Dispersive/Hyperbolic Hydrodynamic Models for Quantum Transport (in Semiconductor Devices)

Carl Gardner & Christian Ringhofer
Arizona State University

- “Smooth” quantum hydrodynamic (QHD) model
- Quantum Maxwellian–\(O(\beta V)\) solution to the Bloch eq.
  \[
  \beta = \frac{1}{T}
  \]
- Derivation of smooth QHD model from moment expansion of Wigner-Boltzmann eq.
- Derivation of “hybrid” QHD model (Chapman-Enskog)
- Numerical methods
- QHD simulations of RTDs
**Technological Problem:**

- Predict performance of submicron transistors & diodes
  \((\sim 5\text{ million/chip})\)

- Quantum tunneling devices (resonant tunneling diodes &
  transistors, HEMTs, MODFETs, superlattice devices)

- Advanced microelectronic applications including multiple-
  state logic & memory devices & high frequency oscillators
  & sensors

- Fundamental approach: Wigner-Boltzmann transport equa-
  tion, but \(f = f(x, p, t)\)

- Hydrodynamic approximation (electrogasdynamics):
  \(n, u, T = \text{functions of } x, t\)
• Smooth QHD model is based on a moment expansion of the Wigner-Boltzmann equation using an $O(\beta V)$ “quantum Maxwellian”

• Feynman: The 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.”

\[ V_{a^2}(x) = \int \frac{dy}{\sqrt{2\pi a^2}} \exp \left\{ -\frac{(x - y)^2}{2a^2} \right\} V(y), \quad a^2 \propto \beta \hbar^2 / m \]

• Smooth QHD model involves a smoothing of the classical potential over space & temperature

• Reproduces the original $O(\hbar^2)$ QHD model for

\[ \epsilon = \frac{\hbar^2 \beta}{ml^2} \ll 1 \]

& recovers classical electrogasdynamics for $\epsilon = 0$

• Possible applications in nuclear physics, superfluidity, & superconductivity

• QHD includes quantum transport effects like particle tunneling through potential barriers & particle buildup in quantum wells
Smooth QHD equations

\[ \frac{\partial n}{\partial t} + \frac{\partial}{\partial x_i}(n u_i) = 0 \]

\[ \frac{\partial}{\partial t}(m n u_j) + \frac{\partial}{\partial x_i}(m n u_i u_j - P_{ij}) = -\frac{n}{\partial x_j} \frac{\partial V}{\partial x_i} - \frac{m n u_j}{\tau_p} \]

\[ \frac{\partial W}{\partial t} + \frac{\partial}{\partial x_i}(u_i W - u_j P_{ij} + q_i) = -\frac{n}{\partial x_i} \frac{\partial V}{\partial x_i} - \frac{(W - W_0)}{\tau_w} \]

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

Stress tensor & energy density

\[ P_{ij} = -nT \delta_{ij} - \frac{\hbar^2 n}{4m T} \frac{\partial^2 V}{\partial x_i \partial x_j} \]

\[ W = \frac{3}{2} nT + \frac{1}{2} m n u^2 + \frac{\hbar^2 n}{8m T} \nabla^2 V \]

where the “quantum potential”

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

Note that

\[ V = V_B + V_P \]

\[ \mathbf{q} = -\kappa \nabla T - \frac{\hbar^2 n}{8m} \nabla^2 \mathbf{u} \quad \text{(Chapman – Enskog)} \]
\[ R = \frac{1}{2}(x + y), \quad s = x - y \]

**Phase space**

\[ f_W(x, p, t) = \int dp f_W(x, p, t) \]

\[ n(x, t) = \rho(R, s, t) \]

**Fourier transform**

\[ W(x, t) = \int dp \frac{p^2}{2m} f_W(x, p, t) \]

\[ W(x, t) = \lim_{s \to 0} \frac{1}{2m} \frac{p^2}{\partial s^2} \rho(R, s, t) \]

Maxwellian distribution function

\[ f_M(x, p) = C \exp \left\{ -\frac{\beta p^2}{2m} - \beta V(x) \right\} \]

\[ \rho_M(x, y) = C \exp \left\{ -\frac{m}{2\beta \hbar^2} (x - y)^2 - \beta V \left( \frac{x + y}{2} \right) \right\} \]
Figure 1: Classical Maxwellian for a 0.1 eV potential step for electrons in GaAs at 300 K.

