Resonant Tunneling in the Quantum Hydrodynamic Model

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The phenomenon of resonant tunneling is simulated and analyzed in the quantum hydrodynamic (QHD) model for semiconductor devices. Simulations of a parabolic well resonant tunneling diode at 77 K are presented which show multiple regions of negative differential resistance (NDR) in the current-voltage curve. These are the first simulations of the QHD equations to show multiple regions of NDR.

Resonant tunneling (and NDR) depend on the quantum interference of electron wavefunctions and therefore on the phases of the wavefunctions. An analysis of the QHD equations using a moment expansion of the Wigner-Boltzmann equation indicates how phase information is retained in the hydrodynamic equations.

Key Words: quantum hydrodynamic model, resonant tunneling diode.

1. INTRODUCTION

Resonant tunneling of electrons in quantum semiconductor devices can be modeled by adding quantum corrections to the classical hydrodynamic equations. The leading $O(\hbar^2)$ quantum corrections include the effects of particle tunneling through potential barriers and particle buildup in potential wells.

I will present simulations of a GaAs/Al$_x$Ga$_{1-x}$As parabolic well resonant tunneling diode at 77 K using the quantum hydrodynamic (QHD) equations. The QHD simulations show multiple regions of negative differential resistance (NDR) in the current-voltage curve. These are the first simulations of the QHD equations to show multiple regions of NDR.

Resonances in the current-voltage curve of the resonant tunneling diode occur as electrons tunnel coherently or sequentially through the double barriers. Sequential tunneling occurs if electrons tunnel through the first barrier, undergo scattering, and then tunnel through the second barrier. Coherent tunneling may be interpreted as the constructive interference of multiply reflected electron waves within the well. Resonant tunneling in actual devices usually involves a mixture of coherent and sequential tunneling. Scattering broadens the resonances and reduces the peak to valley ratios in the current-voltage curve. In this investigation, I will present two sets of simulations of the resonant tunneling diode: in the first set, scattering takes place throughout the device, while in the second set the collision terms in the QHD model are set to zero in the barriers and the well, to insure that the electron tunneling is coherent.

Coherent resonant tunneling and negative differential resistance depend on the quantum interference of electron wavefunctions, and therefore on the phases of the wavefunctions. I will indicate how phase information is retained in the hydrodynamic equations through an analysis of the QHD equations using a moment expansion of the Wigner-Boltzmann equation.

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2. THE QUANTUM HYDRODYNAMIC MODEL

The QHD equations have the same structure [1] as the classical hydrodynamic equations:

\[ \frac{\partial n}{\partial t} + \frac{1}{m} \frac{\partial \Pi_i}{\partial x_i} = 0 \]  
\[ \frac{\partial \Pi_i}{\partial t} + \frac{\partial}{\partial x_i} \left( u_i \Pi_j - P_{ij} \right) = -n \frac{\partial V}{\partial x_j} - \frac{\Pi_j}{\tau_p} \]  
\[ \frac{\partial W}{\partial t} + \frac{\partial}{\partial x_i} (u_i W - u_j P_{ij} + q_i) = - \frac{\Pi_i}{m} \frac{\partial V}{\partial x_i} - \frac{W - \frac{3}{2} n T_0}{\tau_w} \]  
\[ \nabla \cdot (e \nabla V) = e^2 (N_D - N_A - n) \]  

where \( n \) is the electron density, \( m \) is the effective electron mass, \( \Pi_i \) is the momentum density, \( u \) is the velocity, \( P_{ij} \) is the stress tensor, \( V = -e \phi \) is the potential energy, \( \phi \) is the electric potential, \( e > 0 \) is the electronic charge, \( W \) is the energy density, \( q \) is the heat flux, \( \tau_p \) and \( \tau_w \) are the momentum and energy relaxation times, respectively. The heat flux is specified here by Fourier's law \( q = -K \nabla T \), where \( T \) is the electron temperature.

