IL NUOVO CIMENTO Vol. 33 C, N. 1 Gennaio-Febbraio 2010
DOI 10.1393/ncc/i2010-10578-0

Colloquia: ICTT2009

Hydrodynamic subband model for semiconductors based on the maximum entropy principle

G. Mascali(1)(2) and V. Romano(3)

(1) Dipartimento di Matematica, Università della Calabria - Via Ponte Bucci, cubo 30 B Arcavacata di Rende (Cs), Italy
(2) INFN-Gruppo c. Cosenza - Cosenza, Italy
(3) Dipartimento di Matematica e Informatica, Università di Catania - Viale A. Doria 6 I-95125 Catania, Italy

(ricevuto il 30 Ottobre 2009; approvato il 14 Gennaio 2010; pubblicato online il 16 Marzo 2010)

Summary. — A hydrodynamic subband model for semiconductors is formulated by closing the moment system derived from the Schrödinger-Poisson-Boltzmann equations on the basis the maximum entropy principle. Explicit closure relations for fluxes and production terms are obtained taking into account scattering of electrons with acoustic and nonpolar optical phonons and surface scattering.

PACS 73.63.-b – Electronic transport in nanoscale materials and structures.
PACS 05.60.Gg – Quantum transport.
PACS 73.63.Hs – Quantum wells.

1. – Quantum confinement

By shrinking the dimension of electronic devices, effects of quantum confinement are observed, *e.g.*, in MOSFETs the gate voltage and the energy barrier at the Si-SiO$_2$ interface confine the carriers near the oxide-silicon interface. Similarly in double-gate MOSFETs the potential between the two gates confines the electrons. The same effect is present in quantum wells in hetero-structures like AlGa-Ga. For a comprehensive review the reader is referred to [1, 2].

If electrons are quantized in a direction which we call z and free to move in the x-y plane, it is natural to assume the following ansatz for the wave function:

$$\psi(\mathbf{k},\mathbf{r}) = \psi(k_x,k_y,k_z,x,y,z) = \frac{1}{\sqrt{\mathcal{A}}}\,\varphi(z)e^{i\mathbf{k}_{||}\cdot\mathbf{r}_{||}},$$

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.

© Società Italiana di Fisica

Inserting the previous expression of ψ into the Schrödinger equation in the effective-mass approximation

$$\left[-\frac{\hbar^2}{2m^*}\,\Delta + E_C(\mathbf{r})\right]\psi = E\,\psi,$$

gives the following equation for φ:

$$(1)\quad \left[-\frac{\hbar^2}{2m^*}\frac{\mathrm{d}^2}{\mathrm{d}z^2} + E_C\right]\varphi(z) = \left[E - \frac{\hbar^2}{2m^*}(k_x^2 + k_y^2)\right]\varphi(z) = \varepsilon\varphi(z),\ -L/2 \leq z \leq L/2,$$

where $\hbar$ is the reduced Planck constant, m^* is the effective electron mass, E_C is the conduction band minimum, ε is the energy associated with the confinement in the z-direction, and L is the extension in the z-direction.

One finds a countable set of eigen-pairs (subbands) $(\varphi_\nu, \varepsilon_\nu), \nu = 1, 2\ldots$. In each subband the energy is the sum of a longitudinal and transversal contribution

$$E_\nu = \varepsilon_\nu + \frac{\hbar^2}{2m^*}(k_x^2 + k_y^2).$$

In (1) $E_C = -q(V_C + V)$ where V_C is the confining potential and V is the self-consistent electrostatic potential obtained from the Poisson equation

$$(2)\qquad \nabla\cdot(\epsilon\,\nabla V) = -q(C(\mathbf{r}) - n),$$

where q is the absolute value of the electron charge, ϵ is the dielectric constant, $C(\mathbf{r})$ is the doping concentration, and n is the electron density given by

$$n(\mathbf{r}, t) = \sum_{\nu=1}^{+\infty} \rho_\nu(x, y, t)|\varphi_\nu(z, t)|^2,$$

with the areal density of electrons ρ_ν of the ν-subband.

