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An Explicitly Solvable Kinetic Model for Semiconductors

Carlo Cercignani[1,2]

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We consider a simple model for the electron Boltzmann equation in a semiconductor and show that specific boundary value problems can be explicitly solved. Cases of both homogeneous and inhomogeneous electric fields are considered.

KEY WORDS: Boltzman equation, homogeneous electric fields, inhomogeneous electric fields, boundary value problems.

1. INTRODUCTION

When the transport of charges in a semiconductor is considered on a sufficiently large time scale, then the motion of the carriers is decidedly influenced by the short-range interactions with the crystal lattice, which can be described, in a classical picture of the electron gas, by particle collisions. This situation, which occurs in high-density integrated circuits, explains why there has been an increasing interest in understanding the mathematics of an electron gas in submicron structures.[1] The basic tool in this situation is given by the Boltzmann equation,[2] which may exclude the short-range interactions between carriers, which only play a role when the particle density is very large, but can incorporate the Pauli exclusion principle, if necessary. Here we shall not take into account any quantum effects; in particular, we shall ignore the exclusion principle and the fact that we deal with quasiparticles rather than particles. Also we shall assume that we deal with just one species; the extension to a mixture of carriers is possible, if cumbersome.

[1] Institut für Theoretische Physik II, Universität Erlangen, D-91058 Erlangen, Germany.
[2] Permanent address: Dipartimento di Matematica, Politecnico di Milano, I-20133 Milan, Italy.

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Since the Boltzmann equation for classical gases has been used for several years in the study of flight in the upper atmosphere and similar problems occur in the transport of neutrons and radiation, one might try to borrow some of the methods and results.[3,4] One difficulty is that in these areas the body force is ignored or considered to be of secondary importance, while the action of the electric field is of paramount importance in the case of semiconductor devices. It is in fact the circumstance that the electrons are heated up by the electric field that needs to be accurately modeled.[5,6]

The Boltzmann equation for the electron gas in a semiconductor may be written as follows:

$$\frac{\partial f}{\partial t} + \mathbf{v} \cdot \frac{\partial f}{\partial \mathbf{x}} + \frac{e}{m} \mathbf{E} \cdot \frac{\partial f}{\partial \mathbf{v}} = Lf \tag{1.1}$$

where $f = f(\mathbf{x}, \mathbf{v}, t)$ is the distribution function, a function of position $\mathbf{x}$, velocity $\mathbf{v}$, and time t. Here $\mathbf{E}$ is the electric field, sum of the external field (applied or produced by ions) and the field produced by carriers, e the electric charge of a carrier, m its mass, and L the collision operator, assumed to be linear.

A frequently used approximation (the relaxation time approximation) assumes the following model for the collision term:

$$Lf = \left[C \exp(-\beta \, |\mathbf{v}|^2/2) \int (\tau_{\mathbf{v}'})^{-1} f(\mathbf{v}') \, d^3\mathbf{v} - f \right] \Big/ \tau_{\mathbf{v}} \tag{1.2}$$

where $\beta = m/(k_B T)$ (T is the temperature, k_B is Boltzmann's constant) and C is a suitable normalization constant that ensures conservation of particles.

The above expression clearly shows that in the space-homogeneous case the distribution function relaxes to a Maxwell–Boltzmann distribution, proportional to $\exp(-\beta \, |\mathbf{v}|^2/2)$. Please remark that the integral multiplying this distribution is not proportional to the number density of the electrons, as is sometimes stated, unless the relaxation time is independent of $\mathbf{v}$.

In this paper we shall consider steady solutions, depending on just one coordinate x and one velocity component ξ, for a special choice of the relaxation time $\tau = \tau(\mathbf{v})$, which was first considered in connection with a model for a gas molecule wandering inside a solid body, in a layer near the surface.[7] The model is chosen in such a way as to lead to explicit solutions for boundary value problems.

2. THE MODEL AND ITS SOLUTION IN THE ABSENCE OF ELECTRIC FIELDS

As mentioned in the introduction, in order to discuss the behavior of the solutions of the Boltzmann equation in the presence of boundaries, we shall consider a steady problem in a one-dimensional geometry for a model with a relaxation time approximation.