The quantum corrections to the classical hydrodynamic equations appear in the stress tensor and the energy density. As \( \hbar \to 0 \), the quantum corrections can be developed in a power series in \( \hbar^2 \). The actual expansion parameter is \( \hbar^2/8m\Pi^2 \), where \( l \) is a characteristic length scale of the problem [2, 3]. For the resonant tunneling diode in section 3 with \( T \approx T_0 = 77 \text{ K} \) and \( l = 100 \text{ Å} \), the expansion parameter is approximately 0.23.

In Ref. [1], I showed that for the \( O(\hbar^2) \) momentum-shifted thermal equilibrium Wigner distribution function, the momentum density is given by

\[ \Pi_i = mn u_i \]  

3. SIMULATIONS OF MULTIPLE RESONANCES

I will simulate a GaAs resonant tunneling diode with double Al_{0.8}Ga_{0.2}As barriers and a parabolic Al\(_x\)Ga\(_{1-x}\)As quantum well. The diode consists of an \( n^+ \) source (at the left), an \( n \) channel, and an \( n^- \) drain (at the right). The doping density \( N_{D} = 10^{16} \text{ cm}^{-3} \) in the \( n^+ \) source and drain, and \( N_{D} = 5 \times 10^{15} \text{ cm}^{-3} \) in the \( n \) channel (see Figure 1). The channel is 500 Å long, the barriers are 30 Å wide, and the well between the barriers is 300 Å wide. The device has 70 Å spacers between the barriers and the contacts (source and drain) to enhance NDR. The barrier height is set equal to 0.7 eV. In the well, the Al mole fraction \( X \) varies between 0.8 and 0, so that the potential barrier height in the well is (see Figure 2)

\[ \mathcal{B}_{\text{well}} = 0.7 \text{ eV} \left[ x - \frac{1}{2} (x_L + x_R) \right]^2 \]  

where \( x_L \) and \( x_R \) are the coordinates of the left and right edges of the well. The left edge of the first barrier and the right edge of the second barrier are modeled as step functions. (Computationally the step function goes from 0 to 1 over one \( \Delta x \).)
For the classical momentum and energy relaxation times, I use modified Baccarani-Wordemann models:

\[ \tau_p = \tau_{p0} \frac{T_0}{T} \]  \hspace{1cm} (9)

\[ \tau_w = \frac{\tau_p}{2} \left(1 + \frac{3}{2} \frac{T}{m_w^2} \right) \]  \hspace{1cm} (10)

where the low-energy momentum relaxation time \( \tau_{p0} \) is set equal to 0.9 picoseconds from the low-field electron mobility in GaAs at 77 K. For lower valley electrons in GaAs at 77 K, the effective electron mass \( m = 0.063 \ m_e \), where \( m_e \) is the electron mass, and the saturation velocity \( v_s \approx 2 \times 10^7 \) cm/s. I set \( \kappa_0 = 0.4 \) in the Wiedemann-Franz formula for thermal conductivity

\[ q = -\kappa \nabla T, \quad \kappa = \kappa_0 \tau_{p0} n T_0 / m. \]  \hspace{1cm} (11)

The dielectric constant \( \varepsilon = 12.9 \) for GaAs.

I discretize the 1D steady-state QHD equations using the second upwind method and compute the solution using a damped Newton method (see Ref. [1] for details). The barrier height \( \Phi \) is incorporated into the QHD transport equations (1)–(3) by replacing \( V \rightarrow V + \Phi \). Poisson's equation is not changed.

The current voltage curve for the resonant tunneling diode at 77 K is plotted in Figure 3, using a grid.
with 300 $\Delta x$. For these simulations, scattering takes place throughout the device. There are seven resonances and seven regions of negative differential resistance in the current-voltage curve between 0 and 0.5 volts.

Figure 4 presents the current-voltage curve for the same device with the classical collision terms in the momentum and energy equations (2) and (3) turned off in the barriers and the well. Electron tunneling in this case must be purely coherent rather than sequential plus coherent, since there is no scattering in the well or barriers. There are twelve resonances and seven regions of negative differential resistance in the current-voltage curve between 0 and 1 volt.

