Relaxation time approximation for electron-phonon interaction in semiconductors

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Abstract. A Boltzmann equation for semiconductors is considered. Physical assumptions include the parabolic band approximation and a new relaxation time model for electron-phonon interaction. Thermal equilibrium distributions for this scattering mechanism are products of Maxwellian distributions with periodic functions of the energy, where the period is the energy of a phonon. The hydrodynamic limit is considered and a drift-diffusion model is derived by formal asymptotic methods.

Key words: Semiconductors, Boltzmann equation, drift-diffusion limit

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1 Introduction

The subject of this work is the derivation of hydrodynamic limits of kinetic models for the transport of electrons in a semiconductor crystal. The basic character of these hydrodynamic limits is determined by the scattering mechanisms and, in particular, by the corresponding thermal equilibrium distributions. In mathematical terms, the scattering mechanisms are described by an integral operator, and the set of all equilibrium distributions is the kernel of this operator. Statistical mechanics tells us that the equilibrium distribution for electrons is a Fermi-Dirac distribution or, as an approximation for low density situations, a Maxwellian distribution. In both cases the mean velocity is zero and the temperature is equal to the lattice temperature. The electron density (or, equivalently, the chemical potential) remains as the only free parameter. Thus, the set of equilibrium distributions is one-dimensional. In semiconductors, relaxation towards equilibrium is reached via a number of different scattering mechanisms (see [1]). The total scattering operator can be written as a sum of models for the individual scattering mechanisms. In general, these individual scattering terms do not lead to relaxation towards a Fermi-Dirac (or Maxwellian) distribution, but to a less restricted set of distributions. In mathematical terms: The kernel of a scattering operator modelling one scattering mechanism can be larger than the set of Fermi-Dirac (or Maxwellian) distributions. This observation becomes important when one notices that different scattering mechanisms can have strongly different relaxation times in certain situations. This means that for structures of a certain sizes and/or on certain time scales relaxation towards larger sets of equilibrium distributions is relevant.

In this work a situation is considered where the scattering of electrons with phonons of fixed energy is the dominant scattering mechanism (the one with the shortest relaxation time). For simplicity, other scattering mechanisms are neglected. We also deal with a low density approximation. The corresponding (linear) scattering operator has been analyzed by Majorana [2]. The main result is that the kernel consists of all products of Maxwellian distributions with periodic functions of the energy, where the period is the energy of the phonon. In section 2 of this work electron-phonon scattering is modelled by a relaxation time model incorporating the essential features of the original scattering operator. In particular, it has the same kernel and the same collision invariants, i.e. it gives rise to conservation laws for the same quantities.

In section 3, the Cauchy problem for the corresponding Boltzmann equation is considered with equilibrium initial data. The hydrodynamic limit is computed by formally letting a scaled version of the mean free path tend to zero. The result is a drift-diffusion model determining the above mentioned periodic function of the energy and its dependence on position and time. The asymptotics are an adaption of the classical Hilbert expansion applied to the semiconductor case as in, e.g., [7].

The papers [6], [4] parallel to this work, deal with the physical model for electron-phonon scattering as analyzed in [2] and with the nonlinear model (Fermi-Dirac case) considered in [3], respectively.

2 The relaxation time approximation

We consider the transport equation

$$\frac{\partial f}{\partial t} + v \cdot \nabla_x f - \frac{q}{m} E \cdot \nabla_v f = Q(f) \tag{1}$$

for the electron distribution function $f(x, v, t)$, depending on position $x \in \mathbb{R}^3$, velocity $v \in \mathbb{R}^3$ and time $t \geq 0$. The electric field E is assumed to be given in terms of the position dependent electrostatic potential:

$$E(x) = -\nabla_x \Phi(x)$$

The parameters q and m denote the electron charge and effective mass, respectively, and we have used a parabolic band approximation (see [5] for more details). The scattering operator is assumed to have the form

$$\begin{aligned} Q(f)(x, v, t) &= \int_{\mathbf{R}^3} [aW(v, v') + W(v', v)] f(x, v', t)\, dv' \\ &\quad - f(x, v, t) \int_{\mathbf{R}^3} [aW(v', v) + W(v, v')]\, dv' \end{aligned} \tag{2}$$