We shall take the relaxation time to be inversely proportional to $|\xi|$, where ξ denotes the velocity component along the x axis; this might be objectionable, but one may think that a suitable average has been taken with respect to the transverse degrees of freedom.

The Boltzmann equation then reads as follows:

$$\xi \frac{\partial f}{\partial x} + \frac{q}{m} E \frac{\partial f}{\partial \xi} = |\xi| \left[M(\xi) \int |\xi'| f(\xi')\, d\xi' - f \right] \Big/ l \tag{2.1}$$

where l is a sort of mean free path and E the only component of the electric field, whereas $M(\xi)$, the one-dimensional Maxwellian

$$M(\xi) = (\beta/2) \exp(-\beta\xi^2/2) \qquad [\beta = m/(k_B T)] \tag{2.2}$$

is normalized in such a way that

$$\int M(\xi)\, |\xi|\, d\xi = 1 \tag{2.3}$$

This ensures that the particle number is conserved in a collision. We shall also assume that the temperature in the Maxwellian is constant.

Let us first try to solve the equation in the case of a zero electric field. Then we have the following consequences of Eq. (2.1):

$$\begin{aligned} \partial j/\partial x &= 0 \\ \partial k/\partial x &= -j/l \end{aligned} \tag{2.4}$$

where

$$j = \int \xi f\, d\xi; \qquad k = \int |\xi|\, f\, d\xi \tag{2.5}$$

Then j is a constant and

$$k = -jx/l + k_0 \tag{2.6}$$

where k_0 is another constant.

Inserting Eq. (2.6) into Eq. (2.1) (with $E=0$), we obtain

$$\xi\, \partial f/\partial x = |\xi|\, [(k_0 - jx/l)\, M(\xi) - f]/l \tag{2.7}$$

It is convenient to solve the equation separately for $\xi > 0$ and $\xi < 0$; we denote by f^+ and f^- the corresponding solutions. We have

$$f^\pm = [k_0 - j(x/l \mp 1)]\, M(\xi) + A^\pm(\xi)\, e^{\mp x/l} \tag{2.8}$$

where $A^\pm(\xi)$ denote two functions of ξ which are only subjected to the restriction

$$\int_{\pm\xi > 0} \xi A^\pm(\xi)\, d\xi = 0 \tag{2.9}$$

in order to be consistent with Eqs. (2.5)–(2.6).

We thus obtain a solution which has a form similar to the one holding for small mean free paths plus a term which becomes important only near the boundaries and decays on a length of the order of l. Just to give an example, let us assume that the boundary conditions are

$$f^\pm(\mp L) = g_\pm(\xi)\, M(\xi) \tag{2.10}$$

where $g_\pm$ are two given functions. Then

$$[k_0 \pm j(L/l + 1)]\, M(\xi) + A^\pm(\xi)\, e^{L/l} = g_\pm(\xi)\, M(\xi) \tag{2.11}$$

and

$$A^\pm(\xi) = e^{-L/l}\{-[k_0 \pm j(L/l + 1)]\, M(\xi) + g_\pm(\xi)\, M(\xi)\} \tag{2.12}$$

and Eqs. (2.9) determine the values of j and k_0 in terms of $g_\pm$.

3. THE CASE OF A CONSTANT ELECTRIC FIELD

Let us consider now the case of a constant electric field in a slab $-L < x < L$ and let us put $\alpha = qE/m$. Without loss of generality we assume $\alpha > 0$. The first of Eqs. (3.4) still holds, but the second one does not. We then write the equation for the particles with $\xi < 0$ (which travel against the field)

$$\xi\, \partial f^-/\partial x + \alpha\, \partial f^-/\partial \xi = |\xi|\, \{M(\xi)[2k_-(x) + j] - f^-\}/l \tag{3.1}$$

where we have let

$$k_\pm(x) = \int_{\pm\xi > 0} |\xi|\, f^\pm(x, \xi)\, d\xi \tag{3.2}$$

and remarked that $j = k_+ - k_-$ is the constant current.

