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MATHEMATICAL STRUCTURE OF THE TRANSPORT EQUATIONS FOR COUPLED 2D-3D ELECTRON GASSES IN A MOSFET.

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Abstract. In a previous paper [1] we have studied the coexistence of coupled 2DEG and 3DEG in the proximity of a silicon-oxide interface in a MOSFET devising a hydrodynamical model obtained by taking the moment of the kinetic transport equation and by resorting to the maximum entropy principle for the closure relations. Here we classify the model from the point of view of PDEs by showing that it is hyperbolic in the relevant physical region of density, energy, velocity and energy fluxes in each subband and bulk electrons.

1 Introduction

In [1] we have presented a subband transport model for the description of charge transport in a MOSFET. Under the gate oxide, in the channel of the device, there is a quantization in the transversal direction forming a 2D electron gas but far from such a region electrons are 3D. Therefore one has to include the coexistence of both 2D and 3D electron gas inside the channel and only 3D electrons in the remaining part.

Starting from the Boltzmann equations, corresponding moment equations have been written and the closure problem, typical of such a kind of balance equations, has been solved by resorting to the maximum entropy principle. The obtained complete model is constituted by a set of balance equations for average density, velocity, energy and energy flux in each subband and for bulk electrons, coupled with the Schrödinger-Poisson system.

A crucial point has been how to take into account the transition of electrons from the 3DEG to the 2DEG. We have solved the problem inspired by the procedure used in [2]. If an electron belonging to the 2DEG gains an energy above a threshold value after a

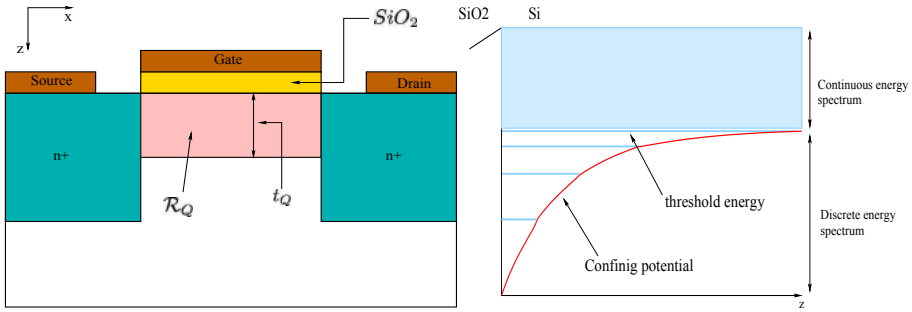

Figure 1: Simulated MOSFET (left). Energy spectrum along the transversal direction (right).

scattering, it is considered as 3D and vice versa if a 3D electron gets an energy below a threshold value after an emission process it is considered into the 2DEG.

Here we show how the range of variation of the threshold energy influences the mathematical structure of the balance equations.

2 Confinement effects in nanoscale MOSFET

In a MOSFET (fig.1-left), in the proximity of the silicon-oxide (Si/SiO_2) interface a two dimensional electron gas (2DEG) is created with a discrete energy spectrum along the z-direction (fig.1-right). Above a fixed energy level, the energy spectrum is continuous and a three dimensional electron gas (3DEG) coexists with the 2DEG. To describe the whole system, we define a spatial quantum region $\mathcal{R}_Q$ where the 2DEG is confined, associated with an energy quantum region $\mathcal{R}_E$ in the wave-vector space. Outside $\mathcal{R}_Q$ electrons are only belonging to the 3DEG.

In the quasi-static approximation, the 2D-charges in $\mathcal{R}_Q$ are described by the steady wave function $\psi_\nu(\mathbf{k},\mathbf{r}) = \psi_\nu(k_x,k_y,k_z,x,y,z) = \frac{1}{\sqrt{\mathcal{A}}}\phi_\nu(\mathbf{r}_{||},z)e^{i\mathbf{k}_{||}\cdot\mathbf{r}_{||}}$ with $\mathbf{k}_{||} = (k_x,k_y)$ and $\mathbf{r}_{||} = (x,y)$ denoting the longitudinal components of the wave-vector $\mathbf{k}$ and the position vector $\mathbf{r}$, respectively, and $\mathcal{A}$ symbolizing the area of the xy cross-section of $\mathcal{R}_Q$.

$\phi_\nu(\mathbf{r}_{||},z)$ is called envelope function and, under the scaling where the ratio between transversal and longitudinal characteristic lengths is small, it is solution of the Schrödinger equation $\left[-\frac{\hbar^2}{2m^*}\frac{d^2}{dz^2} - q(V_C+V)\right]\phi_\nu(\mathbf{r}_{||},z) = \varepsilon_\nu\phi_\nu(\mathbf{r}_{||},z)$ in the effective mass approximation. $\hbar$ is the reduced Planck constant, m^* is the effective electron mass, V_C is the confining potential and V is the self-consistent electrostatic potential which solves the Poisson equation. Note that $\mathbf{r}_{||}$ enters as a parameters.

Under the assumption that the confining potential gives rise to an infinite barrier at the oxide-silicon interface (z=0) and that a fictitious boundary is posed at $z = t_Q$, we solve the Schrödinger equation only inside the $\mathcal{R}_Q$ region by setting $\phi = 0$ at $z = 0$ and $z = t_Q$, the boundary of $\mathcal{R}_Q$. The problem is a self-adjoint problem posed on a limited domain. So one finds a countable set of normalized eigen-pairs (subbands) $(\phi_\nu,\varepsilon_\nu)$.

In each subband the energy E_ν is the sum of a transversal contribution $\varepsilon_\nu(\mathbf{r}_{||})$ and a

longitudinal (kinetic) contribution $\varepsilon_{||} = \frac{\hbar^2}{2m^*}(k_x^2 + k_y^2)$, that is $E_\nu(\mathbf{r}_{||}, \mathbf{k}_{||}) = \varepsilon_\nu(\mathbf{r}_{||}) + \varepsilon_{||}(\mathbf{k}_{||})$ and the corresponding longitudinal velocity is $\mathbf{v}_{||} = \frac{1}{\hbar}\nabla_{\mathbf{k}_{||}}\varepsilon_{||} = \frac{\hbar \mathbf{k}_{||}}{m^*}$.

