Electron Vorticity – Internal Energy Formulation of the Hydrodynamic Model of Electron Transport

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ABSTRACT

The hydrodynamic model of electron transport is revisited. By rearranging the governing equations a new set of equations in terms of the electron vorticity and internal energy is derived. The advantage of the new set of equations is the explicit removal of the electric field from the equations. A scale analysis of the electron vorticity equation is performed and the conditions for the observation of electron vortices in high field transport in submicron devices are predicted.

Keywords: Electron transport, internal energy, hydrodynamic model, electron vorticity.

1 INTRODUCTION

Electron transport in two-dimensional electron gas (2DEG) exists in three regimes: ballistic, quasi-diffusive and diffusive (see Table 1).

The distinction between these three regimes is defined by the relative magnitude of electron-electron scattering length, electron-phonon scattering length and the size of the device. The diffusive transport regime for 2DEG has found application in high electron mobility transistors. There has been extensive research to include quantum mechanical effects [1,2] where the wave nature of electrons plays an important role in the device operation. To this end the ballistic transport regime has been studied extensively with the observation of conductance quantization, quantum Hall effect and fractional quantum Hall effect. The intermediate regime of the quasi-diffusive transport, considered in this study, has been the focus of less attention. The quasi-diffusive transport effects in 2DEG have included shallow water analogy and terahertz sources [3–6]. What distinguishes quasi-diffusive regime is that the electron temperature is high enough so that many energy levels are occupied and there is no conductance quantization or coherent electronic effects. This regime is beyond the Landauer-Buttiker formalism. In addition the electron density is high enough for the electron-electron scattering distance to be the shortest length scale in the system.

In our previous work [7, 8] we focused on the quasi-diffusive transport through hydrodynamic model of electron transport. We drove the electron vorticity[1] transport equations. The electron vorticity transport equations derived in [8] does not provide a closed system of equations. One needs another independent equation involving higher moments of the Boltzmann transport equation. This could be in the form of an energy balance equation. We derive an equation for the evolution of the internal energy of electrons that does not involve the applied electric field. Then the new set of equations for the electron vorticity, $\vec{\omega}$, and the internal energy could potentially substitute the the hydrodynamic model in terms of the primitive variables.

2 GOVERNING EQUATIONS

We start with the Boltzmann transport equation for electrons moving with the group velocity $\mathbf{u}$ in an electric field $\mathbf{E}$ can be represented as

$$\frac{\partial f}{\partial t} + \mathbf{u} \cdot \nabla_{\mathbf{x}} f - \frac{e}{m} \mathbf{E} \cdot \nabla_{\mathbf{u}} f = C, \qquad (1)$$

where e is the electron charge, m the effective electron mass, C the Collision term, $f(\mathbf{x}, \mathbf{u}, t)$ the distribution function for the electrons, $\mathbf{x}$ the space variable, and t is time.

The first five moments of the Boltzmann transport equation (1) in the velocity space are the balance equations for the flux of electron, momentum, and energy. These equations are represented as follows:

$$\frac{\partial n}{\partial t} + \nabla \cdot (n\mathbf{v}) = C_n, \qquad (2)$$

$$\frac{\partial \mathbf{p}}{\partial t} + \mathbf{v}(\nabla \cdot \mathbf{p}) + (\mathbf{p} \cdot \nabla)\mathbf{v} = -en\mathbf{E} - \nabla \cdot \mathbf{P} + \mathbf{C_p}, \qquad (3)$$

[1] We define electron vorticity as $\vec{\omega} = \nabla \times \mathbf{v}$, where $\mathbf{v}$ is the translational velocity. Helmholtz's first theorem states that a vector (in our case $\mathbf{v}$) is uniquely specified by giving its curl (vorticity $\nabla \times \mathbf{v}$) and its divergence (dilatation $\nabla \cdot \mathbf{v}$) within a region and its normal component over the boundary.