The description of the electron transport along the longitudinal direction is included by adding the system of coupled Boltzmann equations for the distributions $f_\nu(x, y, k_x, k_y, t)$ of electrons in the subbands

$$(3)\qquad \frac{\partial f_\nu}{\partial t} + \frac{1}{\hbar}\nabla_{\mathbf{k}_{||}}E_\nu\cdot\nabla_{\mathbf{r}_{||}}f_\nu - \frac{q}{\hbar}\mathbf{E}_\nu^{\mathrm{eff}}\cdot\nabla_{\mathbf{k}_{||}}f_\nu = \sum_{\mu=1}^{\infty} C_{\nu,\mu}[f_\nu, f_\mu], \quad \nu = 1, 2, \ldots$$

where $\mathbf{E}_\nu^{\mathrm{eff}} = \frac{1}{q}\nabla_{\mathbf{r}_{||}}\varepsilon_\nu(\mathbf{r}_{||})$. ρ_ν is expressed in terms of f_ν by $\rho_\nu = \int_{B_2} f_\nu(\mathbf{r}_{||}, \mathbf{k}_{||}, t)\mathrm{d}^2\mathbf{k}_{||}$, with B_2 indicating the 2D Brillouin zone, which will be approximated with $\mathbb{R}^2$ consistently with the effective-mass approximation. In the non-degenerate approximation, each term contributing to the collision term has the general form

$$C_{\nu,\mu}[f_\nu, f_\mu] = \int_{B_2}\left[S(\mathbf{k}_{||}^\mu, \mathbf{k}_{||}^\nu)\,f_\mu - S(\mathbf{k}_{||}^\nu, \mathbf{k}_{||}^\mu)\,f_\nu\right]\mathrm{d}^2\mathbf{k}_{||}^\mu.$$

When $\mu = \nu$ we have intra-subband scattering; when $\mu \neq \nu$ we have inter-subband scatterings. $S(\mathbf{k}_{||}^\mu, \mathbf{k}_{||}^\nu)$ is the transition rate from the longitudinal state with wave vector

$\mathbf{k}_{||}^{\mu}$ to the longitudinal state with wave vector $\mathbf{k}_{||}^{\nu}$. The relevant 2D scattering mechanisms in Si are acoustic phonon scattering, nonpolar phonon scattering, and surface scattering. Scattering with impurities will be not considered in this paper, but it is relevant only at low temperature or low field.

For the acoustic phonon scattering in the elastic approximation, the transition rate is given by

$$S^{(\mathrm{ac})}(\mathbf{k}_{||}^{\nu}, \mathbf{k}_{||}^{\mu}) = A^{(\mathrm{ac})} G_{\nu\mu} \delta(E_{\mu}(\mathbf{k}_{||}^{\mu}) - E_{\nu}(\mathbf{k}_{||}^{\nu})),$$

$A^{(\mathrm{ac})}$ is a physical constant, while the $G_{\nu\mu}$'s are the interaction integrals

$$G_{\nu\mu} = \int_{-\infty}^{\infty} |I_{\nu\mu}(q_z)|^2 \mathrm{d}q_z, \qquad I_{\nu\mu}(q_z) = \int_{L/2}^{L/2} \overline{\varphi_{\nu}(z)} \varphi_{\mu}(z) e^{iq_z z}\, \mathrm{d}z,$$

with $\mathbf{q}$ denoting the 3D-phonon wave vector, and the bar indicating the symbol for complex conjugation. We note that $G_{\nu\mu} = G_{\mu\nu}$ holds.

Similarly for nonpolar optical phonon scattering one has

$$S^{(\mathrm{no})}(\mathbf{k}_{||}^{\nu}, \mathbf{k}_{||}^{\mu}) = A^{(\mathrm{no})} G_{\nu\mu} \left(N_q + \frac{1}{2} \mp \frac{1}{2} \right) \delta(E_{\mu}(\mathbf{k}_{||}^{\mu}) - E_{\nu}(\mathbf{k}_{||}^{\nu}) \mp \hbar\omega),$$

where $A^{(\mathrm{no})}$ is a physical constant, N_q is the Bose-Einstein distribution of the phonons and $\hbar\omega$ is the phonon energy.

At last, we recall that scattering at a surface is due to the roughness of the interface between oxide and silicon in the MOSFET and it produces fluctuation in the transverse component of the electric potential. It is very relevant at high gate voltage. If the fluctuation of the thickness is assumed to have an exponential autocorrelation function with a root mean square amplitude Δ and a correlation length L_C, the transition probability has the form

$$S^{(\mathrm{sur})}(\mathbf{k}_{||}^{\nu}, \mathbf{k}_{||}^{\mu}) = \frac{2\pi}{\hbar} (q\tilde{E}_{\mu\nu})^2 \pi \Delta^2 L_C^2 \frac{1}{1 + L_C^2 (\mathbf{k}_{||}^{\nu} - \mathbf{k}_{||}^{\mu})^2 / 2} \delta(E_{\mu} - E_{\nu}),$$

$\tilde{E}_{\mu\nu}$ being the effective electric field given by

$$q\tilde{E}_{\mu\nu} = \int_{-L/2}^{L/2} \overline{\varphi}_{\mu} q E_z \varphi_{\nu} \mathrm{d}\, z,$$

with E_z transverse component of the electric field.