Figure 2: Smooth quantum Maxwellian for a 0.1 eV potential step for electrons in GaAs at 300 K.
In thermal equilibrium, \( \rho \) satisfies the Bloch equation

\[
\frac{\partial \rho}{\partial \beta} = -\frac{1}{2}(H_x + H_y)\rho = \frac{\hbar^2}{4m} \left( \nabla_x^2 + \nabla_y^2 \right) \rho - \frac{1}{2} \left[ V(\mathbf{x}) + V(\mathbf{y}) \right] \rho
\]

where \( H_x = -\hbar^2 \nabla_x^2 / 2m + V(\mathbf{x}) \)

Green’s function for the Bloch equation (6D heat equation):

\[
G(\beta, \mathbf{x}, \mathbf{y}; \beta', \mathbf{x}', \mathbf{y}') = 
\left( \frac{m}{\pi(\beta - \beta')\hbar^2} \right)^3 \exp \left\{ -\frac{m}{(\beta - \beta')\hbar^2} \left[ (\mathbf{x} - \mathbf{x}')^2 + (\mathbf{y} - \mathbf{y}')^2 \right] \right\} \theta(\beta - \beta')
\]

Initial condition \( \rho(0, \mathbf{x}, \mathbf{y}) = \delta^{(3)}(\mathbf{x} - \mathbf{y}) \)

We obtain

\[
\rho(\beta, \mathbf{x}, \mathbf{y}) = \rho_0(\beta, \mathbf{x}, \mathbf{y}) - \frac{1}{2} \int_0^\beta d\beta' \int d^3x' d^3y' \left( \frac{m}{\pi(\beta - \beta')\hbar^2} \right)^3 \times 
\exp \left\{ -\frac{m}{(\beta - \beta')\hbar^2} \left[ (\mathbf{x} - \mathbf{x}')^2 + (\mathbf{y} - \mathbf{y}')^2 \right] \right\} \left[ V(\mathbf{x}') + V(\mathbf{y}') \right] \rho(\beta', \mathbf{x}', \mathbf{y}')
\]

where the free-particle (\( V = 0 \)) density matrix is

\[
\rho_0(\beta, \mathbf{x}, \mathbf{y}) = \left( \frac{m}{2\pi\beta\hbar^2} \right)^{3/2} \exp \left\{ -\frac{m}{2\beta\hbar^2}(\mathbf{x} - \mathbf{y})^2 \right\}
\]
Next solve for $\rho$ iteratively: set $\rho = \rho_0$ inside the integral to get

$$R = \frac{1}{2}(x + y), \quad s = x - y$$

$$\rho(\beta, R, s) \approx \left(\frac{m}{2\pi\beta\hbar^2}\right)^{3/2} \exp\left\{-\frac{m}{2\beta\hbar^2}s^2 - \beta \tilde{V}(\beta, R, s)\right\}$$

where

$$\tilde{V}(\beta, R, s) = \frac{1}{2\beta} \int_{0}^{\beta} d\beta' \int d^3X' \left(\frac{2m\beta}{\pi(\beta - \beta')(\beta + \beta')\hbar^2}\right)^{3/2} \times$$

$$\exp\left\{-\frac{2m\beta}{(\beta - \beta')(\beta + \beta')\hbar^2}X'^2\right\} \left[V\left(X' + R + \frac{\beta'}{2\beta}s\right) + V\left(X' + R - \frac{\beta'}{2\beta}s\right)\right]$$
Dynamic evolution of $\rho$ (including departures from thermal equilibrium) is governed by the Wigner-Boltzmann equation

$$i\hbar \frac{\partial \rho}{\partial t} + \frac{\hbar^2}{m} \nabla_R \cdot \nabla_s \rho =$$

$$\left[ V \left( R + \frac{S}{2} \right) - V \left( R - \frac{S}{2} \right) \right] \rho - i\hbar \frac{1}{\tau} S \cdot \nabla_s \rho - i\frac{m(2w_0/3)}{\hbar \tau} S^2 \rho$$

