QUANTUM HYDRODYNAMIC EQUATIONS FOR A TWO-BAND WIGNER-KANE MODEL

STEFANO BIONDINI, GIOVANNI FROSALI
AND FRANCESCO MUGELLI
Dipartimento di Elettronica e Telecomunicazioni and
Dipartimento di Matematica Applicata "G.Sansone"
Università di Firenze

1. Introduction

The numerical simulations of semiconductor devices are usually based on hydrodynamic models formulated in terms of macroscopic quantities such as charge density, current, energy, and so on. In the classical frame, hydrodynamic models are derived from the hierarchy of the moments of the Boltzmann equation. Starting from the pionieristic paper by Bløtekjær[1], in the 70's, the literature on hydrodynamic modeling, both theoretical and numerical, is very extensive. The reader interested in hydrodynamic modeling can refer to the papers quoted in the review by Anile and Romano[2].

As it is well known, the fluid dynamical description begins to fail when the carriers involved (i.e. electrons and holes) are few and the quantum aspects become not negligible or even predominant. Nevertheless it is worthwhile to recall that keeping an hydrodynamic formulation would still present some relevant advantages (also in the previously mentioned situation), since fluid dynamical equations are preferable on the computational side. Moreover, it easier to face the boundary conditions problem when macroscopic quantities are involved rather than the Wigner distribution function or the wave function. On the other hand, in practical applications, approaches based on microscopic models are not completely satisfactory, and it is useful to formulate semi-classical models in terms of macroscopic variables. Such models are generally built from a hierarchy of coupled moment equations and referred to as quantum hydrodynamic models.

In this context some very interesting results are present in literature,

where a quantum hydrodynamic set of equations capable to describe the behaviour of nanometric devices like resonant tunneling diodes is introduced. We recall here the "smooth" quantum hydrodynamic model proposed by Gardner and Ringhofer[3], who derive the fluid dynamical formulation from moment expansion of a Wigner–Boltzmann equation, and the approach by Jüngel[4], whose starting point is the ansatz of a peculiar type of solutions to the Schrödinger equation. Published results are generally devoted to single-band problems.

Quantum mechanical phenomena are essential in nanometer scale semiconductor devices, as for the Resonant Interband Tunneling Diode (RITD), whose properties differ from those of the Resonant Tunneling Diode (RTD) because of the role played by the valence band electrons in the control of the current flow[5]. For the new family of heterojunction resonant interband tunneling diodes, which make use of resonant interband tunneling through potential barriers, we have to consider the multi-band structure in the transport computation of the current.

In this context, a simple model introduced by E.O.Kane[6] in the early 60's describes the electron behaviour in a system equipped with two allowed energy bands separated by a forbidden region. The Kane model is the simplest framework capaple of including one conduction band and one valence band in each material of a heterogeneous device and it is formulated as the coupling of two Schrödinger-like equations for the conduction and the valence band wave (envelope) functions[7]. The typical band diagram structure of a tunneling diode is characterized by a band alignment such that the valence band of the positive side of the semiconductor device lies above the conduction band of the negative one.

In this paper, we face the problem of a fluid dynamical formulation for a semiconductor device characterized by a two–band (i.e. conduction and valence band) structure where the carriers dynamics is driven by interband tunneling. We start from the formulation of the Kane model in terms of Wigner functions[7], and derive formally a system for the zeroth, first and second velocity moments.

Finally, a short discussion in given on such model and on related problems, such as closure and numerical implementation.

2. Wigner formulation of the Kane model

Let $\psi_c(x,t)$ be the conduction band electron wave (envelope) function and $\psi_v(x,t)$ be the valence band electron wave (envelope) function.

In the one-dimensional case, the Kane model reads as follows[6,7]

$$\begin{cases} i\hbar\dfrac{\partial\psi_c}{\partial t} = \left[-\dfrac{\hbar^2}{2m}\dfrac{\partial^2}{\partial x^2} + V_c\right]\psi_c - \dfrac{\hbar^2}{m}P\dfrac{\partial\psi_v}{\partial x} \\ i\hbar\dfrac{\partial\psi_v}{\partial t} = \left[-\dfrac{\hbar^2}{2m}\dfrac{\partial^2}{\partial x^2} + V_v\right]\psi_v + \dfrac{\hbar^2}{m}P\dfrac{\partial\psi_c}{\partial x} \end{cases} .$$