Note that there are five resonant “shoulders” in the current-voltage curve between 0 and 0.33 volts, and that the sixth through twelfth resonances become more pronounced as $V$ increases. Ref. [7] explains this effect, which was observed in an experimental device: Below 0.33 volts, electrons tunnel out of the well through the thick portion of the parabolic well in Figure 2, and the transmission resonance widths are small. As the voltage bias increases above 0.33 volts, the transmission resonance widths rapidly increase because (i) the right barrier height is progressively reduced and (ii) electrons tunnel out of the well through the thin portion of the parabolic well.

The resonant peaks of the current-voltage curve occur as the electrons tunneling through the first barrier come into resonance with the energy levels of the quantum well. The locations of the resonances can be qualitatively understood from the
energy levels of an infinite parabolic well. For an
infinite well,
\[ E_\lambda = \left( \lambda + \frac{1}{2} \right) \hbar \sqrt{\frac{8E}{m_0^2}} \approx \left( \lambda + \frac{1}{2} \right) 0.087 \text{ eV} \quad (12) \]
where \( x_0 = 300 \text{ Å} \) is the width of the finite well and \( \lambda \) is a non-negative integer. The energy levels of the
infinite parabolic well are linearly spaced in \( \lambda \) with
a spacing of 87 meV, compared with the linear
spacings of approximately 70 mV (with scattering
throughout the device) and 100 mV (with scattering
turned off in the barriers and the well) for the
computed peaks in the current-voltage curves. The
first peak with scattering throughout the device oc-
curs at 0.030 volts, compared with \( E_0 = 0.044 \text{ eV} \).

The overall shape of the current-voltage curve in
Figure 3—the rise to a peak at 0.11 volts and the
fall to the valley at 0.58—is determined by the
negative differential resistance of a 0.7 eV high
double barrier square well with an effective width of
approximately 75 Å. The energy levels of the
parabolic well modulate this basic shape.

The time spent by electronics in the well is shown
in Figure 5. The “dwell” time has relative maxima at
voltages corresponding to valleys (relative minima)
of the current-voltage curve. The absolute maximum
of the dwell time occurs at the global valley of the
current-voltage curve at 0.58 volts; the dwell time
subsequently decreases rapidly toward zero (Cf. Ref.
[1], Figure 5). The dwell time mimics \( 1/|j| \), where
\( j = -enu \) is the current density, since the peak
electron density in the well increases monotonically
with applied voltage. Microscopic quantum calcula-
tions predict that the electron dwell time is maxi-
mum at resonance. The QHD model presents a
different “macroscopic” interpretation of the dwell
time (see the discussion in Ref. [1]).

4. PHASE INFORMATION
IN THE QHD MODEL

The computations of multiple resonances and re-
gions of negative differential resistance naturally
raise the question: how do the hydrodynamic equa-
tions, expressed in terms of macroscopic variables \( n, u, \) and \( T \), “know” about quantum interference, which
depends on the microscopic phases of the electron
wavefunctions? By analyzing the first three moments
of the Wigner-Boltzmann equation, I will show how
the phases of the electron wavefunctions are present
in the hydrodynamic equations.

For a mixed quantum mechanical state described
by wavefunctions \( \psi_\lambda(x, t)(\lambda = 1, 2, \ldots) \) with occupa-
tion numbers \( a_\lambda \), the Wigner distribution function is
defined as
\[
\begin{align*}
  f_w(x, p, t) = (\pi \hbar)^{-3} & \sum_\lambda a_\lambda \int d^3y \\
  & \times \psi_\lambda^*(x + y, t) \psi_\lambda(x - y, t) e^{2ip\cdot y/\hbar}.
\end{align*}
\]
(13)
The sum of the occupation numbers \( \sum_\lambda a_\lambda = M \),
where \( M \) is the total number of electrons in the
system. In general the \( a_\lambda \)'s may vary slowly with \( x \)
and \( t \). For the purposes of the derivation below, I
will assume the $a_{\lambda}$'s are constant. (For a mixed state in thermal equilibrium with a heat bath at temperature $T = 1/\beta, a_{\lambda} \propto e^{-BE_{\lambda}}$.) I will normalize the wavefunctions so that $\int d^3x \psi_{\lambda}^* \psi_{\lambda} = 1$.

