

# THE SEMICONDUCTOR STEADY BOLTZMANN EQUATION: A VARIATIONAL FORMULATION WITH AN APPLICATION TO MOBILITY

A.M. ANILE

*Dipartimento di Matematica ed Informatica,  
Università degli Studi di Catania, Italy,  
E-mail: anile@dmi.unict.it*

G. ALÌ

*Istituto per le Applicazioni del Calcolo "M. Picone", sez. di Napoli,  
Consiglio Nazionale delle Ricerche,  
via Pietro Castellino 111, 80131 Napoli, Italy,  
and INFN-Gruppo c. Cosenza, Italy,  
E-mail: g.ali@iac.cnr.it*

G. MASCALI

*Dipartimento di Matematica, Università della Calabria,  
ponte Bucci, cubo 30 B, 87036 Arcavacata di Rende, Italy  
and INFN-Gruppo c. Cosenza, Italy,  
E-mail: g.mascali@unical.it*

We consider a variational formulation of the steady Boltzmann equation for semiconductors. We apply this formulation to the calculation of an approximate expression of the electron mobility, valid for electric fields up to  $1-1.5 \frac{V}{\mu m}$ .

*Keywords:* Semiclassical Boltzmann equation; Semiconductors; Variational formulation; Mobility.

## 1. Introduction

The semiclassical Boltzmann (BE) equation is the reference model for charge transport in semiconductors.<sup>1-3</sup> In fact, not only the results of simulations by other models are usually compared with BE simulations, but most of the existing models in microelectronics have been or can be derived from BE.<sup>1,4</sup>

In the past, calculus of variations has been extensively applied to transport theory, mainly to obtain estimates of physical quantities or to derive

approximate methods for transport problems.<sup>5,6</sup> These variational approach has been particularly fruitful in the field of kinetic models of plasmas, with application in nuclear engineering and reactor analysis.<sup>7</sup>

Despite of the great interest of the Boltzmann equation in semiconductor applications, so far variational methods have not been applied to this model, with few exceptions. Isolated attempts in this direction can be found in Ref. 8, where a variational formulation of the BTE is introduced to evaluate an approximate expression of the mobility for a bulk semiconductor, and, more recently, in Ref. 9, where the mathematical setting of the variational formulation has been clarified.

In this paper, after a brief review of the variational formulation of the steady-state BE, we show how this formulation can be used for studying the behavior of the electron mobility in bulk silicon as a function of the electron average energy. The formula is valid at low energies, more general approximations are under investigation and will be presented as soon as possible.

## 2. Boltzmann transport equation

At kinetic level a family of carriers in an infinitely extended semiconductor is described by a distribution function

$$f(\mathbf{x}, \mathbf{k}, t), \text{ with } \mathbf{x} \in \mathbb{R}^3, \mathbf{k} \in \mathcal{B} \subset \mathbb{R}^3, \text{ and } t \in \mathbb{R}^+.$$

Here,  $\mathcal{B}$  is a bounded set, the first Brillouin region of the inverse lattice of the semiconductor crystal. The carrier energy is expressed in terms of the wave vector  $\mathbf{k}$  by means of a dispersion relation  $\mathcal{E}(\mathbf{k})$ , it is determined by the band structure of the semiconductor, and satisfies the following symmetry property

$$\mathcal{E}(-\mathbf{k}) = \mathcal{E}(\mathbf{k}), \quad (1)$$

due to the time reversibility of the Schrödinger equation.<sup>10</sup> Moreover, we assume that:

$$\text{the isoenergetic surfaces, } \mathcal{E}(\mathbf{k}) = \text{constant}, \text{ are closed and bounded.} \quad (2)$$

The dispersion relation defines the group velocity of the carriers (Bloch electrons or holes),

$$\mathbf{v}(\mathbf{k}) = \frac{1}{\hbar} \nabla_{\mathbf{k}} \mathcal{E}(\mathbf{k}),$$

which in the semiclassical approximation is identified with the carrier velocity.