Table 1. Multiple Scale Electron Transport in Doped Semiconductors

	$L << l_{e\text{-}ph}$			$L \sim l_{e\text{-}ph}$	$L >> l_{e\text{-}ph}$
	$L<\lambda$	$L < l_{e\text{-}e}$	$L >> l_{e\text{-}e}$		
Transport Regime	Quantum	Ballistic	Fluid	Fluid	Diffusive
Scattering	Rare	Rare	e-e (Many), e-ph (Few)		Many
Model:					
Drift / Diffusion					
Hydrodynamic	Quantum Hydrodynamic				
Monte Carlo					
Schrod. / Green's Function	Wave				
Applications	Quantum wells Superlattices	Ballistic Transistor	**Not much explored**	**Not much explored**	Current ICs

L = Characteristic Length Scale of film/device
$l_{e\text{-}ph}$ = Average Mean Free Path due to Electron /Phonon interaction
$l_{e\text{-}e}$ = Average Mean Free Path due to Electron /Electron interaction
λ = Wavelength of Electrons. Typically $\lambda \sim l_{e\text{-}e} << l_{e\text{-}ph}$ in the case of moderately doped semiconductors.

$$\frac{\partial(nw)}{\partial t} + \nabla\cdot(nw\mathbf{v}) + \nabla\cdot(\mathbf{v}\mathbf{P}) = -en\mathbf{v}\cdot\mathbf{E} - \nabla\cdot\mathbf{q} + C_W, \quad (4)$$

where
$$w = me_I + \frac{1}{2}m|\mathbf{v}|^2, \quad (5)$$

is the total energy density. Here, n is the electron concentration, $\mathbf{v}$ is the translational velocity, $\mathbf{p}$ is the momentum density $mn\mathbf{v}$, $\mathbf{P}$ is the pressure tensor, $\mathbf{q}$ is the heat flux, e_I is the internal energy, and C_n, $\mathbf{C_p}$, and C_W represent moments of C, *i.e.* moments of the collision terms. These equations are supplemented by the Poisson equation (in quasi-electrostatic limit) for the electric potential ϕ

$$\mathbf{E} = -\nabla\phi, \quad (6)$$
$$\nabla\cdot(\epsilon\nabla\phi) = -\sum e_i n_i - k_1, \quad (7)$$

where k_1 := doping concentration and ϵ := dielectric constant. For devices in which the quasi-electrostatic approximation is not accurate enough one needs to use the full Maxwell's equations (see *e.g.* , [9]). We refer to Lundstrom [10] for a derivation of the hydrodynamic model of electron transport and for more references. A commonly used simplification for the collision integrals is the relaxational time approximation [10]. Although, this will not affect our technique it might simplifies the computations in some cases. Therefore, the collision terms are modeled as

$$C_n = -R, \quad (8)$$
$$\mathbf{C_p} = -\mathbf{p}/\tau_p, \quad (9)$$
$$C_W = -(W - W_0)/\tau_w, \quad (10)$$

where R is the recombination rate and τ_p and τ_w are the momentum and energy relaxation times, respectively. In the following sections we derive an alternative set of equations for the hydrodynamic model in terms of electron vorticity and internal energy.

3 INTERNAL ENERGY EQUATION

An interesting question is how to make statements about the electron velocity field which do not involve the electric field. This can be done by removing the electric field from equations (3) and (4). First note that

$$\mathbf{v}\cdot\frac{\partial\mathbf{p}}{\partial t} = m\mathbf{v}\cdot\frac{\partial(n\mathbf{v})}{\partial t} = m\mathbf{v}\cdot\left(n\frac{\partial\mathbf{v}}{\partial t} + \mathbf{v}\frac{\partial n}{\partial t}\right). \quad (11)$$

By substituting from the continuity equation one can show that

$$\mathbf{v}\cdot\frac{\partial\mathbf{p}}{\partial t} = \frac{mn}{2}\frac{\partial|\mathbf{v}|^2}{\partial t} + m|\mathbf{v}|^2\left(C_n - \nabla\cdot(n\mathbf{v})\right) = m|\mathbf{v}|^2 C_n - |\mathbf{v}|^2\nabla\cdot\mathbf{p} \quad (12)$$

The evolution equation for the kinetic energy is, then calculated as

$$\frac{mn}{2}\frac{\partial|\mathbf{v}|^2}{\partial t} + m|\mathbf{v}|^2 C_n + \mathbf{v}\cdot(\mathbf{p}\cdot\nabla)\mathbf{v} = -en\mathbf{v}\cdot\mathbf{E} - \mathbf{v}\cdot(\nabla\cdot\mathbf{P}) - \mathbf{v}\cdot\mathbf{C_p} \quad (13)$$