I will assume that the electron flow can be approximated by a single-particle effective mass Schrödinger equation with a self-consistent many-body field:

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

where the wavefunctions have energies $E_{\lambda}$ and $V(x)$ is the self-consistent potential energy. In the effective mass approximation, Schrödinger's equation with the free electron mass and the total potential energy (the periodic potential energy of the semiconductor lattice plus $V$) is rewritten with the total potential energy replaced by $V$ and the electron mass replaced by the effective electron mass.

The local average value of an observable $X$ is defined in the Wigner formalism as

$$\langle X(x,t) \rangle = \int d^3p \chi(x,p,t) \phi(w(x,p,t)).$$

The first three moments of the Wigner-Boltzmann equation are obtained [8, 1] by setting $X$ equal to 1, $p$, and $p^2/2m$:

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

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

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

where

$$\langle p_i \rangle = \Pi_i$$

$$\left( \frac{p_i p_j}{m} \right) = u_{ij} \Pi - P_{ij}$$

$$\langle \frac{p^2}{2m} \rangle = W$$

$$\left( \frac{p_i p^2}{2m^2} \right) = u_{ij} W - u_{ij} p_{ij} + q_{ij}$$

define $\Pi_i, P_{ij}, W,$ and $q$. The quantum conservation laws have the same form as their classical counterparts. Explicit factors of $\hbar$ enter only at the fourth and higher moments.

To calculate the average values in the first three moment equations, in Ref. [1] I used the momentum-shifted version of the $O(\hbar^2)$ thermal equilibrium solution [4] to the Wigner-Boltzmann equation. The momentum-shifted $O(\hbar^2)$ $\phi(w)$ need only approximate the actual Wigner distribution function closely enough for the average values in Eqs. (16)–(18) to be close to the actual values. Using this approach, I derived the three-dimensional QHD equations (1)–(3) with $\Pi_i, P_{ij}$, and $W$ given by Eqs. (5)–(7).

Since here I am concerned with how phases appear in the QHD equations, I will instead evaluate average values by writing the wavefunction $\psi_{\lambda}$ in terms of its magnitude $A_{\lambda}$ and phase $\theta_{\lambda}$:

$$\psi_{\lambda}(x,t) = A_{\lambda}(x,t) e^{i\theta_{\lambda}(x,t)}.$$
where I have integrated by parts and where the velocity $u_\lambda$ is defined by

$$u_\lambda = \frac{\hbar}{m} \nabla \theta_\lambda. \quad (26)$$

This definition agrees with the standard expression for the semiclassical momentum $p_\lambda = mu_\lambda = \hbar \nabla \theta_\lambda$ of an electron in state $\lambda$. Next I calculate

$$\langle \frac{p_i p_j}{m} \rangle = u_i \Pi_j - P_{ij} = \int d^3p \frac{p_i p_j}{m} f_w(x, p, t)$$

$$= -\frac{\hbar^2}{4m} \sum_\lambda a_\lambda \int \frac{d^3p}{(\pi \hbar)^3} d^3y \, e^{i p \cdot y / \hbar} \times \frac{\partial^2}{\partial y_i \partial y_j} \left\{ A_\lambda(x + y) A_\lambda(x - y) + i e^{-i \theta(x+y)+i \theta(x-y)} \right\}$$

$$= \hbar^2 \sum_\lambda a_\lambda \left[ (\nabla A_\lambda)^2 - A_\lambda \nabla^2 A_\lambda + 2 A_\lambda^2 (\nabla \theta_\lambda)^2 \right]$$

$$= \sum_\lambda \frac{1}{2} m n_\lambda u_\lambda^2 - \frac{\hbar^2}{8m} \sum_\lambda n_\lambda \nabla^2 \log(n_\lambda). \quad (27)$$