We assume that above a threshold energy E_T electrons are 3D and therefore only the subbands with $E_\nu < E_T$ are retained. We will denote by ν_T the threshold subband index. Then $\mathbf{k}_{||} = (k_x, k_y) \in B_2^\nu$, where $B_2^\nu = \left\{(k_x, k_y) \in \mathbb{R}^2 : 0 \leq \frac{\hbar^2}{2m^*}(k_x^2 + k_y^2) \leq E_T - \varepsilon_\nu\right\}$ is the selected Brillouin zone for 2D electrons in the ν-th subband.

The Brillouin zone for the 3D electrons is $B_3^* = \{(k_x, k_y, k_z) \in \mathbb{R}^3 : \mathcal{E}(\mathbf{k}) \geq E_T\}$ where we are assuming a Kane dispersion relation $\mathcal{E}(\mathbf{k})\left[1 + \alpha\mathcal{E}(\mathbf{k})\right] = \frac{\hbar^2 k^2}{2m^*}$ in order to take into account the effetcs of nonparabolicity at high energies.

Under the assumption that the channel length is no shorter than few tents of nanometers, the transport of the carriers is assumed to be well described by semiclassical Boltzmann equations. 2D electrons in each subband are considered as different populations and for each subband it is introduced a distribution function $f_\nu(\mathbf{x}_{||}, \mathbf{k}_{||}, t)$ obeying the Boltzmann equation

$$\frac{\partial f_\nu(\mathbf{x}_{||}, \mathbf{k}_{||}, t)}{\partial t} + \mathbf{v}_{||} \cdot \nabla_{\mathbf{r}} f_\nu(\mathbf{x}_{||}, \mathbf{k}_{||}, t) - \frac{q}{\hbar}\mathbf{E}_\nu^{eff} \cdot \nabla_{\mathbf{k}} f_\nu(\mathbf{x}_{||}, \mathbf{k}_{||}, t) = C_\nu^{2D}, \quad \mathbf{k} \in B_2^\nu \tag{1}$$

where $\mathbf{E}_\nu^{eff} = \frac{1}{q}\nabla_{\mathbf{r}}\varepsilon(\mathbf{r}_{||})$ and C_ν^{2D} describes the scattering with phonons, including the mechanisms pushing 2D electrons into the 3DEG.

The 3DEG in the region $\mathcal{R}_Q$ is described by the Boltzmann equation

$$\frac{\partial f(\mathbf{x}, \mathbf{k}, t)}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{r}} f(\mathbf{x}, \mathbf{k}, t) - \frac{q}{\hbar}\mathbf{E} \cdot \nabla_{\mathbf{k}} f(\mathbf{x}, \mathbf{k}, t) = C^{3D}, \quad \mathbf{k} \in B_3^* \tag{2}$$

where $\mathbf{v} = \frac{1}{\hbar}\nabla_{\mathbf{k}}\mathcal{E} = \frac{1}{m^*}\frac{\hbar \mathbf{k}}{1+2\alpha\mathcal{E}}$ is the electron group velocity.
C^{3D} represents the scattering of 3D electrons with phonons, including the mechanisms pushing 3D electrons into the 2DEG. $\mathbf{E} = -\nabla_{\mathbf{r}} V$ is the self-consistent electric field which is related to the electron distributions function through Poisson's equation $\nabla\left(\epsilon\nabla V\right) = -q\left(n_d(\mathbf{r}) - n_T(\mathbf{r})\right)$, with ϵ the relative permittivity, $n_d(\mathbf{r})$ the doping concentration and $n_T(\mathbf{r})$ the total charge density given by $n_T(\mathbf{r}, t) = n(\mathbf{r}, t) + \sum_{\nu=1}^{\nu_T} \rho_\nu(x, y, t)|\phi_\nu(z, t)|^2$ with $n(\mathbf{r}, t) = \int_{B_3^*} f(\mathbf{x}, \mathbf{k}, t) d^3\mathbf{k}$ the density of the bulk electrons, and $\rho^\nu\left(\mathbf{r}_{||}, t\right) = \int_{B_2^\nu} f_\nu(\mathbf{r}_{||}, \mathbf{k}_{||}, t) d^2\mathbf{k}_{||}$ the areal density of electrons in the ν-th subband.

All the main scattering processes have been considered, that is those due to acoustic phonons in the elastic approximation and non polar optical phonons, that cause the particles exchange between 2DEG and 3DEG. The reader is referred to [1] for the details.

3 The moment system and its closure by the MEP

We now write a system of moment equations deduced from Boltzmann transport equations under suitable closure relations. Let us define the generic moment associated with electrons in the subband ν with respect to a weight function $a(\mathbf{k}_{||})$ as

$$M_a\left(\mathbf{r}_{||}, t)\right) = \int a(\mathbf{k}_{||}) f(\mathbf{r}, \mathbf{k}_{||}, t) d^2\mathbf{k}_{||}.$$

In particular we take as basic moments for the 2DEG the following ones

$$\text{areal density} \quad \rho^\nu\left(\mathbf{r}_{||},t\right)\big) = \int_{B_2^\nu} f_\nu(\mathbf{r}_{||},\mathbf{k}_{||},t)d^2\mathbf{k}_{||}$$

$$\text{longitudinal mean velocity} \quad \mathbf{V}^\nu\left(\mathbf{r}_{||},t\right)\big) = \frac{1}{\rho^\nu\left(\mathbf{r}_{||},t\right)}\int_{B_2^\nu} \mathbf{v}_{||} f_\nu(\mathbf{r}_{||},\mathbf{k}_{||},t)d^2\mathbf{k}_{||}$$

$$\text{longitudinal mean energy} \quad W^\nu\left(\mathbf{r}_{||},t\right)\big) = \frac{1}{\rho^\nu\left(\mathbf{r}_{||},t\right)}\int_{B_2^\nu} \varepsilon_{||} f_\nu(\mathbf{r}_{||},\mathbf{k}_{||},t)d^2\mathbf{k}_{||}$$

$$\text{longitudinal mean energy flux} \quad \mathbf{S}^\nu\left(\mathbf{r}_{||},t\right)\big) = \frac{1}{\rho^\nu\left(\mathbf{r}_{||},t\right)}\int_{B_2^\nu} \varepsilon_{||}\mathbf{v}_{||} f_\nu(\mathbf{r}_{||},\mathbf{k}_{||},t)d^2\mathbf{k}_{||}$$