The time evolution of the distribution function  $f$  is determined by the semiclassical Boltzmann-Poisson system

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \nabla_{\mathbf{x}} f + \frac{q_c}{\hbar} \mathbf{E} \cdot \nabla_{\mathbf{k}} f = C[f], \quad (3)$$

$$-\nabla_{\mathbf{x}} \cdot (\epsilon_s \nabla_{\mathbf{x}} \phi) = Q_{\text{bi}} + q_c \int_{\mathcal{B}} f d\mathbf{k}, \quad (4)$$

where  $\mathbf{E}$  is the electric field,  $C[f]$  the collision operator,  $\phi$  the electric potential,  $q_c$  the carrier's charge,  $Q_{\text{bi}}$  the built-in charge, related to the dopant concentration.

The electric field is related to the electric potential by the usual relation

$$\mathbf{E} = -\nabla_{\mathbf{x}} \phi. \quad (5)$$

The collision operator takes into account various scattering mechanisms, in particular carrier-phonon scattering and carrier-impurity scattering. In the non-degenerate case, it can be written in the general form:

$$C[f] = \int_{\mathcal{B}} [P(\mathbf{k}', \mathbf{k}) f(\mathbf{x}, \mathbf{k}', t) - P(\mathbf{k}, \mathbf{k}') f(\mathbf{x}, \mathbf{k}, t)] d\mathbf{k}', \quad (6)$$

where the kernel  $P(\mathbf{k}', \mathbf{k})$ , which is the transition probability per unit time from a state  $\mathbf{k}$  to a state  $\mathbf{k}'$ , satisfies the detailed balance principle

$$P(\mathbf{k}', \mathbf{k}) \exp[-\mathcal{E}(\mathbf{k}')/k_B T_L] = P(\mathbf{k}, \mathbf{k}') \exp[-\mathcal{E}(\mathbf{k})/k_B T_L], \quad (7)$$

and the symmetry condition

$$P(-\mathbf{k}', -\mathbf{k}) = P(\mathbf{k}', \mathbf{k}). \quad (8)$$

Equations (3), (4) are defined for  $\mathbf{x} \in \mathbb{R}^3$ . The same equations can be considered in a bounded subset  $\Omega \subset \mathbb{R}^3$ . In this case, appropriate boundary conditions are needed. In general, the boundary can be split as  $\partial\Omega = \Gamma_D \cup \Gamma_N$ , where  $\Gamma_D$  comprises the Ohmic boundaries and  $\Gamma_N$  the insulating boundaries, with  $\Gamma_D \cap \Gamma_N = \emptyset$ . We denote by  $\boldsymbol{\nu}(\mathbf{x})$  the external normal to the boundary at  $\mathbf{x} \in \partial\Omega$ , and introduce the following notation:

$$\begin{aligned} \mathcal{B}^{\pm}(\mathbf{x}) &= \{\mathbf{k} \in \mathcal{B} \mid \pm \mathbf{v}(\mathbf{k}) \cdot \boldsymbol{\nu}(\mathbf{x}) > 0\}, \\ \Sigma_{D,N}^{\pm} &= \{(\mathbf{x}, \mathbf{k}) \in \Gamma_{D,N} \times \mathcal{B} \mid \mathbf{k} \in \mathcal{B}^{\pm}(\mathbf{x})\}, \quad \Sigma^{\pm} = \Sigma_D^{\pm} \cup \Sigma_N^{\pm}, \\ f^{\pm} &= f|_{\Sigma^{\pm} \times \mathbb{R}^+}. \end{aligned}$$

The boundary conditions are assigned on the incoming carriers, that is, on the function  $f^-$ . For the Ohmic boundaries, one usually assigns Dirichlet conditions of the form:

$$f^-(\mathbf{x}, \mathbf{k}, t) = \bar{f}(\mathbf{x}, \mathbf{k}, t), \quad (\mathbf{x}, \mathbf{k}) \in \Sigma_D^-, \quad t > 0, \quad (9)$$

where  $\bar{f}$  is a given function, usually the lattice temperature Maxwellian. For insulating boundaries, it is appropriate to assign Neumann conditions of the form:

$$f^-(\mathbf{x}, \mathbf{k}, t) = \tilde{\mathcal{K}}_N[f^+](\mathbf{x}, \mathbf{k}, t), \quad (\mathbf{x}, \mathbf{k}) \in \Sigma_N^-, t > 0, \quad (10)$$