with the parameter

$$a = \exp\left(\frac{\hbar\omega}{k_B T}\right)$$

and

$$W(v,v') = K(v,v')\delta(\varepsilon(v') - \varepsilon(v) - \hbar\omega)\,.$$

Here $\hbar\omega$, k_B and T are the energy of a phonon, the Boltzmann constant and the lattice temperature, respectively. By δ we denote the Dirac distribution and by $\varepsilon(v) = m|v|^2/2$ the kinetic energy. Physically relevant models for the overlap factor K are given by

$$K(v,v') = A\left(|v - v'|^2 + \beta\right)^{-n} \tag{3}$$

with $A > 0$, $\beta \geq 0$ and $n > 0$. The most important property of K is the $O(3)$-invariance:

$$K(Sv, Sv') = K(v,v') \qquad \text{for every orthogonal matrix } S.$$

As a first step a scaling of (1) is introduced. We use a reference length L, reference velocity $v_0 = \sqrt{2\hbar\omega/m}$ and reference voltage $V_0 = \hbar\omega/q$. For the overlap factor we assume that it can be written in the form

$$K(v,v') = K_0 k\left(\frac{v}{v_0}, \frac{v'}{v_0}\right)$$

with a dimensionless function k. For the model (3) we have

$$K_0 = A\left(\frac{m}{2\hbar\omega}\right)^n, \qquad k(w,w') = \left(|w - w'|^2 + m\beta/(2\hbar\omega)\right)^{-n}.$$

Then a factor

$$1/\tau = \frac{2K_0}{m}\sqrt{\frac{2\hbar\omega}{m}}$$

can be taken out of the scattering integral, where τ is a characteristic value for the mean free flight time between collisions. Finally, we introduce the reference time $t_0 = L^2 m/(2\hbar\omega\tau)$. Then the scaled transport equation reads

$$\alpha^2\frac{\partial f}{\partial t} + \alpha\left(v\cdot\nabla_x f + \frac{1}{2}\nabla_x\Phi\cdot\nabla_v f\right) = Q(f)\,, \tag{4}$$

where the same symbols are used for scaled and unscaled variables. The dimensionless parameter

$$\alpha = \frac{\tau}{L}\sqrt{\frac{2\hbar\omega}{m}}$$

can be interpreted as a scaled version of the mean free path of an electron having the energy of a phonon. In the subsequent sections we shall be concerned with the limit $\alpha \to 0$.

The scaled scattering operator Q has the form (2) with

$$W(v, v') = k(v, v')\delta\left(|v'|^2 - |v|^2 - 1\right) .$$

An analysis of Q can be found in [2]. Here we only list those properties that will be needed in the sequel (assuming sufficient regularity of the function k):

(P1) H-Theorem: Let $\kappa : \mathbb{R} \longrightarrow \mathbb{R}$ be an increasing function. Then

$$\int_{\mathbf{R}^3} Q(f)\kappa\left(a^{|v|^2} f\right) dv \leq 0 .$$

Equality holds iff $f(v) = a^{-|v|^2} P(|v|^2)$, where P is a 1-periodic function, i.e. $P(u+1) = P(u)\ \forall u \geq 0$. Note that $a^{-|v|^2}$ is the scaled version of the Maxwellian distribution.

(P2) Nullspace: $Q(f) = 0$ iff $f(v) = a^{-|v|^2} P(|v|^2)$ with a 1-periodic function P.

(P3) Symmetry:

$$\int_{\mathbf{R}^3} Q(f_1) f_2 a^{|v|^2} dv = \int_{\mathbf{R}^3} Q(f_2) f_1 a^{|v|^2} dv .$$

(P4) Collision invariants:

$$\int_{\mathbf{R}^3} Q(f) P(|v|^2)\, dv = 0$$

for all 1-periodic functions P.

Obviously, (P2) implies that zero is an eigenvalue of infinite multiplicity of the operator Q. This degeneracy is caused by the fact that the scattering rate

$$S(v',v) = aW(v,v') + W(v',v)$$

is singular (more precisely, a measure). It is well known that zero is an eigenvalue of multiplicity 1 if the scattering rate is a positive bounded function (which is such that Q satisfies the principle of detailed balance). The eigenspace then is spanned by the Maxwellian $a^{-|v|^2}$ (see [7]).