The corresponding moment system is obtained by multiplying the Boltzmann equation by the weight functions entering into the definition of the fundamental moments and by integrating with respect to $\mathbf{k}_{||}$. Explicitly we get

$$\frac{\partial\rho^\nu}{\partial t} + \nabla_{\mathbf{r}_{||}}\cdot(\rho^\nu\mathbf{V}_\nu) + \rho^\nu L_0^\nu = \rho^\nu C_{\rho_\nu}^{(ac)} + \rho^\nu C_{\rho_\nu}^{(no)} + \rho^\nu C_{\rho_\nu}^{(no),3D} \tag{3}$$

$$\frac{\partial}{\partial t}(\rho^\nu\mathbf{V}^\nu) + \nabla_{\mathbf{r}_{||}}\cdot(\rho^\nu\mathbf{F}^{(0)\nu}) + (\rho^\nu\mathbf{G}^{(0)\nu})\cdot\nabla_{\mathbf{r}_{||}}\varepsilon_\nu = \rho^\nu C_{\mathbf{V}^\nu}^{(ac)} + \rho^\nu C_{\mathbf{V}^\nu}^{(no)} + \rho^\nu C_{\mathbf{V}^\nu}^{(no),3D} \tag{4}$$

$$\frac{\partial}{\partial t}(\rho^\nu W^\nu) + \nabla_{\mathbf{r}_{||}}\cdot(\rho^\nu\mathbf{S}^\nu) + (\rho^\nu\mathbf{V}^\nu)\cdot\nabla_{\mathbf{r}_{||}}\varepsilon_\nu + \rho^\nu L_1^\nu = \rho^\nu C_W^{(ac)} + \rho^\nu C_W^{(no)} + \rho^\nu C_W^{(no),3D} \tag{5}$$

$$\frac{\partial}{\partial t}(\rho^\nu\mathbf{S}^\nu) + \nabla_{\mathbf{r}_{||}}\cdot(\rho_\nu\mathbf{F}^{(1)\nu}) + (\rho_\nu\mathbf{G}^{(1)\nu})\cdot\nabla_{\mathbf{r}_{||}}\epsilon_\nu = \rho_\nu C_{\mathbf{S}^\nu}^{(ac)} + \rho_\nu C_{\mathbf{S}^\nu}^{(no)} + \rho_\nu C_{\mathbf{S}^\nu}^{(no),3D} \tag{6}$$

where

$$\begin{pmatrix}\mathbf{F}^{(0)\nu}\\ \mathbf{F}^{(1)\nu}\end{pmatrix} = \frac{1}{\rho^\nu}\int_{B_2^\nu}\begin{pmatrix}1\\ \varepsilon_{||}\end{pmatrix}\mathbf{v}_{||}\otimes\mathbf{v}_{||}\, f_\nu(\mathbf{r}_{||},\mathbf{k}_{||},t)\, d^2\mathbf{k}_{||},$$

$$\begin{pmatrix}\mathbf{G}^{(0)\nu}\\ \mathbf{G}^{(1)\nu}\end{pmatrix} = -\frac{1}{\rho^\nu}\int_{B_2^\nu}\begin{pmatrix}\frac{1}{\hbar}\mathbf{v}_{||}\nabla_{\mathbf{k}_{||}}\\ \frac{1}{\hbar}\varepsilon_{||}\mathbf{v}_{||}\nabla_{\mathbf{k}_{||}}\end{pmatrix} f_\nu(\mathbf{r}_{||},\mathbf{k}_{||},t)\, d^2\mathbf{k}_{||},$$

$$\begin{pmatrix}C_{\rho_\nu}\\ C_{W_\nu}\end{pmatrix} = \frac{1}{\rho^\nu}\int_{B_2^\nu}\begin{pmatrix}1\\ \varepsilon_{||}\end{pmatrix}\left[S_{\mu\nu}(\mathbf{k}'_{||},\mathbf{k}_{||})\, f'_\mu - S_{\nu\mu}(\mathbf{k}_{||},\mathbf{k}'_{||})\, f_\nu\right]\, d^2\mathbf{k}'_{||}\, d^2\mathbf{k}_{||},$$

$$\begin{pmatrix}C_{\mathbf{V}_\nu}\\ C_{\mathbf{S}_\nu}\end{pmatrix} = \frac{1}{\rho^\nu}\int_{B_2^\nu}\begin{pmatrix}\mathbf{v}_{||}\\ \varepsilon_{||}\mathbf{v}_{||}\end{pmatrix}\left[S_{\mu\nu}(\mathbf{k}'_{||},\mathbf{k}_{||})\, f'_\mu - S_{\nu\mu}(\mathbf{k}_{||},\mathbf{k}'_{||})\, f_\nu\right]\, d^2\mathbf{k}'_{||}\, d^2\mathbf{k}_{||}$$

$$L_0^\nu = -\frac{1}{\hbar\rho^\nu}\nabla_{\mathbf{r}_{||}}\varepsilon_\nu\int_{B_2^\nu}\nabla_{\mathbf{k}_{||}} f_\nu d^2\mathbf{k}_{||}, \quad L_1^\nu = -\frac{1}{\hbar\rho^\nu}\nabla_{\mathbf{r}_{||}}\varepsilon_\nu\int_{B_2^\nu}\nabla_{\mathbf{k}_{||}}(\varepsilon_{||} f_\nu)d^2\mathbf{k}_{||}.$$

It is worth to underline here that the two last drift terms (L_0^ν and L_1^ν) are due to the anisotropy of the distribution function. Usually they do not appear in the constitutive

equations of the carriers transport because the boundary of the first Brillouin zone is moved to infinity or the distribution function is symmetric on this boundary.