The trajectory of a particle in the phase plane in the absence of collisions is represented by the parabolas

$$\tfrac{1}{2}\xi^2 - \alpha x = \varepsilon \tag{3.3}$$

Please remark that $\varepsilon \geqslant -\alpha L$. Unless $\varepsilon \geqslant \alpha L$, a particle starting from $x = L$ will reverse its path for $x = -\varepsilon/\alpha$.

Let us now change the independent variables in Eq. (3.1) from (x, ξ) to (y, ε), where $y = x$ and ε is given by Eq. (3.3). Then Eq. (3.1) becomes

$$-l\frac{\partial f^-}{\partial y} = M([2(\varepsilon+\alpha y)]^{1/2})[2k_-(y)+j] - f^- \tag{3.4}$$

and hence

$$f^- = A^-(\varepsilon)\, e^{y/l} + \int_y^L e^{(y-y')/l} M([2(\varepsilon+\alpha y')]^{1/2})[2k_-(y')+j]\, dy'/l, \qquad -\varepsilon/\alpha < y < L \tag{3.5}$$

or, going back to the original variables (x, ξ),

$$f^- = A^-(\tfrac{1}{2}\xi^2 - \alpha x)\, e^{x/l} + \int_x^L e^{(x-x')/l} M([\xi^2 + 2\alpha(x'-x)]^{1/2})[2k_-(x')+j]\, dx'/l \tag{3.6}$$

We can now form an integral equation for k^- by inserting (3.5) into Eq. (3.2). We obtain

$$k^- = k_0^-(x) + \tfrac{1}{2}\int_x^L e^{[(x-x')(1/l+\beta\alpha)]}[2k_-(x')+j]\, dx'/l \tag{3.7}$$

where

$$k_0^-(x) = e^{x/l}\int_{\xi<0} |\xi|\, A^-(\tfrac{1}{2}\xi^2 - \alpha x)\, d\xi \tag{3.8}$$

and we used Eq. (2.2).

If we now multiply Eq. (3.7) by $e^{-x(1/l+\beta\alpha)}$ and differentiate with respect to x, we obtain

$$dk^-/dx - \beta\alpha k_- = d_0(x) - j/(2l) \tag{3.9}$$

where

$$d_0(x) = e^{(x/l+\beta\alpha x)}\frac{d}{dx}[k_0^- e^{-(x/l+\beta\alpha x)}] \tag{3.10}$$

It is easily checked that when $\alpha=0$, $d_0=0$ and Eq. (3.9) with $j=\text{const}$ reproduces Eqs. (2.4).

Let us now consider the particular case when the boundary conditions reduce to Eq. (2.10) with $g_\pm(\xi)=n_\pm$ are constants, or, in other words,

$$f^\pm(\mp L)=n_\pm M(\xi) \tag{3.11}$$

Then it is easy to see that

$$A^-\left(\frac{1}{2}\xi^2-\alpha x\right)=\frac{\beta}{2}n^- e^{-\beta[\xi^2/2-\alpha(x-L)]}e^{-L/l} \tag{3.12}$$

and

$$k_0^-(x)=\tfrac{1}{2}n^- e^{[(x-L)/l+\beta\alpha(x-L)]} \tag{3.13}$$

and Eq. (3.10) shows that $d_0(x)=0$ and hence Eq. (3.9) reduces to

$$dk^-/dx-\beta\alpha k^- = -j/(2l)$$

and hence

$$dk/dx-\beta\alpha k = -j(1/l+\beta\alpha) \tag{3.14}$$

This shows that in this case k is a constant plus an exponential in x:

$$k=J_0+K_0 e^{\beta\alpha x} \tag{3.15}$$

where

$$J_0=j[1/(l\beta\alpha)+1] \tag{3.16}$$

One can easily relate J_0 and K_0 to n^+ and n^-, because

$$k^+=(k+j)/2=j[1+1/(2l\beta\alpha)]+(K_0/2)\,e^{\beta\alpha x}$$

and

$$k^-=(k-j)/2=j/(2l\beta\alpha)+(K_0/2)\,e^{\beta\alpha x} \tag{3.17}$$

and $k^\pm(\mp L)$ must equal $n^\pm/2$. Thus

$$\begin{aligned} j&=2\alpha\beta l\,\frac{n^+e^{\alpha\beta L}-n^-e^{-\alpha\beta L}}{(1+2l\beta\alpha)\,e^{\alpha\beta L}+e^{-\alpha\beta L}}\\ J_0&=\left(\frac{1}{l\beta\alpha}+1\right)\frac{n^+e^{\alpha\beta L}-n^-e^{-\alpha\beta L}}{[1/(2l\beta\alpha)+1]\,e^{\alpha\beta L}+e^{-\alpha\beta L}/(2\alpha\beta l)}\\ K_0&=2\,\frac{n^-(1+2l\alpha\beta)-n^+}{(1+2l\alpha\beta)\,e^{\alpha\beta L}-e^{-\alpha\beta L}} \end{aligned} \tag{3.18}$$

We can now compute $f^-(x,\xi)$ from Eq. (3.6):

$$
\begin{aligned}
f^- &= \frac{\beta}{2} n^- e^{-\beta[\xi^2/2 + \alpha(L-x)]} e^{-(L-x)/l} \\
&\quad + \frac{\beta}{2e^{-\beta\xi^2/2}} \left[J_0 \frac{1 - e^{-(L-x)(\alpha\beta + 1/l)}}{1 + \alpha\beta l} \right. \\
&\quad \left. + K_0 e^{\beta\alpha x} (1 - e^{-(L-x)/l}) \right] \\
&= \beta k^-(x)\, e^{-\beta\xi^2/2}
\end{aligned} \tag{3.19}
$$

The calculation of f^+ is more complicated, because there are two contributions: particles coming directly from the boundary at $x = -L$ and particles which started from $x = L$ but reversed their paths, because their energy (per unit mass) $\varepsilon = \frac{1}{2}\xi^2 - \alpha x$ is less than αL. We thus distinguish two regions in the phase plane, $\frac{1}{2}\xi^2 - \alpha x > \alpha L$ and $\frac{1}{2}\xi^2 - \alpha x < \alpha L$. In the first region we have

$$
\begin{aligned}
f^+ &= \frac{\beta}{2} n^+ e^{-\beta\xi^2/2} e^{-(L+x)(1/l - \alpha\beta)} \\
&\quad + \frac{\beta}{2} e^{-\beta\xi^2/2} \left[J_0 \frac{1 - e^{-(L+x)(1/l - \alpha\beta)}}{1 - \alpha\beta l} \right. \\
&\quad \left. + K_0 e^{\beta\alpha x} (1 - e^{-(L+x)/l}) \right]
\end{aligned} \tag{3.20}
$$

$$
\left(\frac{1}{2}\xi^2 - \alpha x > \alpha L \right)
$$

whereas in the second region, if we take into account that a particle going through x with velocity ξ reversed its path at $x - \xi^2/(2\alpha)$, we obtain

$$
\begin{aligned}
f^+ &= \left\{ n^- \frac{\beta}{2} e^{-\beta\alpha(L-x)} e^{-[(L-x+\xi^2/(2\alpha)]/l} e^{-\beta\xi^2/2} \right. \\
&\quad + \frac{\beta}{2} \left[J_0 \frac{1 - e^{-[L-x+\xi^2/(2\alpha)](\alpha\beta + 1/l)}}{1 + \alpha\beta l} \right. \\
&\quad \left.\left. + K_0 e^{\beta(\alpha x - \xi^2/2)} (1 - e^{-(L-x)/l - \xi^2/(2\alpha l)}) \right] \right\} e^{-\xi^2/(2\alpha l)} \\
&\quad + \frac{\beta}{2} e^{-\beta\xi^2/2} \left[J_0 \frac{1 - e^{-\xi^2/(2\alpha l) + \beta\xi^2/2}}{1 - \alpha\beta l} \right. \\
&\quad \left. + K_0 e^{\beta\alpha x} (1 - e^{-\xi^2/2\alpha l}) \right]
\end{aligned} \tag{3.21}
$$

$$
\left(\frac{1}{2}\xi^2 - \alpha x < \alpha L \right)
$$

It is clear that one has layers close to the boundaries which are extremely thin when the mean free path is small, but tend to invade the entire sample when the mean free path becomes comparable with the size of the latter.