The above quantum picture can present further specific features. For example in the Si-SiO$_2$ interface of a MOSFET, the quantized inversion layer having a (100)-oriented surface has two sets of subbands, called *ladders*: one coming from the projection of the two valleys with longitudinal mass in the direction perpendicular to the interface, the other one originating from the four valleys having a transverse mass in the direction perpendicular to the interface. Here for the sake of simplicity only one ladder will be considered. However our results can be easily generalized in order to include both ladders by taking into account also intervalley scatterings between subbands belonging to different ladders and solving a Schrödinger equations for each effective mass (longitudinal and transversal).

2. – The moment system

A complete description of quantum confinement is obtained by solving the system (1), (2), (3) (see for example [3-5]), but this is a daunting computational task. Therefore simpler macroscopic models are warranted for CAD purposes. These can be obtained as moment equations of the transport Boltzmann equations under suitable closure relations. The moment of the ν-subband distribution with respect to a weight function $a(\mathbf{k}_{||})$ reads

$$M_a^\nu = \int_{B_2} a(\mathbf{k}_{||}) f_\nu(\mathbf{r}_{||}, \mathbf{k}_{||}, t) \mathrm{d}^2\mathbf{k}_{||}.$$

In particular we take as basic moments

$$\begin{aligned}
\text{the areal density} \quad \rho^\nu &= \int_{B_2} f_\nu(\mathbf{r}_{||}, \mathbf{k}_{||}, t)\mathrm{d}^2\mathbf{k}_{||},\\
\text{the longitudinal mean velocity} \quad \mathbf{V}^\nu &= \frac{1}{\rho^\nu}\int_{B_2} \frac{\hbar \mathbf{k}_{||}}{m^*} f_\nu(\mathbf{r}_{||}, \mathbf{k}_{||}, t)\mathrm{d}^2\mathbf{k}_{||},\\
\text{the longitudinal mean energy} \quad W^\nu &= \frac{1}{\rho^\nu}\int_{B_2} \frac{\hbar^2 \mathbf{k}_{||}^2}{2m^*} f_\nu(\mathbf{r}_{||}, \mathbf{k}_{||}, t)\mathrm{d}^2\mathbf{k}_{||},\\
\text{the longitudinal mean energy-flux} \quad \mathbf{S}^\nu &= \frac{1}{\rho^\nu}\int_{B_2} \frac{\hbar \mathbf{k}_{||}}{m^*}\frac{\hbar^2 \mathbf{k}_{||}^2}{2m^*} f_\nu(\mathbf{r}_{||}, \mathbf{k}_{||}, t)\mathrm{d}^2\mathbf{k}_{||}.
\end{aligned}$$

The corresponding moment system reads

$$\begin{aligned}
\frac{\partial \rho^\nu}{\partial t} + \nabla_{\mathbf{r}_{||}} \cdot (\rho^\nu \mathbf{V}^\nu) &= \rho^\nu \sum_\mu C_\rho^{\nu,\mu},\\
\frac{\partial (\rho^\nu \mathbf{V}^\nu)}{\partial t} + \nabla_{\mathbf{r}_{||}} \cdot (\rho^\nu \underline{\underline{\mathbf{U}}}^\nu) + \frac{\rho^\nu}{m^*}\nabla_{\mathbf{r}_{||}}\varepsilon_\nu &= \rho^\nu \sum_\mu C_{\mathbf{V}}^{\nu,\mu},\\
\frac{\partial \rho^\nu W^\nu}{\partial t} + \nabla_{\mathbf{r}_{||}} \cdot (\rho^\nu \mathbf{S}^\nu) + \rho^\nu \nabla_{\mathbf{r}_{||}}\varepsilon_\nu \cdot \mathbf{V}^\nu &= \rho^\nu \sum_\mu C_W^{\nu,\mu},\\
\frac{\partial (\rho^\nu \mathbf{S}^\nu)}{\partial t} + \nabla_{\mathbf{r}_{||}} \cdot (\rho^\nu \underline{\underline{\mathbf{F}}}^\nu) + \rho^\nu \nabla_{\mathbf{r}_{||}}\varepsilon_\nu : \left[\frac{W^\nu}{m^*}\underline{\underline{\mathbf{I}}} + \underline{\underline{\mathbf{U}}}^\nu\right] &= \rho^\nu \sum_\mu C_{\mathbf{S}}^{\nu,\mu},
\end{aligned}$$