where

$$\tilde{\mathcal{K}}_N[f^+](\mathbf{x}, \mathbf{k}, t) = \int_{\mathcal{B}^+(\mathbf{x})} \tilde{R}(\mathbf{k}', \mathbf{k}) f^+(\mathbf{x}, \mathbf{k}', t) d\mathbf{k}',$$

and the kernel  $\tilde{R}(\mathbf{k}', \mathbf{k})$  satisfies the reciprocity property

$$\tilde{R}(\mathbf{k}', \mathbf{k}) |\mathbf{v}(\mathbf{k}) \cdot \boldsymbol{\nu}(\mathbf{x})| = \tilde{R}(-\mathbf{k}, -\mathbf{k}') |\mathbf{v}(\mathbf{k}') \cdot \boldsymbol{\nu}(\mathbf{x})|, \quad \forall \mathbf{k} \in \mathcal{B}^-(\mathbf{x}). \quad (11)$$

The boundary conditions can be rewritten more concisely, as

$$f^- = 1_{\Gamma_N} \tilde{\mathcal{K}}_N[f^+] + 1_{\Gamma_D} \bar{f}, \quad \text{in } \Sigma^- \times \mathbb{R}^+. \quad (12)$$

where  $1_{\Gamma_{N,D}}$  represent the characteristic functions of the sets  $\Gamma_{N,D}$ . Further details can be found in Ref. 11.

### 3. Variational formulation

In this section we derive a variational formulation of the steady Boltzmann equation for semiconductors when  $\phi(\mathbf{x})$  is a time independent externally applied potential.

To start with, we introduce a weighted distribution function,  $h$ , defined by

$$f(\mathbf{x}, \mathbf{k}) = M_\phi(\mathcal{E}(\mathbf{k})) h(\mathbf{x}, \mathbf{k}),$$

where  $M_\phi(\mathcal{E})$  is the Maxwell equilibrium distribution,

$$M_\phi(\mathcal{E}) = \exp \left[ -\frac{\mathcal{E} + q_c \phi}{k_B T_L} \right].$$

Also, we introduce the streaming operator

$$\mathcal{D} = \mathbf{v} \cdot \nabla_{\mathbf{x}} + \frac{q_c}{\hbar} \mathbf{E} \cdot \nabla_{\mathbf{k}}.$$

By using the detailed balance principle (7), and the identity  $\mathcal{D}M_\phi(\mathcal{E}) = 0$ , it is possible to see that the weighted distribution function  $h(\mathbf{x}, \mathbf{k})$  satisfies the modified Boltzmann equation

$$\mathcal{D}h = \mathcal{C}[h], \quad (13)$$

where

$$\mathcal{C}[h] = \int_{\mathcal{B}} P(\mathbf{k}, \mathbf{k}') [h(\mathbf{x}, \mathbf{k}') - h(\mathbf{x}, \mathbf{k})] d\mathbf{k}'.$$

As a result of this change of coordinate, the new collision operator  $\mathcal{C}$  is symmetric with respect to the weighted scalar product

$$((h, g)) = \int_{\Omega} \int_{\mathcal{B}} h(\mathbf{x}, \mathbf{k}) M_{\phi(\mathbf{x})}(\mathcal{E}(\mathbf{k})) g(\mathbf{x}, \mathbf{k}) d\mathbf{k} d\mathbf{x}, \quad (14)$$

that is,

$$((h, \mathcal{C}[g])) = ((\mathcal{C}[h], g)). \quad (15)$$

Unfortunately, the streaming operator  $\mathcal{D}$  is not symmetric with respect to the same scalar product (14). Anyway, by using a well known trick,<sup>5</sup>  $\mathcal{D}$  can be symmetrized by means of the parity operator  $\mathcal{P}$ , defined by

$$\mathcal{P}h(\mathbf{x}, \mathbf{k}) = h(\mathbf{x}, -\mathbf{k}). \quad (16)$$