In $(x,p)$ space,

$$\langle \chi \rangle = \int d^3 p \chi(p)f_W(x,p)$$

In $(R,s)$ space,

$$\langle \chi \rangle = \lim_{s \to 0} \chi \left( \frac{\hbar}{i} \nabla_s \right) \rho(R,s)$$

which can be verified using

$$\rho(R,s) = \int d^3 p \ f_W(R,p)e^{ip \cdot s/\hbar}$$

The moment expansion is obtained by multiplying the Wigner-Boltzmann equation with powers of $\hbar \nabla_s / i$ ($1, \hbar \nabla_s / i, & -\hbar^2 \nabla_s^2 / 2m$) & taking the limit $s \to 0$:

$$\frac{\partial n}{\partial t} + \frac{1}{m} \frac{\partial \langle p_i \rangle}{\partial x_i} = 0$$

$$\frac{\partial \langle p_j \rangle}{\partial t} + \frac{\partial}{\partial x_i} \frac{\langle p_i p_j \rangle}{m} = -n \frac{\partial V}{\partial x_j} - \frac{\langle p_j \rangle}{\tau}$$

$$\frac{\partial}{\partial t} \langle \frac{p_i^2}{2m} \rangle + \frac{\partial}{\partial x_i} \langle \frac{p_i p_j}{2m^2} \rangle = -\frac{\langle p_i \rangle}{m} \frac{\partial V}{\partial x_i} - \frac{\langle p_i^2 / 2m \rangle}{\tau/2} - W_0$$
We now assume that the momentum-shifted
\[ p = m u + p' \]
effective \( \rho \) approximates the actual \( \rho \) well enough for average values in the conservation laws to approximate actual values.

Smooth QHD equations:

\[
\frac{\partial n}{\partial t} + \frac{\partial}{\partial x_i} (n u_i) = 0
\]

\[
\frac{\partial}{\partial t} (m n u_j) + \frac{\partial}{\partial x_i} (m n u_i u_j - P_{ij}) = -n \frac{\partial V}{\partial x_j} - \frac{m n u_j}{\tau_p}
\]

\[
\frac{\partial W}{\partial t} + \frac{\partial}{\partial x_i} (u_i W - u_j P_{ij} + q_i) = -n u_i \frac{\partial V}{\partial x_i} - \frac{(W - W_0)}{\tau_w}
\]

\[
P_{ij} = \lim_{s \to 0} \frac{\hbar^2}{m} \frac{\partial^2 \rho}{\partial s_i \partial s_j} \approx -n T \delta_{ij} - \frac{\hbar^2 n}{4 m T} \frac{\partial^2 \nabla}{\partial x_i \partial x_j}
\]

\[
W = \frac{1}{2} m n u^2 - \lim_{s \to 0} \frac{\hbar^2}{2 m} \nabla^2 \rho \approx \frac{3}{2} n T + \frac{1}{2} m n u^2 + \frac{\hbar^2 n}{8 m T} \nabla^2 \nabla
\]

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

\[
q = -\kappa \nabla T - \frac{\hbar^2 n}{8 m} \nabla^2 u \quad \text{(Chapman – Enskog)}
\]
Figure 3: Smooth effective potential for electrons in GaAs for 50 Å wide unit potential double barriers & 50 Å wide well as a function of $x \& \log_{10}(T/300 \text{ K})$. 
\( O(\hbar^2) \) QHD Model

\[
\bar{V} = \frac{1}{3} V + O(\hbar^2)
\]

\[
P_{ij} = -nT\delta_{ij} - \frac{\hbar^2 n}{4mT} \frac{\partial^2 \nabla}{\partial x_i \partial x_j} \approx -nT\delta_{ij} - \frac{\hbar^2 n}{12mT} \frac{\partial^2 V}{\partial x_i \partial x_j}
\]

\[
W \approx \frac{3}{2} nT + \frac{1}{2} mnu^2 + \frac{\hbar^2 n}{24mT} \nabla^2 V
\]

Use (?) classical thermal equilibrium relation

\[
n \propto \exp(-\beta V)
\]

\[
P_{ij} \approx -nT\delta_{ij} + \frac{\hbar^2 n}{12m} \frac{\partial^2 \ln(n)}{\partial x_i \partial x_j}
\]

\[
W \approx \frac{3}{2} nT + \frac{1}{2} mnu^2 - \frac{\hbar^2 n}{24m} \nabla^2 \ln(n)
\]
Problems with the $O(\hbar^2)$ model

- Dispersive Schrödinger modes
- I-V curves wrong shape near $V = 0$
- Too sensitive to amount of heat conduction (true also for smooth & hybrid QHD models)
Hybrid QHD Model