where

$$\begin{aligned}
\begin{pmatrix} \underline{\underline{\mathbf{U}}}^\nu \\ \underline{\underline{\mathbf{F}}}^\nu \end{pmatrix} &= \frac{1}{\rho^\nu}\int_{B_2} \begin{pmatrix} \frac{\hbar^2}{(m^*)^2} \\ \frac{\hbar^4 \mathbf{k}_{||}^2}{2(m^*)^3} \end{pmatrix} \mathbf{k}_{||} \otimes \mathbf{k}_{||} f_\nu(\mathbf{r}_{||}, \mathbf{k}_{||}, t)\, \mathrm{d}^2\mathbf{k}_{||},\\
\begin{pmatrix} C_\rho^{\nu,\mu} \\ C_W^{\nu,\mu} \end{pmatrix} &= \int_{B_2} \begin{pmatrix} 1 \\ \frac{\hbar^2 \mathbf{k}_{||}^2}{2m^*} \end{pmatrix} \left[S(\mathbf{k}_{||}^\mu, \mathbf{k}_{||}^\nu)\, f_\mu - S(\mathbf{k}_{||}^\nu, \mathbf{k}_{||}^\mu)\, f_\nu\right] \mathrm{d}^2\mathbf{k}_{||},\\
\begin{pmatrix} C_{\mathbf{V}}^{\nu,\mu} \\ C_{\mathbf{S}}^{\nu,\mu} \end{pmatrix} &= \int_{B_2} \begin{pmatrix} \frac{\hbar \mathbf{k}_{||}}{m^*} \\ \frac{\hbar^3 \mathbf{k}_{||}^2}{2(m^*)^2}\mathbf{k}_{||} \end{pmatrix} \left[S(\mathbf{k}_{||}^\mu, \mathbf{k}_{||}^\nu)\, f_\mu - S(\mathbf{k}_{||}^\nu, \mathbf{k}_{||}^\mu)\, f_\nu\right] \mathrm{d}^2\mathbf{k}_{||}.
\end{aligned}$$

The moment system is not closed because there are more unknowns than equations. Therefore constitutive relations in terms of the fundamental variables are needed for fluxes and productions terms.

3. – The maximum entropy principle and the closure relations

The maximum entropy principle (MEP) leads to a systematic way for obtaining constitutive relations on the basis of information theory [6, 7]. According to MEP, if a given number of moments $M^{\nu}_{a_A}$, $A = 1, \dots, N$, are known, the distribution functions f_ν can be estimated by the extremal $f^{\text{MEP}} = (f_1^{\text{MEP}}, f_2^{\text{MEP}}, \cdots)$ of the entropy functional under the constraints

$$\int a_A f_\nu^{\text{MEP}} \mathrm{d}\mathbf{k}_{||} = M^{\nu}_{a_A}, \quad A = 1, \dots, N. \tag{4}$$

Actually, in a semiconductor electrons interact with phonons describing the thermal vibrations of the ions placed at the points of the crystal lattice. However, if one considers the phonon gas as a thermal bath, one has to maximize only the electron component of the entropy. Moreover, since we are considering the electron gas as sufficiently dilute, one can take in each subband the expression of the entropy obtained as semiclassical limit of that arising from the Fermi statistics. We define the entropy of the system as

$$\mathcal{S} = -k_B \sum_{\nu=1}^{+\infty} |\varphi_\nu(z,t)|^2 \int_{B_2} (f_\nu \log f_\nu - f_\nu)\, \mathrm{d}^2\mathbf{k}_{||},$$

and therefore, according to MEP, the f_ν's are estimated with the distributions f_ν^{MEP}'s that solve the problem

$$\text{maximize } \mathcal{S} \text{ under the constraints} \quad M^{\nu}_{a_A} = \int_{B_2} a_A(\mathbf{k}_{||}) f_\nu^{\text{MEP}} \mathrm{d}^2\, \mathbf{k}_{||},$$

where $M^{\nu}_{a_A}$ are the basic moments we have previously considered.

The proposed expression of the entropy combines quantum effects and semiclassical transport along the longitudinal direction, weighting the contribution of each f_ν with the modulus of the $\varphi_\nu(z,t)$'s arising from the Schrödinger-Poisson block. In order to determine the f_ν^{MEP}'s, we introduce the Lagrange transform

$$\mathcal{S}' = \mathcal{S} + \sum_{\nu=1}^{\infty} \sum_A \lambda^{\nu}_{a_A} \left[M^{\nu}_{a_A} - |\varphi_\nu(z,t)|^2 \int a_A f_\nu^{\text{MEP}} \mathrm{d}\mathbf{k}_{||} \right].$$

