonlinear waves [13] in the classical hydrodynamic model corresponding to the four hyperbolic modes: two shock waves with characteristic speeds $u_n \pm c$ and two contact waves with characteristic speed u_n . The two contact waves can be labeled by a jump in the tangential velocity $\mathbf{u}_t$ across the

wave. The contact wave corresponding to a discontinuity in T has disappeared due to the parabolic heat conduction term $\nabla \cdot (\kappa \nabla T)$ in (3).

Case 3. $\hbar \neq 0$, $\kappa > 0$ (QHD model). $\text{Tr } \mathcal{S}_5 \approx \frac{2}{3}k^2\kappa/n$ and $\det \mathcal{S}_5 \approx -(\mathbf{k} \cdot \mathbf{u})^2 k^6 \hbar^2 \kappa / 18 m^2 n$. The eigenvalues of the symbol $\mathcal{S}_5$ and corresponding modes are

$$(47) \quad \begin{array}{ll} \pm ik^2 \frac{\hbar}{\sqrt{12}m} & \text{Schrödinger,} \\ i\mathbf{k} \cdot \mathbf{u} & \text{hyperbolic, multiplicity 2,} \\ \frac{2}{3}k^2\kappa/n & \text{parabolic.} \end{array}$$

There are two contact discontinuities (in $\mathbf{u}_i$) in the QHD model corresponding to the two hyperbolic modes. Note that two of the hyperbolic modes that allow shock discontinuities to form in the classical hydrodynamic model have become Schrödinger modes when the quantum corrections are included.

Well-posed boundary conditions for the two-dimensional (2D) (and by extension 3D) classical hydrodynamic model are formulated in [20], assuming subsonic flow at the inflow and outflow boundaries. In one dimension, the QHD model with heat conduction has two Schrödinger modes, one parabolic mode, and one elliptic mode. Thus eight boundary conditions are necessary. Well-posed boundary conditions for the resonant tunneling diode are $n = N_D$, $\partial n / \partial x = 0$, and $T = T_0$ at $x_{\min}$ and $x_{\max}$, with a bias ΔV across the device: $V(x_{\min}) = T \log(n/n_i)$ and $V(x_{\max}) = T \log(n/n_i) + e \Delta V$, where n_i is the intrinsic electron concentration.

5. The second upwind method for the 1D QHD model. In this section, the 1D steady-state QHD equations are discretized using an upwind method adapted from computational fluid dynamics.⁴ Since the upwind method requires velocity values $u_{-1/2}, u_{1/2}, u_{3/2}, \dots, u_{N-1/2}, u_{N+1/2}$ at the midpoints of the elements l_i ($i = 1, \dots, N$) connecting grid points $i-1$ and i , a staggered grid is used for u . (A computational Neumann boundary condition $du/dx = 0$ at $i = 0$ and $i = N$ is imposed to determine $u_{-1/2}$ and $u_{N+1/2}$.) Defining the velocities at midpoints of elements also resolves waves more sharply by avoiding the averaging of velocities defined at grid points i , $i \pm 1$ to obtain $u_{i-1/2}$ and $u_{i+1/2}$. The variables n , T , and V are defined at the grid points $i = 0, 1, \dots, N-1, N$. The boundary conditions specify n , dn/dx , T , and V at $i = 0$ and $i = N$. (The boundary conditions for dn/dx at $i = 0$ and $i = N$ specify values for n_{-1} and n_{N+1} that appear in the upwind discretization.)

In one dimension, the steady-state QHD model consists of the three nonlinear conservation laws for electron number, momentum, and energy, plus Poisson's equation

$$(48) \quad \begin{bmatrix} f_n \\ f_u \\ f_T \\ f_V \end{bmatrix} = \frac{d}{dx} \begin{bmatrix} ug_n \\ ug_u \\ ug_T \\ 0 \end{bmatrix} + \begin{bmatrix} 0 \\ h_u \\ h_T \\ h_V \end{bmatrix} + \begin{bmatrix} 0 \\ s_u \\ s_T \\ s_V \end{bmatrix} = 0,$$

⁴The second upwind method was applied to hydrodynamic model simulations of electron shock waves in submicron $n^+ - n - n^+$ devices in [10]–[12].

