HYDRODYNAMIC MODEL AND JUMP CONDITIONS FOR DISCONTINUOUS MASS AND ELECTRIC POTENTIAL IN HETEROSTRUCTURE DEVICES

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Abstract

A heterostructure is composed of different materials where in each section effective mass of an electron and the minimum energy of the conduction band are different. To model dynamics of electrons in a heterostructure we derive the hydrodynamic equations for a gas of electrons with position dependent mass moving in a potential field. First we write the Boltzmann equation and then we derive the fluid equations by taking the first three moments of the Boltzmann equation and deriving a generalized hydrodynamic model. The jump conditions at the junction are obtained using two different methods. First method relies on using the conservative form of the equations. The second method is based on solving the problem of motion of one electron as it passes through the junction and deriving the necessary conditions on the density functions on two sides of the junction; By taking moments of the density functions we obtain the jump conditions. Jump conditions are obtained as continuity of flux for number of particles, energy, tangential momentum, and square of the tangential momentum.

I. INTRODUCTION

We are concerned with derivation of the hydrodynamic model for devices with a heterojunction. By the hydrodynamic model we shall mean the first three moments of the Boltzmann equation coupled to the Poisson equation [2]. We derive the hydrodynamic model for a gas of electrons with a differentiable position dependent mass and differentiable electric potential. At the interface between the two material there is a discontinuity in the effective mass of electrons and in the minimum energy of the conduction band. We study the problem of the jump conditions at the discontinuity.

A set of equations similar to the hydrodynamic equations were used by D. Widiger, K. Hess, and J. Coleman in [13] and [14]. The equations were derived by considering the first four moments of the Boltzmann equation and simplifying them in order to obtain a closed system for evolution of density and energy. They model a high electron mobility device (HEMT) by writing two sets of equations, a two dimensional system for the electrons in the bulk and a one dimensional system for the electrons in the channel and then coupling the two through flux relations.

A hydrodynamic model including the effects of the position dependent mass was derived by E. M. Azoff in [1]. Our derived equations are similar to his equations but he does not consider the discontinuity in the mass or the potential energy. T. Shawki, G. Salmer, and O. El-Sayed have done numerical simulations of 2D devices using finite difference methods for a set of equations similar to the ones derived by E. M. Azoff [11]. In their work they replace the discontinuities in the conduction band by a smoothed out profile and use an energy dependent relation for effective mass. A different approach was taken by T. Wang and C-H. Hsieh to model the heterostructure devices [12]. They solve a one dimensional hydrodynamic model in the channel coupled to a Schroedinger equation in the perpendicular direction and to a 2D Poisson equation. The problem of interface conditions for the hydrodynamic model has been considered by Schroeder, [9] and [10]. He assumes a perturbed Maxwellian for the density function and from that he derives the interface conditions by taking the moments.

In this paper we present the derived hydrodynamic model for a position dependent mass and the jump conditions at the interface between the two materials. We investigated the problem of electron transfer at the junction where there is a discontinuity in the effective mass and the potential energy. The jump conditions at the discontinuity can be derived using two different methods. One

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can derive the general conservation laws and write them in conservative form. The jump conditions are readily obtained using mathematical arguments. One can also solve the problem of one single electron passing through the junction and deriving the conditions on the density functions and then deriving the jump conditions by taking moments of the density functions on both sides. The two methods yield the same results.

II. QUANTUM MODEL AND BOLTZMANN EQUATION

An electron in a heterostructure consisting of two different semiconductors can be modeled by an electron in an electric potential $Q(x)$ such that

$$Q(x) = Q^+(x) \text{ for } x_1 \geq 0 \text{ and } Q(x) = Q^-(x) \text{ for } x_1 \leq 0. \tag{1}$$

Here $x = (x_1, x_2, x_3)$ is the spatial coordinate variable and functions Q^+ and Q^- are periodic, possibly with different periods, corresponding to the lattice potential in each semiconductor. The Schroedinger equation for an electron in a heterostructure with an applied external potential ϕ is written as

$$-\frac{\hbar^2}{2m}\Delta\Psi(x) + Q(x)\Psi(x) + \phi(x)\Psi(x) = \lambda\Psi(x). \tag{2}$$

Although the problem is easy to state, analytic or computational solutions of the problem are quite complicated. We have obtained some partial results on the above problem [4].

Our results in this paper are based on modeling the electrons in each semi-space as a semi-classical particle. We assume that in each semi-space each electron has an effective mass corresponding to the underlying lattice potential and is moving in a potential field equal to the energy of the bottom of the conduction band plus the applied electric potential. The laws of motion for such a particle and the BTE equation for an ensemble of such particles are easy to derive. We let (x, y, z) be the position variable, (p, q, r) the momentum variable, t time, and $m(x, y, z)$ be the effective mass of an electron moving in a potential field $F(x, y, z) = E_c(x) + \phi(x, y, z)$, such that $E_c(x)$ is the energy level of the conduction band and discontinuous at $x = 0$ and $\phi(x, y, z)$ is the applied potential and differentiable everywhere. The Hamiltonian for motion of one electron is written as

$$H(x, y, z, p, q, r, t) = (p^2 + q^2 + r^2)/(2m) + E_c(x) + \phi(x, y, z). \tag{3}$$