In fact, by integration by parts, it is possible to show that  $\mathcal{P}\mathcal{D}$  satisfies the symmetry condition

$$((\mathcal{P}\mathcal{D}h, g)) + ((\mathcal{P}h, g))_{\Sigma^-} = ((h, \mathcal{P}\mathcal{D}g)) + ((h, \mathcal{P}g))_{\Sigma^-}, \quad (17)$$

where

$$((h, g))_{\Sigma^-} = \int_{\partial\Omega} \int_{\mathcal{B}^-(\mathbf{x})} h(\mathbf{x}, \mathbf{k}) M_{\phi(\mathbf{x})}(\mathcal{E}(\mathbf{k})) g(\mathbf{x}, \mathbf{k}) |\mathbf{v}(\mathbf{k}) \cdot \boldsymbol{\nu}(\mathbf{x})| d\mathbf{k} d\sigma_x, \quad (18)$$

with  $d\sigma_x$  surface element on the boundary.

Moreover, the symmetry of  $\mathcal{C}$  is not destroyed by the parity operator. In fact, the symmetry condition (8) implies that the operator  $\mathcal{P}\mathcal{C}$  is also symmetric,

$$((h, \mathcal{P}\mathcal{C}[g])) = ((\mathcal{P}\mathcal{C}[h], g)). \quad (19)$$

Then, it is convenient to replace the modified Boltzmann equation (13) with the equivalent, symmetric equation

$$\mathcal{P}\mathcal{D}h = \mathcal{P}\mathcal{C}[h]. \quad (20)$$

This equation is the starting point for a variational formulation of the steady-state Boltzmann equation.

It is tempting to introduce the functional

$$\tilde{J}(h) = ((h, \mathcal{P}\mathcal{D}h - \mathcal{P}\mathcal{C}[h])). \quad (21)$$

Then, by using the symmetry conditions, it is possible to prove that

$$\delta\tilde{J}(h) = 2((\delta h, \mathcal{P}\mathcal{D}h - \mathcal{P}\mathcal{C}[h])) - ((\mathcal{P}\delta h, h))_{\Sigma^-} + ((\delta h, \mathcal{P}h))_{\Sigma^-}. \quad (22)$$

This shows that the solutions of the modified Boltzmann equation (20) are not stationary points of  $\tilde{J}$ . Thus, we need to deal with boundary conditions.

The boundary conditions relative to the insulating boundaries can be written

$$h(\mathbf{x}, \mathbf{k}) = \mathcal{K}_N[h](\mathbf{x}, \mathbf{k}) := \frac{\tilde{\mathcal{K}}_N[M_\phi(\mathcal{E})h](\mathbf{x}, \mathbf{k})}{M_{\phi(\mathbf{x})}(\mathcal{E}(\mathbf{k}))}, \quad (\mathbf{x}, \mathbf{k}) \in \Sigma_N^-.$$

Therefore, taking  $\tilde{f}(\mathbf{x}, \mathbf{k}) = \tilde{\psi}(\mathbf{x})M_\phi(\mathcal{E}(\mathbf{k}))$ , the boundary conditions (12) become

$$h = 1_{\Gamma_N}\mathcal{K}_N[h] + 1_{\Gamma_D}\tilde{\psi}, \quad \text{in } \Sigma^-. \quad (23)$$

By using the reciprocity (11), it is possible to see that  $\mathcal{K}_N$  satisfies the symmetry property

$$((\mathcal{P}g, \mathcal{K}_N[h]))_{\Sigma^-} = ((\mathcal{K}_N[g], \mathcal{P}h))_{\Sigma^-}.$$

In conclusion, introducing the functional

$$J(h) = \tilde{J}(h) + (((\mathcal{P}h, h - 1_{\Gamma_N}\mathcal{K}_N[h] - 1_{\Gamma_D}2\tilde{\psi}))_{\Sigma^-}), \quad (24)$$

it is possible to show that

$$\delta J(h) = 2((\delta h, \mathcal{P}\mathcal{D}h - \mathcal{P}\mathcal{C}[h])) + 2(((\mathcal{P}\delta h, h - 1_{\Gamma_N}\mathcal{K}_N[h] - 1_{\Gamma_D}\tilde{\psi}))_{\Sigma^-}). \quad (25)$$

As a result of (25), the following theorem holds:

**Theorem 1.** *The weighted distribution function  $h$  is solution of the modified Boltzmann equation (20), with boundary conditions (23), if and only if it is a stationary point of the functional  $J$ , that is,*

$$\delta J(h) = 0. \quad (26)$$

#### 4. Mobility in bulk Silicon

In this section, we want to use the variational formulation (26) in order to find an approximate expression for the electron mobility in bulk silicon, that is a uniformly doped piece of semiconductor. Therefore in the following we take  $q_c = -q$ , and  $Q_{\text{bi}} = qN_D$ , with  $q$  the elementary charge and  $N_D$  the donor concentration. The hole mobility can be found in a similar way, by taking  $q_c = q$ , and  $Q_{\text{bi}} = -qN_A$ , with  $N_A$  acceptor concentration.