(Hybrid model can be derived directly from a Chapman-Enskog expansion)

\[ \rho(\beta, \mathbf{R}, \mathbf{s}) \sim \exp\left\{-\frac{m}{2\beta\hbar^2} \mathbf{s}^2 - \beta \tilde{V}(\beta, \mathbf{R}, \mathbf{s})\right\} \]

\[ n \sim \exp\{-\beta(V_P + \tilde{V}_B)\} \]

\[ -\beta V_P \approx \ln(n) + \beta \tilde{V}_B + \text{const} \]

Now using

\[ V = V_B + V_P, \quad \nabla P = \frac{1}{3} V_P + O(\hbar^2) \]

we get

\[ P_{ij} = -nT \delta_{ij} - \frac{\hbar^2 n}{4mT} \frac{\partial^2 V}{\partial x_i \partial x_j} \approx -nT \delta_{ij} - \frac{\hbar^2 n}{12mT} \frac{\partial^2 V_P}{\partial x_i \partial x_j} - \frac{\hbar^2 n}{4mT} \frac{\partial^2 \tilde{V}_B}{\partial x_i \partial x_j} \]

\[ \approx -nT \delta_{ij} + \frac{\hbar^2 n}{12m} \frac{\partial^2 \ln(n)}{\partial x_i \partial x_j} - \frac{\hbar^2 n}{4mT} \frac{\partial^2 \tilde{B}}{\partial x_i \partial x_j} \]

\[ W \approx \frac{3}{2} nT + \frac{1}{2} mnu^2 - \frac{\hbar^2 n}{24m} \nabla^2 \ln(n) + \frac{\hbar^2 n}{8mT} \nabla^2 \tilde{B} \]

where the smoothed barrier potential is

\[ B(\beta, \mathbf{x}) = \int_0^\beta \frac{d\beta'}{\beta} \left\{ \left( \frac{\beta'}{\beta} \right)^2 - \frac{1}{3} \right\} \int d^3 x' \left( \frac{2m\beta}{\pi(\beta - \beta')(\beta + \beta')\hbar^2} \right)^{3/2} \times \]

\[ \exp \left\{ -\frac{2m\beta}{(\beta - \beta')(\beta + \beta')\hbar^2} (\mathbf{x}' - \mathbf{x})^2 \right\} B(\mathbf{x}') \]
**Conservative Upwind Numerical Methods**

<table>
<thead>
<tr>
<th>method</th>
<th>type</th>
<th>CHD</th>
<th>$O(h^2)$ QHD</th>
<th>smooth/hybrid QHD</th>
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* with Fatemi, Jerome, Osher, Shu  
† with Chen, Cockburn, Jerome  
‡ LeVeque’s code, with Hernandez

Smooth QHD & CHD models: hyperbolic + parabolic (heat conduction) + elliptic (Poisson eq.)

$O(h^2)$ & hybrid QHD models: hyperbolic + Schrödinger + parabolic (heat conduction) + elliptic (Poisson eq.)
Figure 4: Current density in kiloamps/cm² vs. voltage comparing the $O(\hbar^2)$ (green), smooth (blue), & hybrid (red) QHD models for the RTD at 300 K. The barrier height is 0.1 eV.

Figure 5: Current density in kiloamps/cm² vs. voltage for the smooth QHD model with various amounts of heat conduction for the RTD at 300 K. $\kappa_0 = 1$ (red), 0.8 (cyan), 0.6 (blue), & 0.4 (violet). The barrier height is 280 meV.
Figure 6: Current density in kiloamps/cm² vs. voltage comparing the smooth QHD (blue), $O(h^2)$ QHD (heavy blue), & (one band one effective mass) NEMO (magenta) models for the RTD at 300 K. $\kappa_0 = 0.6$ for the QHD models. The barrier height is 280 meV.

Figure 7: Current density in kiloamps/cm² vs. voltage for various amounts of heat conduction for the classical $n^+/n/n^+$ diode at 300 K. $\kappa_0 = 2$ (red), 1 (blue), & 0.5 (violet).
Figure 8: Smooth effective potential $U$ in eV for applied voltages between 0 & 400 millivolts for 280 meV double barriers at 300 K. $x$ is in Å.

**Future Work**

- Comparison of smooth & $O(\hbar^2)$ QHD simulations of RTDs with simulations of Wigner-Boltzmann equation
- How many moments are needed for good agreement?
- 2D simulation & analysis of quantum transistors