In a similar way, the basic moments we take for 3D electrons are the following ones

$$\text{density} \quad n(\mathbf{r},t) = \int_{B_3^*} f(\mathbf{r},\mathbf{k},t)d^3\mathbf{k}$$

$$\text{mean velocity} \quad \mathbf{V}(\mathbf{r},t) = \frac{1}{n(\mathbf{r},t)}\int_{B_3^*} \mathbf{v}(\mathbf{k})f(\mathbf{r},\mathbf{k},t)d^3\mathbf{k}$$

$$\text{mean energy} \quad W(\mathbf{r},t) = \frac{1}{n(\mathbf{r},t)}\int_{B_3^*} \varepsilon(\mathbf{k})f(\mathbf{r},\mathbf{k},t)d^3\mathbf{k}$$

$$\text{mean energy flux} \quad \mathbf{S}(\mathbf{r},t) = \frac{1}{n(\mathbf{r},t)}\int_{B_3^*} \varepsilon(\mathbf{k})\,\mathbf{v}(\mathbf{k})f(\mathbf{r},\mathbf{k},t)d^3\mathbf{k}.$$

and the corrisponding moments system reads

$$\frac{\partial n}{\partial t} + \nabla_{\mathbf{r}}\Big(n(\mathbf{r},t)\mathbf{v}(\mathbf{n},t)\Big) = nC_n^{(ac)} + nC_n^{(no)} + nC_n^{(no),2D} \tag{7}$$

$$\frac{\partial}{\partial t}(n\mathbf{v}) + \nabla_{\mathbf{r}}\Big(n\mathbf{F}^{(0)}\Big) + q\mathbf{E}\Big(n\mathbf{G}^{(0)}\Big) = nC_{\mathbf{V}}^{(ac)} + nC_{\mathbf{V}}^{(no)} + nC_{\mathbf{V}}^{(no),2D} \tag{8}$$

$$\frac{\partial}{\partial t}(nW) + \nabla_{\mathbf{r}}\Big(n\mathbf{S}\Big) + q\mathbf{E}\Big(n\mathbf{V}\Big) = nC_W^{(ac)} + nC_W^{(no)} + nC_W^{(no),2D} \tag{9}$$

$$\frac{\partial}{\partial t}(n\mathbf{S}) + \nabla_{\mathbf{r}}(n\mathbf{F}^{(1)}) + q\mathbf{E}(n\mathbf{G}^{(1)}) = nC_{\mathbf{S}}^{(ac)} + nC_{\mathbf{S}}^{(no)} + nC_{\mathbf{S}}^{(no),2D} \tag{10}$$

with analogous definition to the previous ones for $\mathbf{F}^{(0)}, \mathbf{F}^{(1)}, \mathbf{G}^{(0)}, \mathbf{G}^{(1)}$ and the production terms.

The above written moment systems are not closed because there are more unknowns than equations. Therefore, constitutive relations in terms of the fundamentals variables are needed for extra fluxes and production terms. The maximum entropy principle leads to a systematic way for obtaining constitutive relations on the basis of information theory and has been widely used for semiconductor modeling (see for example[3, 4, 5, 6]).

According to the MEP, if a given number of moments of f_ν

$$M_{a_A}^{\nu}\left(\mathbf{r}_{||},\mathbf{k}_{||},t)\right), \quad A = 1,.....,N_\nu \quad \text{and} \quad \nu = 1,2\ldots$$

are known along with a given number of moments of f

$$M_{b_B}\left(\mathbf{r},\mathbf{k},\mathbf{t}\right) \quad B = 1,2,\ldots N$$

the distribution functions $f\left(\mathbf{r},\mathbf{k},\mathbf{t}\right)$, $f_\nu\left(\mathbf{r}_{||},\mathbf{k}_{||},t\right)\big)$, $\nu = 1,2\ldots$, can be estimated by the extremal $(f^{MEP}, f_1^{MEP}, f_2^{MEP}, ...)$ of the entropy functional under the constrains

$$\int_{B_2^\nu} a_A(\mathbf{k}_{||}) f_\nu^{MEP}\left(\mathbf{r}_{||},\mathbf{k}_{||},t)\right) d\mathbf{k} = M_{a_A}^{\nu}\left(\mathbf{r}_{||},t)\right) \quad A = 1,...,N_\nu, \quad \nu = 1,2,\ldots$$

$$\int_{B_3^*} b_B(\mathbf{k})\, f^{MEP}(\mathbf{r},\mathbf{k},t)d^3\mathbf{k} = M_{b_B}\left(\mathbf{r},\mathbf{t}\right) \quad B = 1,2,\ldots N.$$

Following the approach in [3, 4, 5], we assume the following definition

Definition 1 *We define the entropies of the two subsystems, 2DEG and 3DEG, as*

$$\mathcal{S}_{2D} = -k_B \sum_{\nu=1}^{+\infty} |\phi_\nu(z,t)|^2 \int_{B_2^\nu} \left(f_\nu \log \frac{f_\nu}{y} - f_\nu \right) d^2\boldsymbol{k}_{||}, \quad y = \frac{2}{(2\pi)^2},$$
$$\mathcal{S}_{3D} = -k_B \int_{B_3^*} f(\boldsymbol{k}) \left[\log f(\boldsymbol{k}) - 1 \right] d^3\boldsymbol{k}$$