First of all, we can consider  $\Omega$  extended to the whole space so that the boundary conditions can be neglected. We take into account the interactions of the electrons in the six equivalent valleys of the conduction band with phonons and impurities.<sup>12</sup> Some of the interactions with phonons leave the electrons in the same valley as they are before the collision (intravalley transitions), while others of them can drive the electrons into a different valley (intervalley transitions) according to suitable selection rules. The transition rate of the collision operator,  $P(\mathbf{k}, \mathbf{k}')$ , is therefore the sum of

- the transition rate for the electron-acoustical phonon intravalley scattering:

$$P_{ac}(\mathbf{k}, \mathbf{k}') = \mathcal{K}_{ac} \delta(\mathcal{E}' - \mathcal{E}),$$

written in the elastic approximation, which is valid when the thermal energy is much greater than that of the phonon. Here,  $\mathcal{K}_{ac}$  is the acoustical intravalley scattering kernel coefficient and  $\delta$  the Dirac function;

- the six intervalley scattering transition rates:

$$P_{\alpha}(\mathbf{k}, \mathbf{k}') = \mathcal{K}_{\alpha} [n_{\alpha} \delta(\mathcal{E}' - \mathcal{E} - \hbar\omega_{\alpha}) + (n_{\alpha} + 1)\delta(\mathcal{E}' - \mathcal{E} + \hbar\omega_{\alpha})],$$

where  $\alpha$  runs over the three  $g_1, g_2, g_3$  and the three  $f_1, f_2, f_3$  intervalley scatterings.<sup>12</sup> The  $\mathcal{K}_{\alpha}$ 's are the optical or acoustical intervalley scattering kernel coefficients and

$$n_{\alpha} = \frac{1}{\exp\left(\frac{\hbar\omega_{\alpha}}{k_B T_L}\right) - 1}$$

is the occupation number of phonons with frequency  $\omega_{\alpha}$ ;

- the impurity scattering transition rate:

$$P_{imp}(\mathbf{k}, \mathbf{k}') = \frac{\mathcal{K}_{imp}}{[|\mathbf{k} - \mathbf{k}'|^2 + \beta^2]^2} \delta(\mathcal{E}' - \mathcal{E}),$$

with  $\mathcal{K}_{imp}$  scattering kernel coefficient and  $\beta$  inverse Debye length.

Now, we assume that  $f$  has the form

$$f(\mathbf{x}, \mathbf{k}) = f^{(0)}(\mathbf{k}) [1 + \Phi(\mathbf{k})], \quad (27)$$

with

$$f^{(0)}(\mathbf{k}) = \frac{n}{N} \exp(-\lambda_W \mathcal{E}(\mathbf{k})), \quad (28)$$

and

$$\Phi(\mathbf{k}) = -\frac{3q}{|\mathbf{v}(\mathbf{k})|^2} \mu \mathbf{v}(\mathbf{k}) \cdot \mathbf{E}. \quad (29)$$

Here,  $n = \int f d\mathbf{k}$  is the carrier density,  $N$  the normalization factor,  $\mu$  the mobility and  $\lambda_W$  is related to the mean energy  $W = \frac{\int \mathcal{E} f d\mathbf{k}}{\int f d\mathbf{k}}$  through the relation

$$W = \frac{1}{N} \int_{\mathcal{B}} \mathcal{E} \exp(-\lambda_W \mathcal{E}) d\mathbf{k}.$$

We also assume that the dispersion relation is given by the Kane approximation

$$\mathcal{E}(1 + \alpha\mathcal{E}) = \frac{\hbar^2 |\mathbf{k}|^2}{2m^*},$$

with  $\alpha$  non parabolicity factor.