where

$$(49) \quad g_n = n,$$

$$(50) \quad g_u = mnu,$$

$$(51) \quad g_T = \frac{5}{2}nT + \frac{1}{2}mnu^2 - \frac{\hbar^2 n}{8m} \frac{d^2}{dx^2} \log(n) + nV,$$

$$(52) \quad h_u = \frac{d}{dx}(nT) - \frac{d}{dx} \left(\frac{\hbar^2 n}{12m} \frac{d^2}{dx^2} \log(n) \right) + n \frac{dV}{dx},$$

$$(53) \quad h_T = - \frac{d}{dx} \left(\kappa \frac{dT}{dx} \right),$$

$$(54) \quad h_V = \epsilon \frac{d^2 V}{dx^2},$$

$$(55) \quad s_u = \frac{mnu}{\tau_p},$$

$$(56) \quad s_T = \left(\frac{3}{2}nT + \frac{1}{2}mnu^2 - \frac{\hbar^2 n}{24m} \frac{d^2}{dx^2} \log(n) - \frac{3}{2}nT_0 \right) / \tau_w,$$

$$(57) \quad s_V = e^2(N_D - N_A - n).$$

Equations $f_n = 0$, $f_T = 0$, and $f_V = 0$ are enforced at the interior grid points $i = 1, \dots, N-1$, while equation $f_u = 0$ is enforced at the midpoints of the elements l_i , $i = 1, \dots, N$.

In the second upwind method,⁵ the advection terms $d(ug)/dx$ in (48) are discretized using second upwind differences

$$(58) \quad \frac{d}{dx}(ug)_i \approx (u_{i+1/2}g_R - u_{i-1/2}g_L)/\Delta x,$$

where

$$(59) \quad g_R = \begin{cases} g_i & (u_{i+1/2} > 0), \\ g_{i+1} & (u_{i+1/2} < 0), \end{cases} \quad g_L = \begin{cases} g_{i-1} & (u_{i-1/2} > 0), \\ g_i & (u_{i-1/2} < 0), \end{cases}$$

and second-order central differences are used for h_u , h_T , h_V , and s_T .

To linearize the discretized version of (48), we use Newton's method

$$(60) \quad J \begin{bmatrix} \delta n \\ \delta u \\ \delta T \\ \delta V \end{bmatrix} = - \begin{bmatrix} f_n \\ f_u \\ f_T \\ f_V \end{bmatrix} = -f, \quad \begin{bmatrix} n \\ u \\ T \\ V \end{bmatrix} \leftarrow \begin{bmatrix} n \\ u \\ T \\ V \end{bmatrix} + t \begin{bmatrix} \delta n \\ \delta u \\ \delta T \\ \delta V \end{bmatrix},$$

where J is the Jacobian and t is a damping factor [4] between 0 and 1, chosen to insure that the norm of the residual f decreases monotonically.

⁵The second upwind method is a conservative extension of the original first-order upwind method; see, e.g., [24].

6. QHD simulations of the resonant tunneling diode. The QHD model allows efficient simulation of the behavior of quantum devices that depend on particle tunneling through potential barriers and charge buildup in potential wells. Simulations of a GaAs resonant tunneling diode with double $\text{Al}_x\text{Ga}_{1-x}\text{As}$ barriers are presented here. The barrier height $\mathcal{B}$ is set equal to 0.209 eV (the Al mole fraction $x = 0.3$). The diode consists of n^+ source (at the left) and drain (at the right) regions with the doping density $N_D = 10^{18} \text{ cm}^{-3}$ and an n channel with $N_D = 5 \times 10^{15} \text{ cm}^{-3}$ (see Fig. 1). A hyperbolic tangent fitting is used for N_D over $\pm 50 \text{ \AA}$ at the junctions. The channel is $250 \text{ \AA}$ long as indicated by the vertical lines at $x = 0$ and $x = 0.025$ microns in Figs. 3, 4, 6, and 7; the barriers are $50 \text{ \AA}$ wide as indicated by the light gray bands in Figs. 1, 3, 4, 6, and 7; and the quantum well between the barriers is $50 \text{ \AA}$ wide. Note that the device has $50 \text{ \AA}$ spacers between the barriers and the contacts (source and drain).