From Eq. (27), the energy density equals

$$\langle \frac{p^2}{2m} \rangle = W =$$

$$= \frac{\hbar^2}{4m} \sum_\lambda a_\lambda \left[ (\nabla A_\lambda)^2 - A_\lambda \nabla^2 A_\lambda + 2 A_\lambda^2 (\nabla \theta_\lambda)^2 \right]$$

$$= \sum_\lambda \frac{1}{2} m n_\lambda u_\lambda^2 - \frac{\hbar^2}{8m} \sum_\lambda n_\lambda \nabla^2 \log(n_\lambda). \quad (28)$$

Finally

$$\langle \frac{p_i p_j}{2m^2} \rangle = u_i W - u_j P_{ij} + q_i = \int d^3p \frac{p_i p_j}{2m^2} f_w(x, p, t)$$

$$= -\frac{\hbar^3}{16m^2} \sum_\lambda a_\lambda \int \frac{d^3p}{(\pi \hbar)^3} d^3y \, e^{i p \cdot y / \hbar} \times \frac{\partial^3}{\partial y_i \partial y_j^2} \left\{ A_\lambda(x + y) A_\lambda(x - y) + i e^{-i \theta(x+y)+i \theta(x-y)} \right\}$$

$$= \frac{\hbar^3}{8m^2} \sum_\lambda a_\lambda \left[ 2((\nabla A_\lambda)^2 - A_\lambda \nabla^2 A_\lambda) \nabla \theta_\lambda \right.$$}

$$\left. + 4((\nabla A_\lambda) \nabla A_\lambda - A_\lambda \nabla \nabla_A_\lambda) \cdot \nabla \theta_\lambda + A_\lambda^2 (4(\nabla \theta_\lambda)^2 \nabla \theta_\lambda - \nabla \nabla^2 \theta_\lambda) \right]$$

$$= \sum_\lambda \frac{1}{2} m n_\lambda u_\lambda^2$$

$$- \frac{\hbar^2}{8m} \sum_\lambda u_\lambda n_\lambda \nabla^2 \log(n_\lambda)$$

$$- \frac{\hbar^2}{4m} \sum_\lambda u_\lambda n_\lambda \nabla \log(n_\lambda)$$

$$- \frac{\hbar^2}{8m} \sum_\lambda n_\lambda \nabla^2 u_\lambda. \quad (29)$$

The results in Eqs. (24)-(29) are exact, and do not involve an expansion in $\hbar$. However the moment equations (16)-(18) with expressions (24)-(29) do not form a closed set of equations in terms of hydrodynamic state variables (say $n$, $u$ and $T$ or $n_\lambda$, $\Pi_\lambda$, and $W$). Note that although the only explicit occurrence of $\hbar$ is $\hbar^2$, the sums over $\lambda$ will in general involve a functional dependence on $\hbar$.

Spatial derivatives of the wavefunction phases $\theta_\lambda(x, t)$ appear in the expressions for $\Pi_\lambda$, $P_{ij}$, $W$, and $q$ through $u_\lambda$. Only partial phase information is contained in the first three moment equations, since the fluid dynamical quantities (25) and (27)-(29) involve weighted sums of spatial derivatives of $\theta_\lambda$.

To make further progress, define

$$u_\lambda = u + \tilde{u}_\lambda$$

where $u$ is the macroscopic fluid velocity and $\tilde{u}$ is the velocity with respect to the macroscopic fluid flow. I will assume that the $\tilde{u}_\lambda$ are random, i.e., that

$$\sum_\lambda n_\lambda \tilde{u}_\lambda = 0 \quad (31)$$

and that the temperature is defined to leading order by the average of the microscopic kinetic energies of motion relative to the macroscopic fluid flow:

$$\sum_\lambda n_\lambda \frac{1}{2} m \tilde{u}_\lambda^2 = \frac{3}{2} nT + O(\hbar^2). \quad (32)$$
Then I obtain

$$\Pi_i = \sum_\lambda m n_\lambda (u_i + \bar{u}_\lambda) = m n_i$$  \hspace{1cm} (33)

$$W = \sum_\lambda \frac{1}{2} m n_\lambda (u_i + \bar{u}_\lambda)^2 - \frac{\hbar^2}{8m} \sum_\lambda n_\lambda \nabla^2 \log(n_\lambda)$$