Before closing this section, we remark that it is easy to obtain the space-homogeneous solution corresponding to that discussed by Trugman and Taylor[5] for the case of a constant relaxation time. It is given by

$$f^+ = \frac{j}{2\alpha l(1-\beta\alpha l)}\left[(1+\beta\alpha l)\, e^{-\beta\xi^2/2} - 2\beta\alpha l e^{-\xi^2/2\beta\alpha l}\right]$$

$$f^- = \frac{j}{2\alpha l} e^{-\beta\xi^2/2} \qquad (\alpha > 0, \quad j > 0) \tag{3.22}$$

where j is, of course, the current density.

4. THE CASE OF A NONCONSTANT FIELD

The case of nonconstant, monotonous potential can be treated in a similar way. Let us assume that the potential energy is decreasing with x. The fact that the potential energy is monotonously decreasing implies (a) there are no particles with negative velocity that reverse their path, (b) we can invert the analog of Eq. (3.4), which now reads

$$\tfrac{1}{2}\xi^2 + V(x) = \varepsilon \tag{4.1}$$

with

$$x = A(\varepsilon - \tfrac{1}{2}\xi^2) \tag{4.2}$$

where A is the inverse function V^{-1}. In particular, Eq. (3.6) is replaced by

$$f^- = A^-(\tfrac{1}{2}\xi^2 + V(x))\, e^{x/l} + \int_x^L e^{(x-x')/l} M([\xi^2 + 2V(x) - 2V(x')]^{1/2})[2k_-(x') + j]\, dx'/l \tag{4.3}$$

and the integral equation for k^- becomes

$$k^- = k_0^-(x) + \tfrac{1}{2}\int_x^L e^{[(x-x')/l + \beta(V(x') - 2V(x))]}[2k_-(x') + j]\, dx'/l \tag{4.4}$$

where

$$k_0^-(x) = e^{x/l}\int_{\xi<0} |\xi|\, A^-(\tfrac{1}{2}\xi^2 + V(x))\, d\xi \tag{4.5}$$

If we now multiply Eq. (4.4) by $e^{-x/l+\beta V(x)}$ and differentiate with respect to x, we obtain

$$dk^-/dx + \beta V'(x)\, k_- = d_0(x) - j/(2l) \qquad (4.6)$$

where

$$d_0(x) = e^{x/l-\beta V(x)} \frac{d}{dx} (k_0^- e^{-[x/l-\beta V(x)]}) \qquad (4.7)$$

If we consider the particular case when the boundary conditions reduce to Eq. (3.11), then

$$A^- \left(\frac{1}{2}\xi^2 + V(x)\right) = \frac{\beta}{2} n^- e^{-\beta[\xi^2/2 + V(x) - V(L)]} e^{-L/l} \qquad (4.8)$$

and

$$k_0^-(x) = \tfrac{1}{2} n^- e^{(x-L)/l - \beta[V(x) - V(L)]} \qquad (4.9)$$

and Eq. (4.7) shows that $d_0(x) = 0$ and hence Eq. (4.6) reduces to

$$dk^-/dx + \beta V'(x)\, k^- = -j/(2l) \qquad (4.10)$$

and hence k can be obtained through a quadrature.

The remaining calculations can be carried ond, but become cumbersome. The case of a nonmonotonous potential requires a more detailed study.

5. CONCLUDING REMARKS

A kinetic model describing the behavior of carriers in a semiconductor has been used to find exact solutions for boundary value problems. Although the model is extremely simplified, it is felt that the qualitative features of the transport phenomena in small semiconductor devices are correctly described by the present solutions. Further work is of course needed for electric fields more general than those considered here.

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