Substituting $-en\mathbf{v}\cdot\mathbf{E}$ from above into the energy equation (4) and using the identity

$$\frac{\partial mne_I}{\partial t} + \nabla\cdot(mne_I\mathbf{v}) = \frac{D(mne_I)}{Dt} + mne_I\nabla\cdot\mathbf{v} \quad (14)$$

an equation for the evolution of the internal energy of electrons can be written as

$$\frac{D(mne_I)}{Dt} + mne_I\nabla\cdot\mathbf{v} + \nabla\cdot\left(\mathbf{v}\frac{mn|\mathbf{v}|^2}{2}\right) + \nabla\cdot(\mathbf{v}\mathbf{P}) = m|\mathbf{v}|^2 C_n + \mathbf{v}\cdot(\mathbf{p}\cdot\nabla)\mathbf{v} + \mathbf{v}\cdot(\nabla\cdot\mathbf{P}) - \mathbf{v}\cdot\mathbf{C_p} - \nabla\cdot\mathbf{q} + C_w \quad (15)$$

where

$$\frac{D}{Dt} := \frac{\partial}{\partial t} + \mathbf{v}\cdot\nabla, \tag{16}$$

is the total derivative. Note that the electric field is completely removed from this equation. It is interesting to note, however, that the electric field directly contributes to the kinetic energy of electrons in equation (13).

4 ELECTRON VORTICITY TRANSPORT EQUATION

The electron vorticity transport equation is obtained by taking curl of the momentum equation (3) and using equation (2) to obtain

$$n\frac{D}{Dt}\left(\frac{\vec{\omega}}{n}\right) - (\vec{\omega}\cdot\nabla)\mathbf{v} = -\nabla\times\left(\frac{1}{mn}\nabla\cdot\mathbf{P}\right) + \nabla\times\left(\frac{1}{mn}\left(\mathbf{C_p} - mC_n\mathbf{v}\right)\right) - \frac{C_n}{n}\vec{\omega}. \tag{17}$$

For simplicity the collision terms are modeled using the relaxational time approximation in equations (8-10). We also need a constitutional law (moment closure) for the pressure tensor $\mathbf{P}$. For simplicity, we consider an inviscid model, where we assume that the pressure tensor can be represented in terms of the effective carrier temperature T by an ideal gas law relationship $\mathbf{P} = nkT\mathbf{I}$, Here $\mathbf{I}$ is the identity tensor. and k is the Boltzmann constant. Noting that $\nabla\times E = 0$, the vorticity equation can be written as

$$n\left(\frac{\partial}{\partial t} + \mathbf{v}\cdot\nabla\right)\left(\frac{\vec{\omega}}{n}\right) = (\vec{\omega}\cdot\nabla)\mathbf{v} - \frac{k}{m}\nabla\left(\frac{T}{n}\right)\times\nabla n + \left(2\frac{R}{n} - \frac{1}{\tau_p}\right)\vec{\omega} + R\,\nabla\left(\frac{1}{n}\right)\times\mathbf{v}. \tag{18}$$

There are seven terms involved in the vorticity equation (18). This equation shows that the ratio of the electron vorticity to the electron concentration can change with time due to the terms on the right-hand side of equation (18). The two terms on the left hand side form the total derivative of the vorticity density. The third term represents the vortex stretching essential for turbulence. The fourth term is similar to the baroclinic generation of vorticity in classical fluid mechanics and is due to the interaction of the principal part of the pressure tensor $\mathbf{P}$ and the density field n. The last three terms in equation (18) are due to vorticity generation through the collision terms in the continuity and momentum equations.

5 SCALING AND ORDER OF MAGNITUDE ANALYSIS

A comparison of the order of magnitude of each term in the vorticity equation are carried in this section to characterize a regime of electron transport with significant electron vorticity transport effects. We assume that the characteristic scales of the problem *i.e.* , velocity, length, electron concentration, temperature and electric field are given by U, L, n_0, T_0, E_0, respectively. Note that the time scale is given by $\tau = L/U$. All the dependent variables are nondimensionalized using these scales. The nondimensional vorticity equation with the appropriate scaling can be written as

$$n^*\left(\frac{\partial}{\partial t^*} + \mathbf{v}^*\cdot\nabla^*\right)\left(\frac{\vec{\omega}^*}{n^*}\right) = (\vec{\omega}^*\cdot\nabla^*)\mathbf{v}^* - \frac{e\phi_0}{mU^2}\nabla^*\left(\frac{T^*}{n^*}\right)\times\nabla^* n^* + 2\frac{RL}{Un_0}\frac{\vec{\omega}^*}{n^*} - \frac{L}{U\tau_p}\vec{\omega}^* + \frac{RL}{Un_0}\nabla^*\left(\frac{1}{n^*}\right)\times\mathbf{v}^*. \tag{19}$$