where i is the imaginary unit, $\hbar$ is the Planck constant scaled by 2π, m is the bare mass of the carriers, V_c and V_v are the minimum of the conduction band energy and maximum of the valence band energy respectively. Moreover P is the coupling coefficient given by

$$P = \frac{m}{\hbar}\sqrt{\frac{m-m^*}{2mm^*}E_g}$$

which is obtained through the energy dispersion relation and where m^* is the effective electron mass depending, through the $x-$coordinate, on the layer composition, but otherwise isotropic, and $E_g = V_c - V_v$ is the $x-$dependent gap energy. We define the density matrix $\rho_{ij}(r,s,t) = \overline{\psi}_i(r,t)\psi_j(s,t),\ \ i,j = c,v$. Taking formally the derivatives with respect to time t of the density matrix element and using Kane eqs., a set of four coupled evolution equations is derived for the density matrix elements ρ_{ij}. The Wigner function is defined by the inverse Fourier transformation

$$w_{i,j}(x,v,t) = \mathcal{F}^{-1}\rho_{i,j}\left(x + \frac{\hbar}{2m}\eta,\ x - \frac{\hbar}{2m}\eta\right) .$$

Then we obtain the following system, which is the Wigner function formulation of the Kane model

$$\begin{cases} i\hbar\dfrac{\partial w_{cc}}{\partial t} = -i\hbar v\dfrac{\partial w_{cc}}{\partial x} + \Theta_{cc}w_{cc} + \dfrac{\hbar^2 P}{2m}\left[\dfrac{\partial w_{vc}}{\partial x} - \dfrac{\partial w_{cv}}{\partial x}\right] - i\hbar Pv\left[w_{vc} + w_{cv}\right] \\ i\hbar\dfrac{\partial w_{cv}}{\partial t} = -i\hbar v\dfrac{\partial w_{cv}}{\partial x} + \Theta_{vc}w_{cv} + \dfrac{\hbar^2 P}{2m}\left[\dfrac{\partial w_{vv}}{\partial x} + \dfrac{\partial w_{cc}}{\partial x}\right] - i\hbar Pv\left[w_{vv} - w_{cc}\right] \\ i\hbar\dfrac{\partial w_{vv}}{\partial t} = -i\hbar v\dfrac{\partial w_{vv}}{\partial x} + \Theta_{vv}w_{vv} - \dfrac{\hbar^2 P}{2m}\left[\dfrac{\partial w_{cv}}{\partial x} - \dfrac{\partial w_{vc}}{\partial x}\right] + i\hbar Pv\left[w_{cv} + w_{vc}\right] \end{cases}$$

where w_{cc} and w_{vv} are real, $w_{cv} = \overline{w_{vc}}$ and

$$\Theta_{ij}w_{ij} = \frac{1}{2\pi}\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}\left[V_j\left(x - \frac{\hbar}{2m}\eta, t\right) - V_i\left(x + \frac{\hbar}{2m}\eta, t\right)\right]w_{ij}(x,v',t)\mathrm{e}^{i(v-v')\eta}d\eta dv'$$

with $i,j = c,v$.

Let now define the particle density, the current density, the energy density and the third moment, limiting to the 1-dimensional case.

If the quantum mechanical probability densities n_{ij} are defined by

$$n_{ij}(x,t) = \int_{-\infty}^{+\infty} w_{ij}(x,v,t)dv\,, \quad i,j = c,v\,,$$

then n_{cc} and n_{vv} are the probability densities for the positions of electrons in band of conduction and valence, respectively. The interband terms n_{cv} and n_{vc} are complex functions such that $n_{cv} = \overline{n_{vc}}$.

It is worthwhile to remark that only n_{cc} and n_{vv} are real functions, corresponding to probability densities, but also we remark that the Wigner functions arise from the envelope function, not from the wave function and so the physical meaning of this quantities has to be understood in the sense of the envelope theory[8,9].

It is well known that the first order moment of the Wigner function with respect to the velocity and multiplied by the charge $-q$ is the quantum current density. Similarly, in the frame of a two-band system, we define

$$J_{ij} = -q\int_{-\infty}^{+\infty} v w_{ij}(x,v,t)dv\,, \quad i,j = c,v\,.$$

Also in this case we can recover the classical meaning of the conduction (valence) current density J_{cc} (J_{vv}) for electrons in conduction (valence) band.