Since the scattering rate as a function of v' is a measure supported by the union of the spheres with center in the origin and radii $\sqrt{|v|^2+1}$ and $\sqrt{(|v|^2-1)_+}$, respectively, the gain term

$$Q^+(f) = \int_{\mathbf{R}^3} [aW(v,v') + W(v',v)] f(v')\, dv'$$

of the collision operator depends on local values of f in the radial variable $|v|$. It is nonlocal in the angular variable $\omega \in \partial B_1$ (we set $v = |v|\omega$).

Thus, the singularity of the scattering rate causes a defect of compactness of Q^+, which allows for the infinite dimensional nullspace of Q.

Clearly, the non-compactness of Q^+ creates various problems in the derivation and justification of drift-diffusion approximations which, at least partially, are based on solving equations of the type $Q(f) = g$, where g lies in the range of Q. These difficulties are at least to some extent remedied by introducing the so-called relaxation time approximation of the collision operator Q.

The relaxation time approximation is obtained by introducing the projection Π of an appropriately chosen weighted L^2-space onto the nullspace of Q and by setting

$$Q^+(f) = Q^+(\Pi f) + Q^+((I-\Pi)f)\,.$$

The basic modeling step is to replace $Q^+(f)$ by $Q^+(\Pi f)$, which obviously makes sense if the density f represents a state close to thermal equilibrium (where $(I-\Pi)f$ is small).

We introduce the collision frequency

$$\lambda = \int_{\mathbf{R}^3} [aW(v',v) + W(v,v')] dv'\,.$$

A simple calculation using the $O(3)$-invariance of the overlap factor shows that λ depends only on $|v|^2$, i.e. $\lambda = \lambda(|v|^2)$, and

$$\begin{aligned}\lambda(u) &= \frac{a}{2}\sqrt{(u-1)_+}\int_{\partial B_1} k\left(\sqrt{(u-1)_+}\,\omega, \sqrt{u}\,e_1\right) d\omega \\ &\quad + \frac{1}{2}\sqrt{u+1}\int_{\partial B_1} k\left(\sqrt{u}\,e_1, \sqrt{u+1}\,\omega\right) d\omega\,,\end{aligned}$$

where $d\omega$ denotes the surface element on ∂B_1 and $e_1 = (1,0,0)$.

(P2) implies

$$Q^+(\Pi f) = \lambda(|v|^2)\Pi f\,,$$

and we obtain the relaxation time approximation of the collision operator

$$Q_R(f) = \frac{\Pi f - f}{\tau(|v|^2)}\,, \tag{5}$$

where (assuming $\lambda(u) > 0\ \forall u \geq 0$)

$$\tau(u) := \frac{1}{\lambda(u)}$$

denotes the relaxation time. We assume

$$\tau \in C([0,\infty))\,, \qquad 0 < \frac{1}{\tau} \leq M\,. \tag{6}$$

Finally, we choose the projection Π such that the properties (P1), (P3), (P4) of the original collision operator Q carry over to the relaxation time approximation Q_R 'as well as possible' (note that (P2) is satisfied automatically due to the construction of Q_R). For setting up a functional analytic framework, Π is interpreted as an orthogonal projection in a weighted L^2-space $\mathcal{H}$. From (P4) it can be easily deduced that the appropriate choice is

$$\mathcal{H} = L^2\left(\mathbb{R}^3, \frac{a^{|v|^2}}{\tau(|v|^2)}dv\right)\,, \quad \langle f,g\rangle_{\mathcal{H}} = \int_{\mathbb{R}^3} f(v)g(v)\frac{a^{|v|^2}}{\tau(|v|^2)}dv\,.$$

We denote the nullspace of Q_R by

$$\mathcal{N} := \left\{a^{-|v|^2}P(|v|^2) \in \mathcal{H} \mid P(u+1) = P(u) \text{ a.e. in } (0,\infty)\right\}\,.$$

Then $\mathcal{H} = \mathcal{N} \oplus \mathcal{N}^\perp$ and we define Π as the orthogonal projection of $\mathcal{H}$ onto $\mathcal{N}$.

A simple computation gives

$$\int_{\mathbf{R}^3} Q_R(f_1) f_2 a^{|v|^2} dv = -\langle (I - \Pi) f_1, (I - \Pi) f_2 \rangle_{\mathcal{H}}$$

and, thus, Q_R satisfies (P1) with $\kappa(r) = r$, as well as (P3) and (P4).

The following Lemma is immediate:

Lemma 2.1 *The equation $Q_R(f) = g$ has a solution $f \in \mathcal{H}$ iff $\tau(|v|^2) g \in \mathcal{N}^\perp$. Then every solution has the form*

$$f(v) = -\tau(|v|^2) g(v) + h(v)\,,$$

where h is an element of $\mathcal{N}$.