The condition that the first variation must be zero, $\delta\, \mathcal{S}' = 0$, gives

$$0 = \sum_{\nu=1}^{+\infty} \sum_A |\varphi_\nu(z,t)|^2 \int_{B_2} \left[k_B \log f_\nu + \lambda^{\nu}_{a_A} a_A(\mathbf{k}_{||}) \right] \delta\, f_\nu\, \mathrm{d}^2\, \mathbf{k}_{||}, \ \forall \delta f_\nu.$$

With the above choice of the functions $a_A(\mathbf{k}_{||}) = \left(1, \frac{\hbar \mathbf{k}_{||}}{m^*}, \frac{\hbar^2 \mathbf{k}_{||}^2}{2m^*}, \frac{\hbar \mathbf{k}_{||}}{m^*} \frac{\hbar^2 \mathbf{k}_{||}^2}{2m^*}\right)$, one has

$$f_\nu^{\mathrm{MEP}} = \exp\left[-\left(\frac{\lambda^\nu}{k_B} + \lambda_{\mathbf{V}}^\nu \cdot \mathbf{v}_{||}{}^\nu + \left(\lambda_W^\nu + \boldsymbol{\lambda}_{\mathbf{S}}^\nu \cdot \mathbf{v}_{||}{}^\nu\right)(E^\nu - \varepsilon^\nu)\right)\right],$$

$\mathbf{v}_{||}{}^\nu$ being the longitudinal velocity of electrons belonging to the ν-subband, given by the quantum-mechanical relation $\mathbf{v}_{||}{}^\nu = \frac{1}{\hbar}\nabla_{\mathbf{k}_{||}} \frac{\hbar^2 \mathbf{k}_{||}^2}{2m^*} = \frac{\hbar \mathbf{k}_{||}{}^\nu}{m^*}$.

In order to complete the procedure one has to insert the f_ν^{MEP} into the constraint relations (4) and express the Lagrangian multipliers as functions of the basic moments ρ^ν, $\mathbf{V}^\nu$, W^ν, $\mathbf{S}^\nu$. However such a procedure requires a numerical inversion, which is not practical for numerical simulations of electron devices, since it must be performed at each time or iteration step (see [8] for the semiclassical case). Following the same approach as in [9-11], we assume a small anisotropy of the distribution function and expand up to first order

$$f_\nu^{\mathrm{MEP}} \approx \exp\left[-\frac{\lambda^\nu}{k_B} - \lambda_W^\nu\,(E^\nu - \varepsilon^\nu)\right]\left[1 - \left(\lambda_{\mathbf{V}}^\nu \cdot \mathbf{v}_{||}{}^\nu + \left(\lambda_W^\nu + \lambda_{\mathbf{S}}^\nu \cdot \mathbf{v}_{||}{}^\nu\right)(E^\nu - \varepsilon^\nu)\right)\right].$$

Inserting the previous expression into the constraints for the density and the energy, one finds in polar coordinates

$$\rho^\nu = \int_0^{2\pi}\int_0^{+\infty} \exp\left[-\lambda^\nu/k_B - \lambda_W^\nu \frac{\hbar^2 k_{||}^2}{2m^*}\right] k_{||}\,\mathrm{d}k_{||}\,\mathrm{d}\phi,$$
$$\rho^\nu W^\nu = \int_0^{2\pi}\int_0^{+\infty} \frac{\hbar^2 k_{||}^2}{2m^*} \exp\left[-\lambda^\nu/k_B - \lambda_W^\nu \frac{\hbar^2 k_{||}^2}{2m^*}\right] k_{||}\,\mathrm{d}k_{||}\,\mathrm{d}\phi,$$

wherefrom $\lambda^\nu = -k_B \log \frac{\hbar^2 \rho^\nu}{2\pi m^* W^\nu}$ and $\lambda_W^\nu = \frac{1}{W^\nu}$.

Similarly, substituting it into the remaining constraints for the velocity and the energy-flux, one has

$$\boldsymbol{\lambda}_{\mathbf{V}}^\nu = -\frac{3m^*}{W^\nu}\mathbf{V}^\nu + \frac{m^*}{(W^\nu)^2}\mathbf{S}^\nu,$$
$$\boldsymbol{\lambda}_{\mathbf{S}}^\nu = \frac{m^*}{(W^\nu)^2}\mathbf{V}^\nu - \frac{m^*}{2(W^\nu)^3}\mathbf{S}^\nu.$$

Note the symmetry of the coefficients which reminds us of the Onsager reciprocity conditions. The obtained distribution functions will be used to get the needed closure relations for fluxes and production terms. For the fluxes we find

$$\mathbf{U}_{ij}^\nu = \frac{1}{m^*} W^\nu \delta_{ij}, \qquad \mathbf{F}_{ij}^\nu = \frac{2}{m^*}(W^\nu)^2 \delta_{ij}.$$