Then the Boltzmann equation for a gas of such electrons is written as

$$\partial_t f + \partial_x(p/mf) + \partial_y(q/mf) + \partial_z(r/mf) +$$

$$\partial_q(-H_x f) + \partial_q(-H_y f) + \partial_r(-H_z f) = C(f, f) \tag{4}$$

where $f(x, y, z, p, q, r, t)$ is the density function,

$$\nabla H = (H_x, H_y, H_z) = -\nabla m(p^2 + q^2 + r^2)/(2m^2) + \nabla E_c + \nabla\phi, \tag{5}$$

and $C(f, f)$ is the collision operator of all the scattering mechanisms present. The fluid equations can be derived from the above Boltzmann equation. This derivation is standard for constant mass, [5], but here we also have calculated the extra terms coming from the dependence of the mass on position.

III. HYDRODYNAMIC MODEL

We present the derived hydrodynamic model of electrons in a heterostructure in this section, please see [4] for the details. We use as dependent variables:

- Density of Electrons, n

- Momentum, $mnu = (mnu, mnv, mnw)$

- Energy, e_c

- Electric Potential, ϕ.

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Temperature, T, is defined using the main variables by

$$\frac{3}{2}nT = e_c - \frac{1}{2}mn(u^2 + v^2 + w^2). \tag{6}$$

The other quantities are defined in terms of the above or are specified.

- charge of an electron, $e > 0$

- conduction band minimum energy, $E_c(x)$

- number of ionized donors, $N_D^+(x, y, z)$

- momentum relaxation time, τ_p

- and energy relaxation time, τ_w

Then the hydrodynamic model is written in the following form:

$$n_t + \nabla \cdot (n\mathbf{u}) = 0 \tag{7}$$

$$(mn\mathbf{u})_t + \nabla \cdot (mn\mathbf{u}^t \cdot \mathbf{u}) + \nabla(nT) - e_c \frac{\nabla m}{m} = en\nabla\phi + n\nabla E_c - \frac{mn\mathbf{u}}{\tau_p} \tag{8}$$

$$e_{ct} + \nabla \cdot (\mathbf{u}e_c + \mathbf{u}nT + (e\phi + E_c)n\mathbf{u}) = (e\phi + E_c)\nabla \cdot (n\mathbf{u}) - \frac{e_c - \frac{3}{2}nT_s}{\tau_w} + \nabla \cdot \mathbf{q} \tag{9}$$

$$\nabla \cdot (\epsilon\nabla\phi) = (N_D^+ - n). \tag{10}$$

The heat conduction vector can be calculated in the first approximation [5],

$$\mathbf{q} = \frac{5\tau nT}{2m}\nabla T + \frac{\tau n}{4m^2}(5m|\mathbf{u}|^2T - 25nT^2)\nabla m. \tag{11}$$

τ is the relaxation time coefficient of the density function and is approximately of order of τ_p. The electric potential satisfies the Poisson equation and ϵ has a discontinuity at the junction but ϕ and the normal component of $\epsilon\nabla\phi$ are continous at the junction. At the interface the following jump conditions are standard

$$[\phi] = 0, \quad [\epsilon\phi_x] = 0. \tag{12}$$

We use the notaion $[\phi] = \phi_2 - \phi_1$ to denote the jump in the variables across the junction. We suggest the following jump conditions for the fluid variables

$$[nu] = 0 \quad [mv] = 0 \quad [mw] = 0 \quad [T] = 0 \quad [m(u^2 + v^2 + w^2) + (3 + \beta(m))T + 2E] = 0. \tag{13}$$

The first jump condition is conservation of number of particles across the jump, the next two are conservation of tangential momentum, and the last two are consequences of conservation of energy, conservation of the square of the tangential momentum, and some assumptions about the shape of the density functions near the junction. The function N_D^+, number of ionized donors, is defined in terms of the electric potential and the Fermi level. β is defined

$$\beta = \frac{3\alpha}{\alpha + 2} \tag{14}$$

and αs for $2/3 < m1/m2 < 3/2$ are defined as

$$\alpha_1 = \frac{m_1/m_2 + 3 - 2m_2/m_1}{m_1/m_2 + m_2/m_1}$$

$$\alpha_2 = \frac{m_2/m_1 + 3 - 2m_1/m_2}{m_2/m_1 + m_1/m_2}. \tag{15}$$

We considered semi-classical dynamics of electrons in a semiconductor where effective mass and minimum energy of the conduction band are functions of position. We have derived the hydrodynamic model for such electrons from the Boltzmann equation. We considered in detail dynamics of electrons as they pass through the junction and the necessary conditions on the density functions at the junction where there is a discontinuity in the mass and electric field. The jump conditions were obtained by taking the moments of the density functions and writing them in terms of the fluid variables invoking the usual closure assumptions for fluid equations. The derived jump conditions for the conservation of mass and energy equations are satisfactory, but the jump conditions for the momentum equation is yet to be shown satisfactory. We have derived the jump conditions here but their numerical implementation and physical implications are subject of a future study.

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