Using ansatz (27), (28) and (29) in the variational formulation amounts to choosing

$$\tilde{h} = \frac{n}{N} \exp\left(\frac{\mathcal{E} - q\mathbf{E}\cdot\mathbf{x}}{k_B T_L} - \lambda_W \mathcal{E}\right) \left[1 - \frac{3q}{|\mathbf{v}|^2} \mu \mathbf{v} \cdot \mathbf{E}\right].$$

Taking variations with respect to  $\mu$ , we obtain the following expression for the mobility

$$\mu = -\frac{((\psi_1, \mathcal{P}(\mathcal{D} - \mathcal{C})[\psi_0]))}{((\psi_1, \mathcal{P}(\mathcal{D} - \mathcal{C})[\psi_1]))}, \quad (30)$$

where

$$\begin{aligned} \psi_0 &= \frac{n}{N} \exp\left(\frac{\mathcal{E} - q\mathbf{E}\cdot\mathbf{x}}{k_B T_L} - \lambda_W \mathcal{E}\right), \\ \text{and} \\ \psi_1 &= -\frac{3n}{N |\mathbf{v}|^2} \exp\left(\frac{\mathcal{E} - q\mathbf{E}\cdot\mathbf{x}}{k_B T_L} - \lambda_W \mathcal{E}\right) \mathbf{v} \cdot \mathbf{E}. \end{aligned}$$

The formula (30) expresses  $\mu$  as a function of  $W, T_L$  and of the doping concentration.

After calculations, we find

$$\mu = \frac{c_1 d(\lambda_W)}{c_2 [d_{ac}(\lambda_W) + \sum_{\alpha} d_{\alpha}(\lambda_W)] + c_3 d_{imp}(\lambda_W)},$$

where

$$c_1 = \frac{\sqrt{2}q}{3\hbar}, \quad c_2 = \frac{4\pi m^{*\frac{5}{2}}}{\hbar^4}, \quad c_3 = \frac{\pi m^{*\frac{1}{2}}}{8},$$

and

$$d = \lambda_W \int_0^\infty e^{-\mathcal{E}(2\lambda_W - \lambda_W^0)} (1 + 2\alpha\mathcal{E}) \sqrt{\mathcal{E}(1 + \alpha\mathcal{E})} d\mathcal{E},$$

$$d_{ac} = \kappa_{ac} \int_0^\infty e^{-\mathcal{E}(2\lambda_W - \lambda_W^0)} (1 + 2\alpha\mathcal{E})^4 d\mathcal{E},$$

$$d_\alpha = \kappa_\alpha \int_0^\infty e^{-\mathcal{E}(2\lambda_W - \lambda_W^0)} \left\{ n_\alpha (1 + 2\alpha\mathcal{E})^3 (1 + 2\alpha\mathcal{E}_\alpha^+) \sqrt{\frac{\mathcal{E}_\alpha^+ (1 + \alpha\mathcal{E}_\alpha^+)}{\mathcal{E}(1 + \alpha\mathcal{E})}} \right. \\ \left. + (n_\alpha + 1) (1 + 2\alpha\mathcal{E}_\alpha^+)^3 (1 + 2\alpha\mathcal{E}) \sqrt{\frac{\mathcal{E}(1 + \alpha\mathcal{E})}{\mathcal{E}_\alpha^+ (1 + \alpha\mathcal{E}_\alpha^+)}} \right\} d\mathcal{E},$$

$$d_{imp} = \kappa_{im} \int_B e^{-\mathcal{E}(2\lambda_W - \lambda_W^0)} (1 + 2\alpha\mathcal{E})^4 \frac{[1 + g(\mathcal{E})] \ln[1 + g(\mathcal{E})] - g(\mathcal{E})}{[1 + g(\mathcal{E})] \mathcal{E}^2 (1 + \alpha\mathcal{E})^2} d\mathcal{E},$$

with  $\lambda_W^0 = \frac{1}{k_B T_L}$ ,  $\mathcal{E}_\alpha^+ = \mathcal{E} + \hbar\omega_\alpha$ ,  $g(\mathcal{E}) = 8a\mathcal{E}(1 + \alpha\mathcal{E})$ ,  $a = \frac{m^*}{\hbar^2 \beta^2}$ .