The total entropy is of course $\mathcal{S} = \mathcal{S}_{2D} + \mathcal{S}_{3D}$. Therefore, according to MEP and our choice of the basic moments in the case we are dealing with, f and the f_ν's are estimated with the distributions f^{MEP} and f_ν^{MEP}'s that solve the problem:

maximize $\mathcal{S}$ under the constraints

$$\int_{B_3^*} f^{MEP}(\mathbf{r},\mathbf{k},t) d^3\mathbf{k} = n(\mathbf{r},t), \int_{B_3^*} \mathbf{v}(\mathbf{k}) f^{MEP}(\mathbf{r},\mathbf{k},t) d^3\mathbf{k} = n(\mathbf{r},t)\mathbf{V}(\mathbf{r},t) \tag{11}$$
$$\int_{B_3^*} \varepsilon(\mathbf{k}) f^{MEP}(\mathbf{r},\mathbf{k},t) d^3\mathbf{k} = n(\mathbf{r},t)\, W(\mathbf{r},t), \int_{B_3^*} \varepsilon\mathbf{v} f^{MEP}(\mathbf{r},\mathbf{k},t) d^3\mathbf{k} = n(\mathbf{r},t)\, \mathbf{S}(\mathbf{r},t) \tag{12}$$

and for $\nu = 1, 2, \ldots$

$$\int_{B_2^\nu} f_\nu(\mathbf{r}_{||},\mathbf{k}_{||},t) d^2\mathbf{k}_{||} = \rho^\nu\left(\mathbf{r}_{||},t\right), \int_{B_2^\nu} \mathbf{v}_{||} f_\nu(\mathbf{r}_{||},\mathbf{k}_{||},t) d^2\mathbf{k}_{||} = \rho^\nu\left(\mathbf{r}_{||},t\right) \mathbf{V}^\nu\left(\mathbf{r}_{||},t\right)\big) \tag{13}$$
$$\int_{B_2^\nu} \varepsilon_{||} f_\nu(\mathbf{r}_{||},\mathbf{k}_{||},t) d^2\mathbf{k}_{||} = \rho^\nu\left(\mathbf{r}_{||},t\right) W^\nu\left(\mathbf{r}_{||},t\right), \tag{14}$$
$$\int_{B_2^\nu} \varepsilon_{||}\mathbf{v}_{||} f_\nu(\mathbf{r}_{||},\mathbf{k}_{||},t) d^2\mathbf{k}_{||} = \rho^\nu\left(\mathbf{r}_{||},t\right) \mathbf{S}^\nu\left(\mathbf{r}_{||},t\right) \tag{15}$$

One has

$$f_\nu^{MEP} = \exp\left[-\left(\lambda^\nu + \lambda_{\mathbf{V}}^\nu \cdot \mathbf{v}_{||} + \left(\lambda_W^\nu + \lambda_{\mathbf{S}}^\nu \cdot \mathbf{v}_{||}\right)\varepsilon_{||}\right)\right] \quad \nu = 1, 2, \ldots \tag{16}$$
$$f^{MEP} = \exp\left[-(\lambda + \lambda_{\mathbf{V}} \cdot \mathbf{v} + (\lambda_W + \lambda_{\mathbf{S}} \cdot \mathbf{v})\varepsilon)\right] \tag{17}$$

Now, following the same approach as in [4, 5], we assume a small anisotropy of the distribution functions and expand them up to first order with respect to the lagrangian multipliers relative to velocity and energy-flux

$$f_\nu^{MEP} \approx \exp\left(-\lambda^\nu - \lambda_W^\nu \varepsilon_{||}\right)\left[1 - \left(\lambda_{\mathbf{V}}^\nu \cdot \mathbf{v}_{||} + \lambda_{\mathbf{S}}^\nu \cdot \mathbf{v}_{||}\varepsilon_{||}\right)\right], \tag{18}$$
$$f^{MEP} \approx \exp(-\lambda^B - \lambda_W^B \varepsilon)[1 - (\lambda_{\mathbf{V}}^B \cdot \mathbf{v} + \lambda_{\mathbf{S}}^B \cdot \mathbf{v}\varepsilon)] \tag{19}$$

Inserting the above-written expansions into the constraints (11)-(15), it is possible to get analytical explicit expressions of the lagrangian multipliers and in turn to get the closure relations for the moment system.

4 Closure relations for the 2DEG

The Lagrange's multipliers of the subbands into the 2DEG are

$$\rho^\nu = \frac{2\pi m^*}{\hbar^2} e^{-\lambda^\nu} I_0^\nu, \quad W^\nu = \frac{1}{\lambda_W^\nu}\left[1 + \frac{\lambda_W^\nu (E_T - \varepsilon_\nu)}{1 - e^{\lambda_W^\nu (E_T - \varepsilon_\nu)}}\right], \tag{20}$$

$$\lambda_{\mathbf{V}}^\nu = b_{11}(W^\nu)\mathbf{V}^\nu + b_{12}(W^\nu)\mathbf{S}^\nu, \quad \lambda_{\mathbf{S}}^\nu = b_{21}(W^\nu)\mathbf{V}^\nu + b_{22}(W^\nu)\mathbf{S}^\nu \tag{21}$$

where

$$b_{11} = -\frac{m^*\mathcal{I}_0^\nu}{\Delta_\nu}\mathcal{I}_3^\nu,\ b_{22} = -\frac{m^*\mathcal{I}_0^\nu}{\Delta_\nu}\mathcal{I}_1^\nu, b_{12} = b_{21} = \frac{m^*\mathcal{I}_0^\nu}{\Delta_\nu}\mathcal{I}_2^\nu, \quad \Delta_\nu = \mathcal{I}_1^\nu\mathcal{I}_3^\nu - (\mathcal{I}_2^\nu)^2$$

with

$$\mathcal{I}_0^\nu = \frac{1 - e^{-\lambda_W^\nu (E_T - \varepsilon_\nu)}}{\lambda_W^\nu}, \quad \mathcal{I}_n^\nu = (-1)^n \frac{d^n}{d(\lambda_W^\nu)^n}\mathcal{I}_0^\nu, \quad n = 0, 1, 2, ...$$

Once the lagrangian multipliers have been obtained, we can calculate the extra fluxes and the drift and production terms. The fluxes read

$$\mathbf{F}^{(0)\nu} = \frac{\mathcal{I}_1^\nu}{m^*\mathcal{I}_0^\nu}\mathbf{I}, \quad \mathbf{F}^{(1)\nu} = \frac{\mathcal{I}_2^\nu}{m^*\mathcal{I}_0^\nu}\mathbf{I}, \tag{22}$$

for the other expressions the reader is referred to [1]. A crucial point is that there exists [1] the critical values $W_c^\nu = \dfrac{E_T - \varepsilon_\nu}{2}$ such that $\lambda_W^\nu(W_c^\nu) = 0$. Therefore the allowed values of the longitudinal average energy are $k_B T_L < W^\nu < W_c^\nu$.