Concerning the production terms, for the acoustic phonon scattering one has

$$
\begin{aligned}
C_\rho^\nu &= \frac{2\pi m^*}{\hbar^2} \sum_{\mu=1}^{+\infty} C_{\nu\mu} \left[\frac{\rho_\mu}{\rho_\nu} \exp\left[-\frac{\Delta_{\nu\mu} + a_{\nu\mu}}{W^\mu} \right] - \exp\left[-\frac{a_{\nu\mu}}{W^\nu} \right] \right], \\
C_{\mathbf{V}}^\nu &= \frac{2\pi}{\hbar^2} \sum_{\mu=1}^{+\infty} C_{\nu\mu} \exp\left[\frac{-a_{\nu\mu}}{W^\nu} \right] \left[\lambda_{\mathbf{V}}^\nu \left(a_{\nu\mu} + W^\nu \right) + \lambda_{\mathbf{S}}^\nu \left(a_{\nu\mu}^2 + 2a_{\nu\mu} W^\nu + 2(W^\nu)^2 \right) \right], \\
C_W^\nu &= \frac{2\pi m^*}{\hbar^2} \sum_{\mu=1}^{+\infty} C_{\nu\mu} \left[\frac{\rho_\mu}{\rho_\nu} \exp\left[-\frac{\Delta_{\nu\mu} + a_{\nu\mu}}{W^\mu} \right] (a_{\nu\mu} + W^\mu) - \exp\left[-\frac{a_{\nu\mu}}{W^\nu} \right] (a_{\nu\mu} + W^\nu) \right], \\
C_{\mathbf{S}}^\nu &= \frac{2\pi}{\hbar^2} \sum_{\mu=1}^{+\infty} C_{\nu\mu} \exp\left[\frac{-a_{\nu\mu}}{W^\nu} \right] \left[\lambda_{\mathbf{V}}^\nu \left(a_{\nu\mu}^2 + 2a_{\nu\mu} W^\nu + 2(W^\nu)^2 \right) \right. \\
&\quad \left. + \lambda_{\mathbf{S}}^\nu \left(a_{\nu\mu}^3 + 3a_{\nu\mu}^2 W^\nu + 6a_{\nu\mu}(W^\nu)^2 + 6(W^\nu)^3 \right) \right],
\end{aligned}
$$

where $\Delta_{\nu\mu} = \varepsilon_\nu - \varepsilon_\mu$ and $a_{\nu\mu} = \max(0, \varepsilon_\mu - \varepsilon_\nu)$ and $C_{\nu\mu} = A^{(\mathrm{ac})} G_{\nu\mu}$.

For the nonpolar optical phonon scattering one has

$$
\begin{aligned}
C_\rho^\nu &= \frac{2\pi m^*}{\hbar^2} \sum_{\mu=1}^{+\infty} D_{\nu\mu} N_{\mathrm{op}} \left[\frac{\rho_\mu}{\rho_\nu} \left(\exp\left[\frac{\hbar\omega}{k_B T_L} - \frac{\Delta_{\nu\mu}^+ + a_{\nu\mu}^-}{W^\mu} \right] + \exp\left[-\frac{\Delta_{\nu\mu}^- + a_{\nu\mu}^+}{W^\mu} \right] \right) \right. \\
&\left. - \exp\left[\frac{\hbar\omega}{k_B T_L} - \frac{a_{\nu\mu}^-}{W^\nu} \right] - \exp\left[-\frac{a_{\nu\mu}^+}{W^\nu} \right] \right], \\
C_{\mathbf{V}}^\nu &= \frac{2\pi}{\hbar^2} \sum_{\mu=1}^{+\infty} D_{\nu\mu} N_{\mathrm{op}} \left[\lambda_{\mathbf{V}}^\nu \left(\exp\left[\frac{\hbar\omega}{k_B T_L} \right] B^{(1)}\left(\lambda_W^\nu, a_{\nu\mu}^- \right) + B^{(1)}\left(\lambda_W^\nu, a_{\nu\mu}^+ \right) \right) \right. \\
&\left. + \lambda_{\mathbf{S}}^\nu \left(\exp\left[\frac{\hbar\omega}{k_B T_L} \right] B^{(2)}\left(\lambda_W^\nu, a_{\nu\mu}^- \right) + B^{(2)}\left(\lambda_W^\nu, a_{\nu\mu}^+ \right) \right) \right], \\
C_W^\nu &= \frac{2\pi m^*}{\hbar^2} \sum_{\mu=1}^{+\infty} D_{\nu\mu} N_{\mathrm{op}} \left[\frac{\rho_\mu}{\rho_\nu} \left(\exp\left[\frac{\hbar\omega}{k_B T_L} - \frac{\Delta_{\nu\mu}^+}{W^\mu} \right] B^{(1)}\left(\lambda_W^\mu, a_{\nu\mu}^- \right) \right. \right. \\
&\left. \left. + \exp\left[-\frac{\Delta_{\nu\mu}^-}{W^\mu} \right] B^{(1)}\left(\lambda_W^\mu, a_{\nu\mu}^+ \right) \right) - \exp\left[\frac{\hbar\omega}{k_B T_L} \right] B^{(1)}\left(\lambda_W^\nu, a_{\nu\mu}^- \right) - B^{(1)}\left(\lambda_W^\nu, a_{\nu\mu}^+ \right) \right], \\
C_{\mathbf{S}}^\nu &= \frac{2\pi}{\hbar^2} \sum_{\mu=1}^{+\infty} D_{\nu\mu} N_{\mathrm{op}} \left[\lambda_{\mathbf{V}}^\nu \left(\exp\left[\frac{\hbar\omega}{k_B T_L} \right] B^{(2)}\left(\lambda_W^\nu, a_{\nu\mu}^- \right) + B^{(2)}\left(\lambda_W^\nu, a_{\nu\mu}^+ \right) \right) \right. \\
&\left. + \lambda_{\mathbf{S}}^\nu \left(\exp\left[\frac{\hbar\omega}{k_B T_L} \right] B^{(3)}\left(\lambda_W^\nu, a_{\nu\mu}^- \right) + B^{(3)}\left(\lambda_W^\nu, a_{\nu\mu}^+ \right) \right) \right],
\end{aligned}
$$