In Fig.1, we show the behavior of mobility as a function of the average energy, neglecting the contribution from the scattering with impurities.

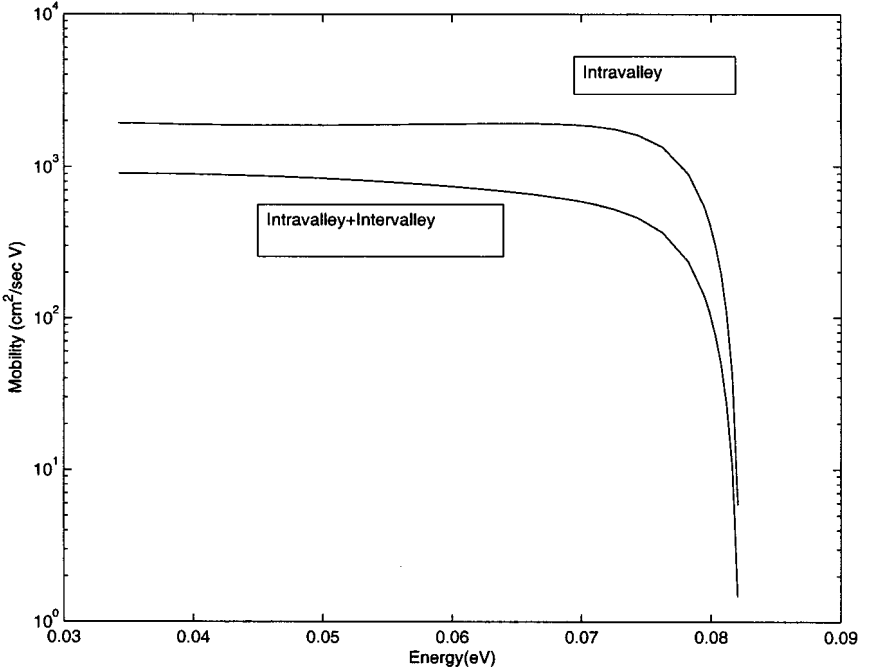


Fig. 1. Mobility vs energy (bulk Silicon).

## 5. Conclusions

As we have anticipated in the introduction, the main aim of this paper is to attract attention on variational methods in semiclassical transport models. We believe that these methods could be used for developing new numerical approximations of the semiclassical Boltzmann equation for semiconductors. In this respect, the main mathematical problem is the lack of any coercivity property of the functional  $J$ .

As regards the application which we have considered in greater extent in this paper, the main drawback of our implementation is the lack of validity for  $\lambda_W \geq \frac{1}{2k_B T_L}$ , due to presence of the weight function in the functional. This means that the ansatz used for our approximation is good only for low electric fields, up to  $1-1.5 \frac{V}{\mu m}$ . However this problem can be tackled by making a more suitable ansatz. For example, one could take the distribution function in the form suggested by the Maximum Entropy Principle (MEP)<sup>13</sup>

$$f(\mathbf{k}) = \exp \left( - \sum_{n=0}^N \lambda_{W_n} \mathcal{E}^n - \mathbf{v} \cdot \sum_{m=0}^M \lambda_{S_m} \mathcal{E}^m \right)$$

where  $N \geq 2$  and  $M$  can be suitably chosen and the  $\lambda_W$ 's and  $\lambda_S$ 's, Lagrange multipliers, depend on the correspondent moments of the MEP distribution

$$n = \int f d\mathbf{k}, \quad W_n = \frac{\int \mathcal{E}^n f d\mathbf{k}}{\int f d\mathbf{k}}, \quad n = 1, \dots, N,$$

$$S_m = \frac{\int \mathcal{E}^m \mathbf{v} f d\mathbf{k}}{\int f d\mathbf{k}}, \quad m = 0, \dots, M,$$

$W_1$  is the energy,  $S_0$  and  $S_1$  the velocity and energy flux respectively.

With this ansatz for the distribution function, the problem is reduced to finding the stationary points of a function of  $N+3M-1$  variables:  $\lambda_{W_n}$ ,  $\lambda_{S_m}$ ,  $n = 1, \dots, N$ ,  $m = 0, \dots, M$ ,  $\lambda_{W_0}$  being determined in terms of the remaining  $\lambda_W$ 's by the condition  $n = N_D$ .