The three nondimensional numbers that appear on the right hand side of equation (19) are of fundamental importance in our analysis. The nondimensional number $e\phi_0/mU^2$ of the baroclinic term is the ratio of the absorbed energy of a free electron from the external potential ϕ_0 to the average thermal energy of electrons. One can obtain an estimate for this nondimensional number by using equation (3). If assuming that the order of the driving force $\frac{e}{m}\mathbf{E}$, is the same as the acceleration term $\frac{D\mathbf{v}}{Dt}$, and using $E_0 = \phi_0/L_d$ we obtain $mU^2 \approx e\phi_0$. This implies that the the baroclinic term is of the same order as the vorticity acceleration and vortex stretching terms. The nondimensional number $L/U\tau_p = \tau/\tau_p$ in front of the momentum relaxation source term is in fact the ratio of the transit time to the momentum relaxation time. Note that the recombination rate can be represented as $R \approx n_0/\tau_r$. Therefore, the nondimensional number $RL/Un_0 = \tau/\tau_r$ in front of the recombination term in equation (19) can be interpreted as the ratio of the transit time in the device to the recombination relaxation time.

In most cases one can neglect the vorticity generation by the recombination term; τ/τ_r is usually a very small number. Since the momentum relaxation term acts as a sink of electron vorticity, one expects to observe the transport of electron vortices in a regime in which this term is smaller than the other remaining source terms, *i.e.* , it is of the order of one or less. A simple calculation of τ/τ_p for a semiconductor material with $\tau_p = 1ps$ (*e.g.* , GaAs at low temperatures) show that for easily achievable feature sizes (0.1-1.5 μm) and applied electric potentials (0.1-1V), the order of magnitude of this term is around one and significant electron vorticity generation and convection can be observed.

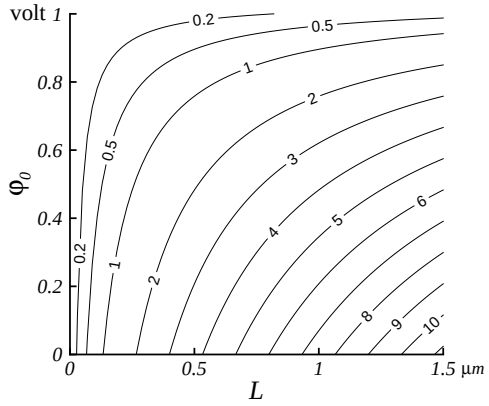

Figure 1: Contour plot of τ/τ_p with $\tau_p = 1ps$.

This is presented in figure 1. By increasing the characteristic length of the device while fixing the electric potential or by decreasing the electric potential for a given device size the contribution of the momentum relaxation term in damping electron vortices increases. In order to verify that this regime of transport falls within the range of hydrodynamic flow assumption, the electron mean-free-path due to electron-electron ($L_{\text{e-e}}$) and electron-phonon ($L_{\text{e-ph}}$) scatterings are calculated by a completely independent calculations. See [7] for details.

6 DISCUSSION

In this study dynamical statements were made in a form that did not involve the electric field **E**. It is interesting to note that although the applied electric field is the cause of electron motion, we made mathematical progress best by eliminating it from the analysis. This is somewhat similar to the elimination of the pressure from the incompressible flows by writing the equations in terms of vorticity (curl of the velocity field). The electron vorticity equation (17) and the electron internal energy (15) could substitute the momentum equation (3) and the energy equation (4) without any explicit reference to the electric field. The Poisson equation for the electric potential (6) needs to be solved only if one needs the distribution of the electric potential in the device.

A scale analysis of the electron vorticity equation is performed and the relative order of magnitude of each source of vorticity is found. Our analysis predicts conditions for the observation of electron vortices in high field transport in submicron devices. Our investigation is set in the regime of validity of hydrodynamic models, *i.e.* , the characteristic length scales are so that the quantum mechanical effects can be neglected and the electron-electron scattering is fast enough so that one cannot make the independent electron approximation. In order to observe electron vortices, electron transit time in a device should be of the same order as the momentum relaxation time. In addition, the device geometry, boundary effects and material parameters should be chosen appropriately.

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