$$= \frac{1}{2} m n u^2 + \frac{3}{2} n T - \frac{\hbar^2}{8m} \sum_\lambda n_\lambda \nabla^2 \log(n_\lambda) + O(\hbar^2)$$  \hspace{1cm} (34)

$$P_{ij} = u_i \Pi_j - \sum_\lambda (u_i + \bar{u}_\lambda) m n_\lambda (u_j + \bar{u}_\lambda)$$

$$+ \frac{\hbar^2}{4m} \sum_\lambda n_\lambda \nabla_i \nabla_j \log(n_\lambda)$$

$$= - \sum_\lambda \bar{u}_\lambda m n_\lambda \bar{u}_\lambda + \frac{\hbar^2}{4m} \sum_\lambda n_\lambda \nabla_i \nabla_j \log(n_\lambda)$$

$$= - \delta_{ij} n T + \frac{\hbar^2}{4m} \sum_\lambda n_\lambda \nabla_i \nabla_j \log(n_\lambda) + O(\hbar^2)$$  \hspace{1cm} (35)

$$\mathbf{q} = \sum_\lambda \bar{u}_\lambda \frac{1}{2} m n_\lambda \bar{u}_\lambda^2 - \frac{\hbar^2}{8m} \nabla^2 \mathbf{u}$$

$$= - \kappa \nabla T - \frac{\hbar^2 n}{8m} \nabla^2 \mathbf{u} + O(\hbar^2).$$  \hspace{1cm} (36)

Eq. (35) follows if the Wigner distribution function in the classical limit $\hbar = 0$ is a momentum-shifted Maxwell-Boltzmann distribution (see e.g. Ref. [9], pp. 99–100). In writing the last equation, I have assumed that

$$\sum_\lambda \bar{u}_\lambda n_\lambda \nabla^2 \log(n_\lambda) = 0,$$

$$\sum_\lambda \bar{u}_\lambda n_\lambda \nabla \nabla_j \log(n_\lambda) = 0,$$

$$\sum_\lambda n_\lambda \nabla \bar{u}_\lambda = 0.$$  \hspace{1cm} (37)

The classical heat flux vanishes if the distribution function is a momentum-shifted Maxwell-Boltzmann distribution. The Fourier term $-\kappa \nabla T$ in Eq. (36) is obtained if the Wigner distribution function in the classical limit is the momentum-shifted Maxwell-Boltzmann distribution plus the first-order Chapman-Enskog correction (see Ref. [9], pp. 99–100 and 103–106). Note that I have not used the quantum correction to the heat flux in the simulations presented here.

Even with these simplifications and with $\mathbf{q} = -\kappa \nabla T$, the moment equations (16)–(18) with expressions (24) and (33)–(35) do not form a closed set of equations in terms of hydrodynamic state variables, due to the quantum terms in $P_{ij}$ and $W$.

The quantum terms in the stress tensor and the energy density were evaluated in Ref. [1] to leading order in $\hbar^2$ by Eqs. (6) and (7). Then the moment equations (16)–(18) do form a closed set in terms of hydrodynamic state variables (say $n$, $\mathbf{u}$, and $T$).

The moment equations simplify to a great extent for a pure quantum mechanical state, in which all the $a_i$’s except one (say $a_1$) vanish, and $a_1 = 1$. For the pure state,

$$n = A^2$$  \hspace{1cm} (38)

$$\mathbf{u} = \frac{\hbar}{m} \nabla \theta$$  \hspace{1cm} (39)

$$P_{ij} = -\frac{\hbar^2}{2m} \left[ \nabla_i A \nabla_j A - A \nabla_i \nabla_j A \right]$$

$$= \frac{\hbar^2 n}{4m} \nabla \nabla_j \log(n)$$  \hspace{1cm} (40)

$$W = \frac{\hbar^2}{4m} \left[ (\nabla A)^2 - A \nabla^2 A \right] + \frac{\hbar^2}{2m} A^2 \{\nabla \theta\}^2$$

$$= \frac{1}{2} m n u^2 - \frac{\hbar^2 n}{8m} \nabla^2 \log(n)$$  \hspace{1cm} (41)

$$\mathbf{q} = -\frac{\hbar^3}{8m^2} A^2 \nabla \nabla \theta = -\frac{\hbar^2 n}{8m} \nabla^2 \mathbf{u}. \hspace{1cm} (42)$$

The expression (42) for $\mathbf{q}$ is written down in Ref. [10], but within a different interpretational framework.