where $a_{\nu\mu}^\mp = \max(0, \varepsilon_\mu - \varepsilon_\nu \mp \hbar\omega)$, $\Delta_{\nu\mu}^\pm = \varepsilon_\nu - \varepsilon_\mu \pm \hbar\omega$, $D_{\nu\mu} = A^{(\mathrm{no})} G_{\nu\mu}$ and

$$
B^{(\mathrm{n})}(x, y) = (-1)^n \, x \frac{\mathrm{d}^n}{\mathrm{d}x^n} \int_0^\infty e^{-x(t+y)\mathrm{d}t} \quad \text{for} \quad x > 0.
$$

For the scattering at a surface one has

$$C^{\nu}_{\rho} = \frac{2\pi m^*}{\hbar^2} D_S \sum_{\mu=1}^{+\infty} (q\tilde{E}_{\mu\nu})^2 \left(\frac{\rho_\mu}{\rho_\nu} \exp\left[-\frac{\Delta_{\nu\mu}}{W^\nu} \right] B_1\left(\lambda^{\mu}_{W}, a_{\nu\mu}\right) - B_1\left(\lambda^{\nu}_{W}, a_{\nu\mu}\right) \right),$$

$$C^{\nu}_{\mathbf{V}} = \frac{2\pi}{\hbar^2} D_S \sum_{\mu=1}^{+\infty} (q\tilde{E}_{\mu\nu})^2 \Bigg\{ \lambda^{\nu}_{\mathbf{V}} B^{(1)}_2\left(\lambda^{\nu}_{W}, a_{\nu\mu}\right) + \lambda^{\nu}_{\mathbf{S}} B^{(2)}_2\left(\lambda^{\nu}_{W}, a_{\nu\mu}\right)$$
$$-\frac{\rho_\mu}{\rho_\nu} \exp\left[-\frac{\Delta_{\nu\mu}}{W^\mu} \right] \left[\lambda^{\boldsymbol{\mu}}_{V} B_2\left(\lambda^{\mu}_{W}, a_{\nu\mu}\right) + \lambda^{\nu}_{\mathbf{S}} \left(\Delta_{\nu\mu} B_2\left(\lambda^{\mu}_{W}, a_{\nu\mu}\right) + B^{(1)}_2\left(\lambda^{\mu}_{W}, a_{\nu\mu}\right) \right) \right] \Bigg\},$$

$$C^{\nu}_{W} = \frac{2\pi m^*}{\hbar^2} D_S \sum_{\mu=1}^{+\infty} (q\tilde{E}_{\mu\nu})^2 \left(\frac{\rho_\mu}{\rho_\nu} \exp\left[-\frac{\Delta_{\nu\mu}}{W^\mu} \right] B^{(1)}_1\left(\lambda^{\mu}_{W}, a_{\nu\mu}\right) - B^{(1)}_1\left(\lambda^{\nu}_{W}, a_{\nu\mu}\right) \right),$$