5 Closure relations for the 3DEG

In the same manner as for the 2DEG, explicit formulas for the closure relations of the 3DEG part of the moment system are obtained. The lagrangian multipliers are given by the following relationships

$$n = \frac{4\pi m^* \sqrt{2m^*}}{\hbar^3} e^{-\lambda^B}\mathcal{I}(E_T, \lambda_W^B), \quad W = -\frac{d}{d\lambda_W^B}\ln \mathcal{I}(E_T, \lambda_W^B) \tag{23}$$

$$\lambda_{\mathbf{V}}^B = B_{11}\mathbf{V} + B_{12}\mathbf{S}, \quad \lambda_{\mathbf{V}}^B = B_{21}\mathbf{V} + B_{22}\mathbf{S} \tag{24}$$

with

$$B_{11} = -\frac{3m^*}{2\Delta}\mathcal{I}(E_T, \lambda_W^B)\mathcal{L}^{(2)}(E_T, \lambda_W^B),\ B_{22} = -\frac{3m^*}{2\Delta}\mathcal{I}(E_T, \lambda_W^B)\mathcal{L}^{(0)}(E_T, \lambda_W^B),$$

$$B_{12} = B_{21} = \frac{3m^*}{2\Delta}\mathcal{I}(E_T, \lambda_W^B)\mathcal{L}^{(1)}(E_T, \lambda_W^B),$$

$$\Delta = \mathcal{L}^{(0)}(E_T, \lambda_W^B)\mathcal{L}^{(2)}(E_T, \lambda_W^B) - (\mathcal{L}^{(1)}(E_T, \lambda_W^B))^2$$

$$\mathcal{I}(x, \beta) = \int_x^{+\infty} (1 + 2\alpha\varepsilon)\sqrt{\varepsilon(1 + \alpha\varepsilon)}e^{-\beta\varepsilon}d\varepsilon$$

$$\mathcal{L}^{(0)}(x, \beta) = \int_x^{+\infty} e^{-\beta\varepsilon}\frac{[\varepsilon(1 + \alpha\varepsilon)]^{3/2}}{1 + 2\alpha\varepsilon}d\varepsilon,\ \mathcal{L}^{(n)}(x, \beta) = (-1)^n\frac{d^n}{d(\beta)^n}\mathcal{L}^{(0)}(x, \beta)$$

Once λ_W has been obtained via a numerical inversion, the extra fluxes and production terms can be obtained. Here we show only the flux expressions (see [1] for others details).

$$\mathbf{F}^{(0)} = \frac{2}{3m^*\mathcal{I}(E_T,\lambda_W^B)}\mathcal{L}^{(0)}(E_T,\lambda_W^B),\ \mathbf{F}^{(1)} = \frac{2}{3m^*\mathcal{I}(E_T,\lambda_W^B)}\mathcal{L}^{(1)}(E_T,\lambda_W^B)$$

At variance with the 2DEG, no upper limit for the energy density arises.

6 Mathematical structure of the moment system closed with MEP

We want to give *a strong numerical evidence that the moment system of the subbands and bulk electrons augmented with the MEP closure relations forms a quasilinear hyperbolic system* in the time direction in the physically relevant range of W^ν. This preliminary analysis is crucial for the development of appropriate numerical schemes.

Since the differential part of each subband and of the 3DEG is decoupled in the moment system, we can limit our analysis to the study of a single subband and the 3DEG. Let us consider the quasilinear system of PDEs

$$\frac{\partial}{\partial t}\mathcal{F}^{(0)}(\mathbf{U}) + \sum_{i=1}^{2}\frac{\partial}{\partial x^i}\mathcal{F}^{(i)}(\mathbf{U}) = \mathcal{P}(\mathbf{U},\mathbf{x},t), \tag{25}$$

with $\mathbf{U}(\mathbf{x},t)$ vector field belonging to a connected open set $\Omega \subset \mathbb{R}^m$, $\forall\, t > 0$ and $\forall\, \mathbf{x}$ belonging to a domain $D \subseteq \mathbb{R}^k$ with $k = 2$ for th 2DEG or $k = 3$ for the 3DEG, and $\mathcal{F}^{(\beta)} : \Omega \mapsto \mathbb{R}^m,\quad \beta = 0,\ldots,k$ sufficiently smooth functions. Defining the Jacobian matrices

$$\mathcal{A}^{(\beta)} = \nabla_{\mathbf{U}}\mathcal{F}^{(\beta)},\quad \beta = 0,\ldots,k,$$

we recall that the system (25) is said to be *hyperbolic in the t-direction* if $\det\left(\mathcal{A}^{(0)}(\mathbf{U})\right) \neq 0$ and the eigenvalue problem

$$\det\left(\sum_{i=1}^{2} n_i\mathcal{A}^{(i)}(\mathbf{U}) - \lambda\mathcal{A}^{(0)}(\mathbf{U})\right) = 0 \tag{26}$$

has real eigenvalues and the eigenvectors span $\mathbb{R}^m$ for all unit vectors $\mathbf{n} = (n_1,\ldots,n_k)$ of $\mathbb{R}^k$. Will first treat the case of a generic subband and then the 3DEG case.

6.1 Iperbolicity of the generic subband subsystem

In the case under consideration, by omitting the subband index, we have

$$\mathbf{U} = \begin{pmatrix} \rho \\ V^1 \\ V^2 \\ W \\ S^1 \\ S^2 \end{pmatrix},\quad \mathcal{F}^{(0)} = \rho\begin{pmatrix} 1 \\ V^1 \\ V^2 \\ W \\ S^1 \\ S^2 \end{pmatrix},\quad \mathcal{F}^{(1)} = \rho\begin{pmatrix} V^1 \\ F^{(0)} \\ 0 \\ S^1 \\ F^{(1)} \\ 0 \end{pmatrix},\quad \mathcal{F}^{(2)} = \rho\begin{pmatrix} V^2 \\ 0 \\ F^{(0)} \\ S^2 \\ 0 \\ F^{(1)} \end{pmatrix},$$