The barrier height $\mathcal{B}$ is incorporated into the QHD transport equations (1)–(3) by replacing $V \rightarrow V + \mathcal{B}$. (Poisson's equation is not changed.)

We use modified Baccarani–Wordemann models [3], [12] for the classical momentum and energy relaxation times in the QHD model

$$(61) \quad \tau_p = \tau_{p0} \frac{T_0}{T},$$

$$(62) \quad \tau_w = \frac{\tau_p}{2} \left(1 + \frac{\frac{3}{2}T}{\frac{1}{2}mv_s^2} \right),$$

where the low-energy momentum relaxation time τ_{p0} is set equal to 0.9 ps from the low-field electron mobility in GaAs at 77 K. The low-field electron mobility μ_{n0} is related to τ_{p0} by $\tau_{p0} = m\mu_{n0}/e$, where $\mu_{n0} = 25,000 \text{ cm}^2/\text{Vs}$ (see [28] and [7]). The effective electron mass $m = 0.063m_e$, where m_e is the electron mass, and the saturation velocity $v_s \approx 2 \times 10^7 \text{ cm/s}$ for lower valley electrons in GaAs at 77 K. The dielectric constant $\epsilon = 12.9$ for GaAs.

Continuation in voltage ΔV was found to be necessary in generating the solutions: that is, to find the solution at $\Delta V = 0.1$ volts, for example, the solutions are

FIG. 1. Doping/ 10^{18} cm^{-3} .

generated at $\Delta V_1 = 0.001$ volts, $\Delta V_2 = 0.002$ volts, ..., at each stage using the previous solution at ΔV_j as the initial guess for the Newton method in computing the solution at ΔV_{j+1} . An algorithm for choosing the ΔV_j 's is used that attempts to maximize the voltage increments while keeping the number of Newton iterations small. Typical simulations on a grid with 250 Δx require 1–3 minutes of CPU time on a Sun SPARCstation 10.

Current-voltage curves for the resonant tunneling diode at 77 K are plotted in Fig. 2 for three different values of κ_0 in the Wiedemann–Franz expression for thermal conductivity

$$(63) \quad \mathbf{q} = -\kappa \nabla T, \quad \kappa = \kappa_0 \tau_{p0} n T_0 / m.$$

The region of negative differential resistance extends from the peak to the valley of the current-voltage curve. These are the first simulations of the full QHD equations to show NDR in the resonant tunneling diode.

The peak of the current-voltage curve occurs as the electrons tunneling through the first barrier come into resonance with the ground state of the quantum well. Note the presence of a “shoulder” in the current-voltage curve around $\Delta V = 0.25$ volts (cf. [29]). The shoulder signals the location of the first virtual state of the quantum well. The location of the peak and shoulder can be qualitatively understood from the energy levels of a square well. For an infinite well, $E_n = (n+1)^2 \pi^2 \hbar^2 / 2m x_0^2$, where x_0 is the width of the well and where n is a nonnegative integer. For a 50 Å wide GaAs infinite well, the ground state energy $E_0 = 0.24$ eV and the energy of the first excited state $E_1 = 0.96$ eV. For a 50 Å wide 0.209 eV high GaAs finite square well (see, e.g., Leighton [18]), there is just one bound state, and the energy level is shifted to $E_0 = 0.079$ eV. The energy of the first virtual state of the well is 0.24 eV.

Note that the main effect of larger values of κ_0 is to shift the peak of the current-voltage curve to the right. With lower values of κ_0 , the electrons have a

FIG. 2. Current density in kiloamps/cm² versus voltage for the resonant tunneling diode at 77 K. $\kappa_0 = 0.2$ (black), 0.4 (gray), and 0.6 (light gray). The dots represent computed solution points.

higher average energy as they impinge upon the first barrier, and therefore resonate with the well at a lower applied voltage.

A physically relevant value of κ_0 is approximately 0.4 for this device. The peak-to-valley current ratio of 1.95 agrees quantitatively with experimental ratios for similar devices (see, e.g., [21], [23]). In fact, for the device parameters of [23], the QHD code predicts a peak-to-valley current ratio of 2.65 (with $\kappa_0 = 1$), compared with the experimental value of approximately 2.5. The experimental (computational) peak occurs at $\Delta V = 0.18$ (0.11) volts, and the experimental (computational) valley occurs at $\Delta V = 0.35$ (0.30) volts.