$$C^{\nu}_{\mathbf{S}} = \frac{2\pi}{\hbar^2} D_S \sum_{\mu=1}^{+\infty} (q\tilde{E}_{\mu\nu})^2 \Bigg\{ \lambda^{\nu}_{\mathbf{V}} B^{(2)}_2\left(\lambda^{\nu}_{W}, a_{\nu\mu}\right) + \lambda^{\nu}_{\mathbf{S}} B^{(3)}_2\left(\lambda^{\nu}_{W}, a_{\nu\mu}\right)$$
$$-\frac{\rho_\mu}{\rho_\nu} \exp\left[-\frac{\Delta_{\nu\mu}}{W^\mu} \right] \left[\lambda^{\mu}_{\mathbf{V}} B^{(1)}_2\left(\lambda^{\mu}_{W}, a_{\nu\mu}\right) + \lambda^{\mu}_{\mathbf{S}} \left(\Delta_{\nu\mu} B^{(1)}_2(\lambda^{\mu}_{W}, a_{\nu\mu}) + B^{(2)}_2(\lambda^{\mu}_{W}, a_{\nu\mu}) \right) \right] \Bigg\},$$

where $D_S = \frac{2\pi^2}{\hbar} \Delta^2 L^2_C$ and

$$B^{(n)}_1(x,y) = x(-1)^n \frac{\mathrm{d}^n}{\mathrm{d}x^n} \int_0^\infty e^{-(t+y)x} \beta_0(t+y)^{-1} \mathrm{d}\, t,$$
$$B^{(n)}_2(x,y) = x(-1)^n \frac{\mathrm{d}^n}{\mathrm{d}x^n} \int_0^\infty e^{-(t+y)x} \beta_1(t+y)^{-1} \mathrm{d}\, t,$$
$$\beta_0(x) = \left(1 + \frac{2m^* L^2_C}{\hbar^2}(2x+\Delta_{\nu\mu}) - \frac{4(m^*)^2 L^4_C}{\hbar^4}(x+\Delta_{\nu\mu})x + \frac{(m^*)^2 L^4_C}{\hbar^4}(2x+\Delta_{\nu\mu})^2 \right)^{1/2},$$
$$\beta_1(x) = \left[1 + \frac{m^* L^2_C (2x+\Delta_{\nu\mu})}{\hbar^2} - \beta_0(x) \right] \left(\frac{2m^* L^2_C}{\hbar^2} \beta_0(x) \right)^{-1}.$$

We remark that only the subbands with the lower energies are populated and therefore only a finite number of moment equations will be relevant. Moreover it is a simple matter to check that the moment system, augmented with the closure relations given by MEP, forms a quasi-linear hyperbolic system provided that $W^\nu > 0$ for each $\nu = 1, 2, \ldots$, that is the case in all the physical regions of the variable space.

* * *

The authors acknowledge the financial support by the EU Marie Curie RTN project COMSON grant n. MRTN-CT-2005-019417. One of the authors (GM) also acknowledges support by Gruppo Nazionale di Fisica Matematica (Modelli matematici per il trasporto di cariche in micro e nanoelettronica, Progetti Giovani Ricercatori 2009).

REFERENCES

[1] Datta S., *Quantum Phenomena*, Vol. **VIII** of the *Modular Series on Solid State Devices* (Addison-Wesley Publishing, Reading, MA) 1989.

[2] Lundstrom M., *Fundamentals of Carrier Transport* (Cambridge University Press, Cambridge, UK) 2000.

[3] Polizzi E. and Abdallah N. B., *J. Comput. Phys.*, **202** (2005) 150.

[4] Galler M. and Schuerrer F., *A deterministic Solver to the Boltzmann-Poisson System Including Quantization Effects for Silicon-MOSFETs*, in *Progress in Industrial Mathematics at ECMI 2006, Series: Mathematics in Industry* (Springer) 2008, pp. 531-536.

[5] Abdallah N. B., Caceres M. J., Carrillo J. A. and Vecil F., *J. Comput. Phys.*, **228** (2009) 6553.

[6] Jaynes E. T., *Phys. Rev. B*, **106** (1957) 620.

[7] Wu N., *The Maximum Entropy Method* (Springer-Verlag, Berlin) 1997.

[8] La Rosa S., Mascali G. and Romano V., *SIAM J. Appl. Math.*, **70** (2009) 710.

[9] Anile A. M. and Romano V., *Continuum Mech. Thermodyn.*, **11** (1999) 307.

[10] Romano V., *Continuum Mech. Thermodyn.*, **12** (2000) 31.

[11] Mascali G. and Romano V., *Continuum Mech. Thermodyn.*, **14** (2002) 405.