For $i,j = c,v$, the set of the higher order moments is

$$\mathcal{E}_{ij}(x,t) = \frac{m}{2}\int_{-\infty}^{+\infty} v^2 w_{ij}(x,v,t)dv,$$

$$M_{ij}^{(3)}(x,t) = \int_{-\infty}^{+\infty} v^3 w_{ij}(x,v,t)dv\,.$$

The equations for the moments of the Wigner functions can be derived by multiplying the equations of Wigner system by 1, v and v^2 and by integrating over the velocity space.

The first set of equations for the evolutions of the position number densities reads as follows

$$\begin{cases} \dfrac{\partial n_{cc}}{\partial t} = \dfrac{1}{q}\dfrac{\partial J_{cc}}{\partial x} + i\dfrac{\hbar P}{2m}\left[\dfrac{\partial n_{cv}}{\partial x} - \dfrac{\partial n_{vc}}{\partial x}\right] + \dfrac{P}{q}\left[J_{cv} + J_{vc}\right] \\ \dfrac{\partial n_{cv}}{\partial t} = \dfrac{1}{q}\dfrac{\partial J_{cv}}{\partial x} + \dfrac{i}{\hbar}\left[V_c(x,t) - V_v(x,t)\right] n_{cv} \\ \qquad\qquad - i\dfrac{\hbar P}{2m}\left[\dfrac{\partial n_{cc}}{\partial x} + \dfrac{\partial n_{vv}}{\partial x}\right] - \dfrac{P}{q}\left[J_{cc} - J_{vv}\right] \\ \dfrac{\partial n_{vv}}{\partial t} = \dfrac{1}{q}\dfrac{\partial J_{vv}}{\partial x} + i\dfrac{\hbar P}{2m}\left[\dfrac{\partial n_{cv}}{\partial x} - \dfrac{\partial n_{vc}}{\partial x}\right] - \dfrac{P}{q}\left[J_{cv} + J_{vc}\right] . \end{cases}$$

In the Kane model, in which only interactions among the conduction and the valence bands are allowed and all the others are neglected, the wave function ψ is expressed by

$$\psi_c(x)u_0^c(x) + \psi_v(x)u_0^v(x)$$

where u_0^c and u_0^v are Bloch functions[8,9,7]. Then, for the two-band Schrödinger-like Kane model, the total density is

$$n_{tot}(x,t) = |\psi|^2 = |\psi_c|^2 + |\psi_v|^2 = n_{cc}(x,t) + n_{vv}(x,t)$$

and the quantum continuity equation takes the form

$$\frac{\partial\ (n_{cc} + n_{vv})}{\partial t} = \frac{1}{q}\mathrm{div}\, J_{tot}.$$

Using the expressions for the wave function in terms of Bloch functions, in the spirit of the envelope theory, the total current density for the two-band system is

$$J_{tot}(x,t) = -\frac{i\hbar q}{2m}(\psi\nabla\bar{\psi} - \bar{\psi}\nabla\psi) = J_{cc} + J_{vv} - \frac{2\hbar qP}{m}\,\mathrm{Im}\, n_{cv}\,.$$

The second set of equations in the quantum hydrodynamic model for the two-band Kane system is given by the following first order moments equations :

$$\frac{\partial J_{cc}}{\partial t} = \frac{2q}{m}\frac{\partial \mathcal{E}_{cc}}{\partial x} + \frac{q}{m}V_c^{'}(x,t)n_{cc} + i\frac{\hbar P}{2m}\frac{\partial}{\partial x}(J_{cv} - J_{vc}) + \frac{2qP}{m}(\mathcal{E}_{cv} + \mathcal{E}_{vc})$$

$$\frac{\partial J_{cv}}{\partial t} = \frac{2q}{m}\frac{\partial \mathcal{E}_{cv}}{\partial x} + \frac{q}{2m}[V_c^{'}(x,t) + V_v^{'}(x,t)]n_{cv}$$
$$+ i\frac{1}{\hbar}[V_c(x,t) - V_v(x,t)]J_{cv} - i\frac{\hbar P}{2m}\frac{\partial}{\partial x}(J_{cc} + J_{vv}) + \frac{2qP}{m}(\mathcal{E}_{cc} - \mathcal{E}_{vv})$$

$$\frac{\partial J_{vv}}{\partial t} = \frac{2q}{m}\frac{\partial \mathcal{E}_{vv}}{\partial x} + \frac{q}{m}V_v^{'}(x,t)n_{vv} + i\frac{\hbar P}{2m}\frac{\partial}{\partial x}(J_{cv} - J_{vc}) - \frac{2qP}{m}(\mathcal{E}_{cv} + \mathcal{E}_{vc})\,.$$

The equations for the current densities (first order moments) contain the second order moments $\mathcal{E}_{ij}(x,t)$, which can be interpreted as energy density terms.