The numerical solution of this problem, for various values of  $N$  and  $M$ , is still in progress and will be presented in a forthcoming paper.<sup>11</sup>

## Dedication

*τυγχάνω γάρ ἐκ παιδὸς ἐπιθυμῶν κτήματός του, ὡς περ ἄλλος ἄλλου. ὁ μὲν γὰρ τις ἵππους. ἐπιθυμεῖ κτᾶσθαι, ὁ δὲ κύνας, ὁ δὲ χρυσίον, ὁ δὲ τιμᾶς: ἐγὼ δὲ πρὸς μὲν ταῦτα πρᾶως ἔχω, πρὸς δὲ τὴν τῶν φίλων κτήσιν πάνυ ἐρωπικῶς, καὶ βουλομένη ἂν μοι φίλου ἀγαθὸν γενέσθαι μᾶλλον ἢ*

τὸν ἀριστὸν ἐν ἀνθρώποις ὄρνυγα ἢ ἄλεκτρούνα, καὶ ναὶ μὰ Δία ἐγὼ γε  
 μᾶλλον ἢ ἵππου τε καὶ κύνᾳ — οἶμαι δέ, νῆ τὸν κύνᾳ, μᾶλλον ἢ τὸ  
 Δαρεῖον χρυσοῦν κτήσασθαι δεξαίμην πολὺ πρότερον ἔταιρον, μᾶλλον  
 <δὲ> ἢ αὐτὸν Δαρεῖον — οὕτως ἐγὼ φιλέταιρός τις εἰμι. ὑμᾶς

*All people have their fancies; some desire horses, and others dogs; and some are  
 fond of gold, and others of honour. Now, I have no violent desire of any of these  
 things; but I have a passion for friends; and I would rather have a good friend  
 than the best cock or quail in the world: I would even go further, and say the best  
 horse or dog. Yea, by the dog of Egypt, I should greatly prefer a real friend to all  
 the gold of Darius, or even to Darius himself: I am such a lover of friends as that.*

Socrates, in *Lysis* (Plato)

DEDICATED TO MY FRIEND ANTONIO GRECO WHO INTRODUCED ME TO THE INTRICACIES AND THE BEAUTIES OF ASYMPTOTIC METHODS IN NONLINEAR WAVE PHENOMENA (A. M. Anile)

## References

1. P. A. Markowich, C. A. Ringhofer and C. Schmeiser, *Semiconductor Equations* (Springer, 1990).
2. C. Jacoboni, P. Lugli, *The Monte Carlo Method for Semiconductor Device Simulations* (Springer, 1989).
3. K. Tomizawa, *Numerical simulation of submicron semiconductor devices* (Artech House, Boston, 1993).
4. J. W. Jerome, *Analysis of charge transport. A mathematical study of semiconductor devices* (Springer, 1995).
5. C. Cercignani, *Rarefied Gas Dynamics* (Cambridge University Press, 2000).
6. J. J. Duderstadt and W. R. Martin, *Transport Theory* (Wiley, New York, 1979).
7. W. M. Stacey Jr., *Variational Methods in Nuclear Reactor Physics* (Academic Press, New York, 1974).
8. A. Schenk, *Advanced Physical Models for Silicon Device Simulation* (Springer, Wien, 1998).
9. G. Ali, A. M. Anile and G. Mascali, *Rendiconti del Circolo Matematico di Palermo*, Serie II, Suppl. **78**, 11-18 (2006).
10. J. J. Sakurai, *Modern Quantum Mechanics* (Benjamin/Cummings, 1985).
11. G. Ali, G. Mascali, *Variational formulation of the steady Boltzmann equation for semiconductors*, in preparation.
12. C. Jacoboni and L. Reggiani, *Rev. Mod. Phys.*, **55**, 645-705 (1983).
13. A. M. Anile, G. Mascali and V. Romano, *Recent developments in hydrodynamical modeling of semiconductors*, in *Lecture Notes in Mathematics, Mathematical problems in semiconductors*, vol. 1823 (Springer, 2003).