In this case, the moment equations (16)–(18) with expressions (25) and (40)–(42) form a closed set in terms of hydrodynamic state variables $n$ and $\mathbf{u}$. Eqs.
(16)-(18) become

$$\frac{\partial n}{\partial t} + \frac{\partial}{\partial x_i}(nu_i) = 0 \quad (43)$$

$$\frac{\partial}{\partial t}(mnui) + \frac{\partial}{\partial x_i}\left(u_imnui - \frac{\hbar^2 n}{4m} \frac{\partial^2}{\partial x_i \partial x_j} \log(n)\right)$$

$$= -n \frac{\partial V}{\partial x_j} \quad (44)$$

$$\frac{\partial}{\partial t}\left(\frac{1}{2} mnui^2 - \frac{\hbar^2 n}{8m} \nabla^2 \log(n)\right)$$

$$+ \frac{\partial}{\partial x_i}\left[u_j\left(\frac{1}{2} mnui^2 - \frac{\hbar^2 n}{8m} \nabla^2 \log(n)\right) - \frac{\hbar^2 n}{4m} \frac{\partial}{\partial x_i \partial x_j} \log(n)\right]$$

$$= -nu_i \frac{\partial V}{\partial x_i} \quad (45)$$

Note that $T = 0$ for the pure state and that the conservation of energy equation (45) follows from the equations for conservation of particles (43) and momentum (44).

For the pure state, then, we have the “hydrodynamic” formulation (see e.g. [11]) of the quantum mechanics of a pure state:

$$\frac{\partial n}{\partial t} + \nabla \cdot (nu) = 0 \quad (46)$$

$$\frac{Du}{m} = -\nabla(V + Q) \quad (47)$$

where the advective derivative $D/Dt = \partial/\partial t + u \cdot \nabla$ and the quantum potential is defined by

$$Q = -\frac{\hbar^2}{2m} \frac{1}{\sqrt{n}} \nabla^2 \sqrt{n} \quad (48)$$

Eqs. (46) and (47) are exact, and follow directly from Schrödinger’s equation.

The reader may check that

$$n(x,t) = \begin{cases} C_1 \exp\left(\frac{1}{\sqrt{2m}}(U - E) x\right) & x < -a \\ C_2 \cos^2\left(\frac{\sqrt{2mE}}{x + \lambda \pi/2}\right) & -a < x < a \\ (-1)^\lambda C_1 \exp\left(-2\sqrt{2m(U - E)} x\right) & x > a \end{cases}$$

is a solution to the “hydrodynamic” equations (46) and (47) for the 1D finite square potential well

$$u(x,t) = 0 \quad (49)$$

and reproduces the bound-state solutions for $\psi(x,t)$ for $0 < E_\lambda < U$, where $E_\lambda(\lambda = 0, 1, 2, \ldots)$ is the energy of the particle (see e.g. Ref. [12], pp. 152–155). The solution in the square well may be thought of as resulting from the interference of a right moving and a left moving wave. In an analogous but more complicated way, the full quantum hydrodynamic equations “sense” the width of the quantum well in the resonant tunneling diode.

5. CONCLUSION

The macroscopic quantum hydrodynamic equations are capable of modeling effects in quantum semiconductor devices that depend on quantum interference. The interference effects appear in the hydrodynamic expressions for the velocity, stress tensor, energy density, and heat flux through sums involving the semiclassical velocities $u_i = \hbar \nabla \theta_i / m$.

The QHD simulations of multiple resonances and multiple regions of NDR in the parabolic well resonant tunneling diode clearly demonstrate the effects of quantum interference and present an intuitive macroscopic picture of electron dwell times in the quantum well.
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References


Biographies

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