and the Jacobian matrices are given by

$$\mathcal{A}^{(0)}=\begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ V^1 & \rho & 0 & 0 & 0 & 0 \\ V^2 & 0 & \rho & 0 & 0 & 0 \\ W & 0 & 0 & \rho & 0 & 0 \\ S^1 & 0 & 0 & 0 & \rho & 0 \\ S^2 & 0 & 0 & 0 & 0 & \rho \end{pmatrix}, \quad \mathcal{A}^{(n)}=\sum_{i=1}^{2} n_i \mathcal{A}^{(i)}=\begin{pmatrix} \mathbf{n}\cdot\mathbf{V} & n_1\rho & n_2\rho & 0 & 0 & 0 \\ n_1F^{(0)} & 0 & 0 & n_1\rho(F^{(0)})' & 0 & 0 \\ n_2F^{(0)} & 0 & 0 & n_2\rho(F^{(0)})' & 0 & 0 \\ \mathbf{n}\cdot\mathbf{S} & 0 & 0 & 0 & n_1\rho & n_2\rho \\ n_1F^{(1)} & 0 & 0 & n_1\rho(F^{(1)})' & 0 & 0 \\ n_2F^{(1)} & 0 & 0 & n_2\rho(F^{(1)})' & 0 & 0 \end{pmatrix},$$

where the prime denotes partial derivation with respect to W.

The equation

$$\det\left(\mathcal{A}^{(n)}-\lambda\mathcal{A}^{(0)}\right)=0$$

gives the eigenvalues

$$\lambda_{1,2}=0, \quad \text{with multiplicity } 2 \tag{27}$$

$$\lambda_{3,4,5,6}=\pm\sqrt{\frac{a(W)\pm\sqrt{a(W)^2-4b(W)}}{2}} \tag{28}$$

where

$$a(W)=F^{(0)}+(F^{(1)})'-W(F^{(0)})', \quad b(W)=F^{(0)}(F^{(1)})'-(F^{(0)})'F^{(1)}.$$

In Fig. 2 the eigenvalues $\lambda_{3,4,5,6}$ are plotted against the longitudinal mean energy W for several values of $E_T-\varepsilon_\nu$ in the range belonging to the realizability region. Since the four eigenvalues $\lambda_{3,4,5,6}$ are real and distinct, each of them has a corresponding eigenspace of dimension one.

Concerning the eigenvalue $\lambda=0$, we observe that whatever $\mathbf{n}$ we take the first and fourth rows of $\mathcal{A}^{(n)}$ are linearly independent, the second and third rows are proportional and similarly the last two rows since $\rho>0$ and n_1 and n_2 cannot be both zero. We observe that

$$\det\begin{pmatrix} F^{(0)} & \rho(F^{(0)})' \\ F^{(1)} & \rho(F^{(1)})' \end{pmatrix}=\rho\, b(W).$$

The fact that the eigenvalues $\lambda_{3,4,5,6}$ are real implies that $b(W)>0$ and therefore the rank of $\mathcal{A}^{(n)}$ is four which means that the eigenspace associated to $\lambda=0$ has dimension two, leading to the hyperbolicity of the system (25) in the physical region $\rho>0$ and $k_BT_L<W^\nu<W_c^\nu$.

In the one dimensional case one has only the eigenvalues $\lambda_{3,4,5,6}$ and by similar computations the hyperbolicity is again guarenteed.

Remark 1 *In the particular case $E_T\mapsto\infty$ we explicitly have*

$$\lambda_{3,4,5,6}=\pm\sqrt{\left(2\pm\sqrt{2}\right)\frac{W}{m^*}}$$

which are real and distinct provided $W>0$ according to [4].

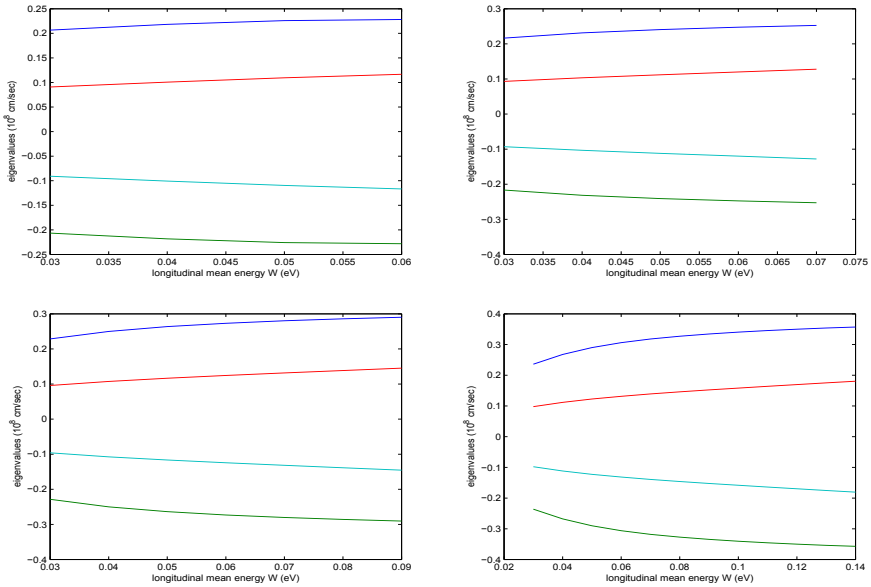

Figure 2: Plot of $\lambda_{3,4,5,6}$ versus the longitudinal mean energy for $E_T - \varepsilon_\nu = 0.125$ (upper left), 015 (upper right), 02 (bottom left), 03 (bottom right) eV.