An explicit representation of the projection Π is easily obtained. We have

$$(\Pi f)(v) = a^{-|v|^2} P_f(|v|^2) \tag{7}$$

with the 1-periodic function P_f given by

$$\begin{aligned} P_f(u) &= \frac{1}{4\pi} \sum_{j=0}^{\infty} \int_{\partial B_1} f\left(\sqrt{u+j}\,\omega\right) d\omega\, \frac{\sqrt{u+j}}{\tau(u+j)} \\ &\quad \times \left(\sum_{j=0}^{\infty} a^{-u-j} \frac{\sqrt{u+j}}{\tau(u+j)} \right)^{-1}, \quad 0 < u < 1. \end{aligned} \tag{8}$$

3 The drift-diffusion approximation

We now consider the formal limit $\alpha \to 0$ in the Cauchy problem for the scaled Boltzmann equation (4), where the collision operator is replaced by the relaxation time model:

$$\begin{aligned} &\alpha^2 f_t + \alpha(v \cdot \nabla_x f + \tfrac{1}{2} \nabla_x \Phi \cdot \nabla_v f) = Q_R(f)\,, \\ &f(x,v,0) = a^{\Phi(x) - |v|^2} \overline{P}(x, |v|^2 - \Phi(x))\,, \end{aligned} \tag{9}$$

where $\overline{P}$ is a 1-periodic function of its second argument. Thus, the initial datum is an element of the nullspace $\mathcal{N}$ of Q_R for every fixed value of x. Expressing it as a function of the energy $|v|^2 - \Phi(x)$ will be convenient below.

We look for a formal asymptotic expansion of f in powers of the perturbation parameter α:

$$f = f_0 + \alpha f_1 + \alpha^2 f_2 + O(\alpha^3)$$

Inserting this expansion into the Boltzmann equation and equating coefficients of equal powers of α gives the equations

$$\begin{aligned} &Q_R(f_0) = 0\,, \\ &Q_R(f_1) = v \cdot \nabla_x f_0 + \tfrac{1}{2}\nabla_x \Phi \cdot \nabla_v f_0\,, \\ &Q_R(f_2) = \tfrac{\partial f_0}{\partial t} + v \cdot \nabla_x f_1 + \tfrac{1}{2}\nabla_x \Phi \cdot \nabla_v f_1\,. \end{aligned} \tag{10}$$

The first equation implies that f_0 lies in $\mathcal{N}$:

$$f_0(x,v,t) = a^{\Phi(x)-|v|^2} P_0(x, |v|^2 - \Phi(x), t)\,,$$

where the function P_0 is 1-periodic in its second argument. Equations for the determination of P_0 will be determined from the higher order equations in (10) being of the form considered in Lemma 2.1.

A straightforward computation gives the right hand side of the equation for f_1:

$$Q_R(f_1) = a^{\Phi-|v|^2} v \cdot \nabla_x P_0$$

The solvability condition of Lemma 2.1 is satisfied and we have

$$f_1 = -\tau a^{\Phi-|v|^2} v \cdot \nabla_x P_0 + a^{\Phi-|v|^2} P_1\,,$$

where P_1 is like P_0. Now the equation for f_2 becomes

$$\begin{aligned} Q_R(f_2) \;=\; & a^{\Phi-|v|^2}\Bigg(\frac{\partial P_0}{\partial t} + v\cdot\nabla_x P_1 - \tau v_i v_j \frac{\partial^2 P_0}{\partial x_i \partial x_j} \\ & -\tau'(v\cdot\nabla_x\Phi)(v\cdot\nabla_x P_0) - \frac{1}{2}\tau\nabla_x\Phi\cdot\nabla_x P_0\Bigg)\,, \end{aligned} \tag{11}$$

where the Einstein summation convention has been used.