Figures 3–7 illustrate the electron density, velocity, and temperature, and the conduction band energy in the resonant tunneling diode for $\kappa_0 = 0.4$. Figure 3 shows the dramatic charge enhancement in the quantum well typical of the resonant tunneling diode for applied voltages of $\Delta V = 0.097$ (peak), 0.191 (valley), and 0.22 volts (just before the shoulder). The electron density at the center of the quantum well increases as ΔV increases and is more than two orders of magnitude larger than the background doping density. Note the depletion of electrons around the channel-drain junction. Figure 4 presents the electron velocities for the same set of applied voltages. Of special note is the fact that the lowest velocity in the well occurs at the voltage ΔV_{valley} at which the current-voltage valley occurs. The electrons spend significantly more time in the quantum well (where the velocity is low) than in the barriers (where the velocity is high) [14].

As illustrated in Fig. 5, the electrons spend the longest time in the quantum well for voltages near ΔV_{valley} . The “dwell” time spent by electrons in the well increases monotonically up to voltages near ΔV_{valley} and then decreases rapidly. Note that the macroscopic QHD dwell time differs qualitatively from dwell times based on microscopic quantum calculations, which predict that the dwell time is maximum at resonance [5], [6], [16].

The electrons cool down to 0.14 ($\Delta V = 0.097$ volts) to 0.35 ($\Delta V = 0.22$ volts) times T_0 as they overcome the first $\text{Al}_x\text{Ga}_{1-x}\text{As}$ potential barrier (see Fig. 6). As the electrons are accelerated near the channel-drain junction, they heat up to 2 ($\Delta V = 0.097$ volts) to 3.5 ($\Delta V = 0.22$ volts) times T_0 and then cool back down to the lattice

FIG. 3. $\text{Log} (\text{Density}/10^{18} \text{ cm}^{-3})$. The curves are for $\Delta V = 0.097$ (light gray), 0.191 (gray), and 0.22 (black) volts.

FIG. 4. $\text{Log}(\text{Velocity}/10^8 \text{ cm/sec})$. The curves are for $\Delta V = 0.097$ (light gray), 0.191 (gray), and 0.22 (black) volts.

temperature in the drain. The conduction band energies $V + \mathcal{B}$ are illustrated in Fig. 7 and show substantial band bending in the well and barriers.

7. Conclusion. The QHD model offers several advantages over other methods for simulating quantum semiconductor devices. Although the Wigner function [17] or density matrix [8] methods for simulating the resonant tunneling diode include quantum effects to all orders in $\hbar$, the QHD method is much less computationally intensive and includes the same physics if the expansion parameter $\hbar^2/8mTl^2$ is small. The more complete quantum mechanical methods also have technical drawbacks: The density matrix has “off-diagonal” terms that are difficult to interpret physically and requires the computation of a set of eigenvalues and eigenfunctions,

FIG. 5. Time in picoseconds (dots) spent by electrons in the quantum well versus voltage. For reference, a scaled version of the current density (solid line) is also shown.

FIG. 6. Temperature in eV. The lattice temperature $T_0 = 77 \text{ K} = 0.0066 \text{ eV}$. The curves are for $\Delta V = 0.097$ (light gray), 0.191 (gray), and 0.22 (black) volts.

while the Wigner function method requires complicated initial conditions for simulations.

Since the QHD equations have the same form as the classical fluid dynamical equations, well-understood classical boundary conditions can be applied in simulating quantum devices. How to impose proper boundary conditions for full quantum mechanical approaches is still an open question (see [9]). Moreover, the QHD equations are expressed in terms of the fluid dynamical quantities density, velocity, and temperature. These classical fluid dynamical concepts enable us to interpret electron behavior in quantum devices in a physically intuitive way. We can define the time spent by an electron in the quantum well or the electron temperature throughout the device in a precise manner. In turn, the intuitive understanding developed through the QHD model sheds light on more fully quantum mechanical descriptions of electron behavior in quantum devices.

FIG. 7. Conduction band energy in eV. The curves are for $\Delta V = 0.097$ (light gray), 0.191 (gray), and 0.22 (black) volts.

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