6.2 Hyperbolicity of the 3DEG subsystem

In a similar way we have for the 3DEG

$$\mathbf{U} = \begin{pmatrix} \rho \\ V^1 \\ V^2 \\ V^3 \\ W \\ S^1 \\ S^2 \\ S^3 \end{pmatrix}, \quad \mathcal{F}^{(0)} = n \begin{pmatrix} 1 \\ V^1 \\ V^2 \\ V^3 \\ W \\ S^1 \\ S^2 \\ S^3 \end{pmatrix}, \quad \mathcal{F}^{(1)} = n \begin{pmatrix} V^1 \\ F^{(0)} \\ 0 \\ 0 \\ S^1 \\ F^{(1)} \\ 0 \\ 0 \end{pmatrix},$$

$$\mathcal{F}^{(2)} = n \begin{pmatrix} V^2 \\ 0 \\ F^{(0)} \\ 0 \\ S^2 \\ 0 \\ F^{(1)} \\ 0 \end{pmatrix}, \quad \mathcal{F}^{(3)} = n \begin{pmatrix} V^3 \\ 0 \\ 0 \\ F^{(0)} \\ S^3 \\ 0 \\ 0 \\ F^{(1)} \end{pmatrix}$$

and the Jacobian matrices are given by

$$\mathcal{A}^{(0)} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ V^1 & n & 0 & 0 & 0 & 0 & 0 & 0 \\ V^2 & 0 & n & 0 & 0 & 0 & 0 & 0 \\ V^3 & 0 & 0 & n & 0 & 0 & 0 & 0 \\ W & 0 & 0 & 0 & n & 0 & 0 & 0 \\ S^1 & 0 & 0 & 0 & 0 & n & 0 & 0 \\ S^2 & 0 & 0 & 0 & 0 & 0 & n & 0 \\ S^3 & 0 & 0 & 0 & 0 & 0 & 0 & n \end{pmatrix},$$

$$\mathcal{A}^{(n)} = \sum_{i=1}^{2} n_i \mathcal{A}^{(i)} = \begin{pmatrix} \mathbf{n}\cdot\mathbf{V} & n_1 n & n_2\rho & n_3 n & 0 & 0 & 0 & 0 \\ n_1 F^{(0)} & 0 & 0 & 0 & n_1 n (F^{(0)})' & 0 & 0 & 0 \\ n_2 F^{(0)} & 0 & 0 & 0 & n_2 n (F^{(0)})' & 0 & 0 & 0 \\ n_3 F^{(0)} & 0 & 0 & 0 & n_3 n (F^{(0)})' & 0 & 0 & 0 \\ \mathbf{n}\cdot\mathbf{S} & 0 & 0 & 0 & 0 & n_1 n & n_2 n & n_3 n \\ n_1 F^{(1)} & 0 & 0 & 0 & n_1 n (F^{(1)})' & 0 & 0 & 0 \\ n_2 F^{(1)} & 0 & 0 & 0 & n_2 n (F^{(1)})' & 0 & 0 & 0 \\ n_3 F^{(1)} & 0 & 0 & 0 & n_3 n (F^{(1)})' & 0 & 0 & 0 \end{pmatrix},$$

where the prime denotes partial derivation respect to W. The equation

$$\det\left(\mathcal{A}^{(n)} - \lambda \mathcal{A}^{(0)}\right) = 0$$

gives the eigenvalues

$$\lambda_{1,2,3,4} = 0, \quad \text{with multiplicity } 4 \tag{29}$$

$$\lambda_{5,6,7,8} = \pm\sqrt{\frac{a(W) \pm \sqrt{a(W)^2 - 4b(W)}}{2}} \tag{30}$$

where, assuming the same notation of the previous case,

$$a(W) = F^{(0)} + (F^{(1)})' - W(F^{(0)})', \quad b(W) = F^{(0)}(F^{(1)})' - (F^{(0)})' F^{(1)}.$$

In Fig. 3 the eigenvalues $\lambda_{5,6,7,8}$ are plotted against the longitudinal mean energy W for several values of E_T. Since the four eigenvalues $\lambda_{5,6,7,8}$ are real and distinct, each of them has a corresponding eigenspace of dimension one.

Concerning the eigenvalue $\lambda = 0$, we use arguments similar to that used previously and, assuming $n_1 = 1, n_2 = n_3 = 0$, observe that

$$\det \begin{pmatrix} \mathbf{nV} & n_1 n & 0 & 0 \\ n_1 F^{(0)} & 0 & n_1 n (F^{(0)})' & 0 \\ \mathbf{nS} & 0 & 0 & n_1 n \\ n_1 F^{(1)} & 0 & n_1 n (F^{(1)})' & 0 \end{pmatrix} = n^3 b(W).$$

The fact that the eigenvalues $\lambda_{5,6,7,8}$ are real implies that $b(W) > 0$ and therefore the rank of $\mathcal{A}^{(n)}$ is four which means that the eigenspace associated to $\lambda = 0$ has dimension four, leading to the hyperbolicity of the system (25) in the physical region $n > 0$.

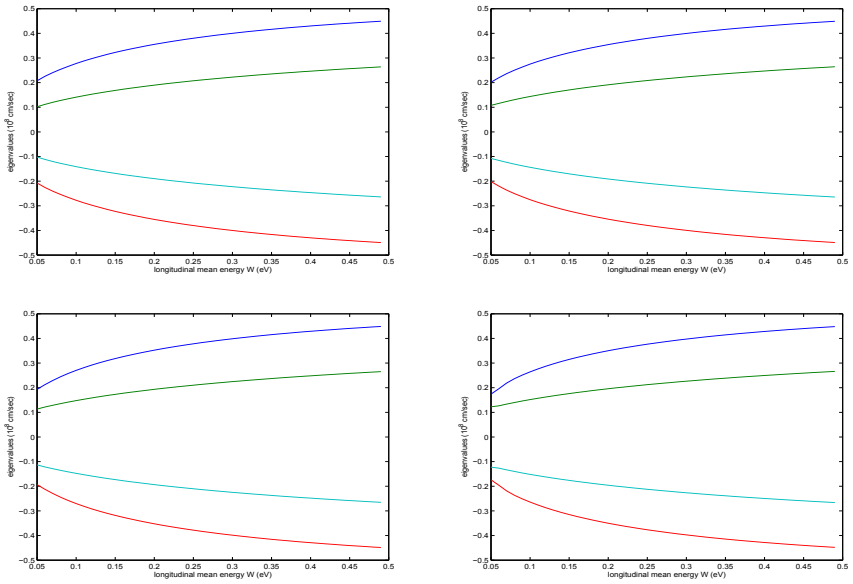

Figure 3: Plot of $\lambda_{3,4,5,6}$ versus the longitudinal mean energy for $E_T = 0.00$ (upper left), 0.10 (upper right), 0.20 (bottom left), 0.30 (bottom right) eV.

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