The desired equation for the determination of P_0 is now obtained as a solvability condition for (11): By Lemma 2.1 the projection of the right hand side multiplied by τ onto the nullspace $\mathcal{N}$ of Q_R has to vanish. A straightforward computation using the representation (7), (8) of the projection leads to the equation

$$G(z,\Phi)\frac{\partial P_0}{\partial t} - \nabla_x \cdot (H(z,\Phi)\nabla_x P_0) = 0\,, \tag{12}$$

where $z = |v|^2 - \Phi(x)$ denotes the second argument of P_0. The functions G and H are 1-periodic in z and for $-\Phi \le z \le 1-\Phi$ defined by

$$\begin{aligned} G(z,\Phi) &= 2\pi \sum_{j=0}^{\infty} a^{-z-j}\sqrt{z+\Phi+j}\,, \\ H(z,\Phi) &= \frac{2\pi}{3}\sum_{j=0}^{\infty} a^{-z-j}\tau(z+\Phi+j)(z+\Phi+j)^{3/2}\,. \end{aligned}$$

It can be easily checked that $G > 0$ and $H > 0$ hold and that G, H and $\partial H/\partial\Phi$ are Hölder continuous with exponent $1/2$ as functions of Φ.

For every fixed value of z, (12) is a parabolic equation for P_0 as a function of x and t. This equation has to be solved subject to the initial condition

$$P_0(x,z,0) = \overline{P}(x,z)\,. \tag{13}$$

The complete determination of P_0 requires solution of the initial value problem (12), (13) for all values of z in an (arbitrary) interval of length 1.

Keeping z fixed means that the diffusion problem (12), (13) is solved along manifolds of constant total energy $z = |v|^2 - \Phi(x)$. The drift and diffusion components of the current density become apparent when the variables x, $u = |v|^2$ and t are used instead of x, z and t. The term $\nabla_x P_0$ then becomes $\nabla_x P_0 + \nabla_x \Phi\, \partial P_0/\partial u$. Derivatives with respect to all the variables x, u and t then appear in the drift-diffusion equation, whereas in the formulation (12) the problem is decoupled in the z-direction.

Approximations for the electron density and the electron flux are given by

$$\begin{aligned} n(x,t) &= \int_{\mathbf{R}^3} f_0(x,v,t)dv = \int_0^1 G(z,\Phi(x))P_0(x,z,t)dz\,, \\ J(x,t) &= \int_{\mathbf{R}^3} v f_1(x,v,t)dv = \int_0^1 H(z,\Phi(x))\nabla_x P_0(x,z,t)dz\,. \end{aligned}$$

Integrating (12) in the z-direction gives the continuity equation

$$\frac{\partial n}{\partial t} + \nabla_x \cdot J = 0\,.$$

An interesting special case occurs when we consider a constant electric field, i.e. $\Phi(x) = -E \cdot x$, and look for stationary, spatially homogeneous solutions of the transport equation. Thus, we are interested in the limits as $\alpha \to 0$ of solutions $f = f(v)$ of the equation

$$-\frac{\alpha}{2} E \cdot \nabla_v f = Q_R(f)\,. \tag{14}$$

The formal limit of f is now written in the form

$$f_0(|v|^2) = a^{-E\cdot x - |v|^2} P_0(x, |v|^2 + E \cdot x)\,,$$

implying $P_0(x,z) = a^z f_0(z - E\cdot x)$, where we use the notation $z = u + E\cdot x = |v|^2 + E\cdot x$. Using (12) we conclude that f_0 is a solution of the equation

$$\frac{d}{du}\left(\tilde{H}(u)\frac{df_0}{du}\right) = 0\,, \qquad 0 < u < 1\,,$$

where

$$\tilde{H}(u) = a^{u+E\cdot x} H(u + E\cdot x, -E\cdot x) = \frac{2\pi}{3}\sum_{j=0}^{\infty} a^{-j}\tau(u+j)(u+j)^{3/2}\,, \qquad 0 < u < 1\,.$$

Thus, defining the 1-periodic functions

$$\begin{aligned} P_1(u) &= a^u \int_0^u \frac{ds}{\tilde{H}(s)}\,, \qquad 0 < u < 1\,, \\ P_2(u) &= a^u\,, \qquad 0 < u < 1\,, \end{aligned}$$

f_0 is given by

$$f_0(u) = a^{-u}(A_1 P_1(u) + A_2 P_2(u))$$

with arbitrary real constants A_1, A_2. The limits of solutions of (14) as $\alpha \to 0$ form a two-dimensional subspace of the infinite-dimensional kernel of the collision operator Q_R. This result should be compared to those for collision operators with regular scattering rates [8]. In this case it can be shown that the solutions of (14) (if they exist!) form a one-dimensional space converging to the (also one-dimensional) kernel of the collision operator as $\alpha \to 0$.

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