A simple quantum hydrodynamic model can be obtained directly from the first two moments, by manipulating the energy terms appearing under the divergence symbol and taking into account that

$$\frac{\partial \mathcal{E}_{ij}}{\partial x} = \frac{m}{2q^2}\frac{\partial}{\partial x}\left(\frac{J_{ij}^2}{n_{ij}}\right) - \frac{\hbar^2}{4m}n_{ij}\frac{\partial}{\partial x}\left[\frac{1}{\sqrt{n_{ij}}}\frac{\partial^2\sqrt{n_{ij}}}{\partial x^2}\right] + \frac{\hbar^2}{2m}\frac{\partial}{\partial x}\left(n_{ij}T_{ij}\right)\,,$$

with $i,j = c,v$, and applying the isothermal closure conditions on the temperatures T_{ij}. The quantum correction term $\dfrac{1}{\sqrt{n_{ij}}}\dfrac{\partial^2\sqrt{n_{ij}}}{\partial x^2}$ can be interpreted as an internal self-potential, the so-called Bohm potential. The temperatures T_{ij} are defined by

$$T_{ij} = \frac{< P_+P_-w_{ij} >}{< w_{ij} >} - \frac{< P_+w_{ij} >< P_-w_{ij} >}{< w_{ij} >^2}\,,$$

where $< \cdot >$ is the mean value and $P_\pm = \dfrac{1}{2}\dfrac{\partial}{\partial x} \pm i\dfrac{mv}{\hbar}$.

For completeness we report the second order moment equations

$$\frac{\partial \mathcal{E}_{cc}}{\partial t} = -\frac{m}{2}\frac{\partial M_{cc}^{(3)}}{\partial x} + \frac{1}{q}V_c^{'}J_{cc} + \frac{i\hbar P}{2m}\frac{\partial}{\partial x}(\mathcal{E}_{cv} - \mathcal{E}_{vc}) - \frac{mP}{2}[M_{vc}^{(3)} + M_{cv}^{(3)}]$$

$$\begin{aligned}\frac{\partial \mathcal{E}_{cv}}{\partial t} = &-\frac{m}{2}\frac{\partial M_{cv}^{(3)}}{\partial x} + \frac{i\hbar}{8m}[V_v^{''} - V_c^{''}]n_{cv} + \frac{1}{2q}[V_v^{'} + V_c^{'}]J_{cv}\\ &- \frac{i}{\hbar}[V_v - V_c]\mathcal{E}_{cv} - \frac{i\hbar P}{2m}\frac{\partial}{\partial x}(\mathcal{E}_{vv} + \mathcal{E}_{cc}) - \frac{mP}{2}(M_{vv}^{(3)} - M_{cc}^{(3)})\end{aligned}$$

$$\frac{\partial \mathcal{E}_{vv}}{\partial t} = \frac{m}{2}\frac{\partial M_{vv}^{(3)}}{\partial x} - \frac{1}{q}V_v^{'}J_{vv} - \frac{i\hbar P}{2m}\frac{\partial}{\partial x}(\mathcal{E}_{cv} - \mathcal{E}_{vc}) - \frac{mP}{2}[M_{cv}^{(3)} + M_{vc}^{(3)}]\,.$$

3. Concluding remarks

A quantum hydrodynamic model is obtained directly from the set of zeroth, first and second order velocity moments of the Wigner equations for a two-band Kane model. In this contribution, we present some preliminary results for a two-band 1-D structure; the future research is oriented towards the

closure of the moment equations and towards the numerical validation of the model. The closure of the previous equations system can be done with different methods. The simpler one consists in assuming that the temperature is constant (isothermal assumption), for the zeroth and first moment equations. Otherwise, a closed set of equations can be obtained by means of the thermal equilibrium Wigner functions for the two-band semiconductor model, in the case of the Kane Hamiltonian[10], or using the maximum entropy principle[11].

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