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An Energy-Transport Model for Semiconductors Derived from the Boltzmann Equation

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An energy-transport model is rigorously derived from the Boltzmann transport equation of semiconductors under the hypothesis that the energy gain or loss of the electrons by the phonon collisions is weak. Retaining at leading order electron–electron collisions and elastic collisions (i.e., impurity scattering and the "elastic part" of phonon collisions), a rigorous diffusion limit of the Boltzmann equation can be carried over, which leads to a set of diffusion equations for the electron density and temperature. The derivation is given in both the degenerate and nondegenerate cases.

KEY WORDS: Semiconductors; kinetic equations; Boltzmann transport equation; degenerate gases; Fermi–Dirac statistics; diffusion approximation; drift-diffusion model; energy transport; hydrodynamic model; Hilbert expansion; Chapman–Enskog expansion.

1. INTRODUCTION

This paper is concerned with the rigorous derivation of an energy-transport model for semiconductors from a suitable diffusion approximation of the Boltzmann transport equation. We first consider a Boltzmann equation in which electron–electron collisions as well as impurity or phonon collisions are incorporated. Then by noting that in typical hot-electron situations, the relative energy gain or loss α^2 of the electrons during a phonon collision is small (i.e., $\alpha^2 \ll 1$), the phonon collision operator is expanded in powers of α^2. The leading-order term of the expansion is an elastic collision operator which can be combined with the impurity collision operator. Thus, the leading-order collision operator is the sum of the electron–electron collision

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operator and of an elastic collision operator. Its equilibrium solutions are Fermi–Dirac or Maxwelliam distributions with arbitrary electron density and temperature, but with zero mean velocity.

The diffusion limit of this Boltzmann equation consists in looking at a space scale of the order of $1/\alpha$ times the kinetic space scale (i.e., the mean free path), while the time scale is $1/\alpha^2$ times the kinetic time scale (i.e., the collision time). This results in a singularly perturbed Boltzmann equation, which can be investigated by the diffusion-approximation procedure. Its solution (formally) converges to a Fermi–Dirac (or Maxwellian) distribution function with time- and space-dependent density and temperature. The density and temperature satisfy a set of drift-diffusion equations, the coefficients of which are rigorously derived from the linearized collision operators. These coefficients appear to be the mobility, heat conductivity, and thermopower coefficients and coincide with the transport coefficients that can be found in the literature.(9, 19) This extended drift-diffusion model can be interpreted as a hydrodynamic model in which the terms involving the electron mass in the momentum transport equation have been dropped.

The usual drift-diffusion model only involves an evolution equation for the density.(29) Its derivation from the Boltzmann equation through the diffusion approximation is treated in many references(26, 10) and mathematically explored in refs. 23, 24, and 15. The hydrodynamic model of semiconductors was first proposed in ref. 7 based on a moment expansion of the distribution function f and closure relations which rely on the perfect-gas equation of state with a heat conductivity term added. Phenomenological relations are used for the momentum and energy relaxation times. The use of the Wiedemann–Franz law for the heat conductivity first appears in ref. 5. Different closure relations are proposed in ref. 4 (where the distribution function is supposed spherically symmetric) or in ref. 18 (where a perturbation in the direction of the field is added to a spherically symmetric Ansatz). An incredible amount of numerical work has been devoted to the solution of the hydrodynamic model and we refer the reader to the bibliography in the above-quoted references.

In most of the real application cases of the hydrodynamic model, the convective terms in the momentum transport equation are neglected and the obtained systems are often called "energy-transport models." The first derivation of an energy-transport model from the Boltzmann equation can be found in ref. 28, under the simplifying assumption that the elastic collisions can be described by an energy-dependent relaxation time. Similar derivations can also be found in refs. 9 and 19. Other derivations are instead based on phenomenological closure relations. This is in particular the case of the recent work by Rudan *et al.*,(27) where an extension of the energy-transport models for arbitrary band structures is performed.

Despite their unquestionable success, these approaches suffer from the lack of a sufficiently general theory supporting the various choices of closure relations that are made. Our approach tries to fill this gap by proposing a rigorous closure of the energy-transport model deduced from the Boltzmann equation. Our framework handles general energy band models and degenerate as well as nondegenerate statistics. It highlights the hypotheses and properties that the collision operators need to fulfill in order for this approach to be valid. The relation between the hydrodynamic and energy-transport models is also clarified. Note a previous attempt to derive directly the hydrodynamic model in ref. 24, based on a high-field drift-diffusion approximation, but this model leads to a somehow nonstandard equation of state.

An intermediate approach between the Boltzmann equation and the hydrodynamic or energy-transport models is the spherical harmonic expansion method (see refs. 14 and 31 and references therein). This approach has been put in the diffusion approximation formalism in ref. 13 under the hypothesis that the relative energy gain or loss of an electron during a phonon collision is very small. We shall use the same hypothesis, with the difference that we consider the electron–electron collision operator to be of the same (leading) order as the elastic collision operator. A somehow similar appraoch to ref. 13 has been applied in refs. 21 and 22, using as leading-order collision operator the optical phonon scattering. In ref. 30 a moment expansion of the spherical harmonic model of ref. 31 or ref. 13 leads to an energy-transport model with a diagonal diffusion matrix, but the moment expansion closure follows from phenomenological considerations.

Other recently introduced intermediate models are the higher order moment models, which consider additional evolution equations for the heat flux, stress tensor deviator, etc. Besides the classical approach,(16,17) the closure relations which have been investigated in semiconductor models issue from the extended thermodynamics theory(1,2) and can be related to the recent models developed for gas dynamics in ref. 20.

This paper is organized as follows: Section 2 gives the setting of the problem, while Section 3 introduces the expansion of the phonon collision operator with respect to the parameter α. In Section 4, we perform the diffusion approximation by using a Hilbert expansion. The connection between the resulting drift-diffusion system in (n, T) and the usual hydrodynamic equation is shown in Section 5. Up to this point, the analysis is carried through in the framework of a degenerate electron gas with an arbitrary band structure. The case of a nondegenerate electron gas with a parabolic band structure (which is a simplification usually assumed in most semiconductor models) is dealt with in Section 6.

A rigorous proof of the convergence of the Hilbert expansion is far beyond the scope of this paper. For a mathematical proof of convergence in a linearized framework, we refer to ref. 6. A proof in the nonlinear case is in progress. Finally, a similar model can be derived for electrons in a plasma.(11)

2. BOLTZMANN EQUATION FOR DEGENERATE ELECTRON GAS IN A SEMICONDUCTOR

We consider the electron distribution function $f(x, k, t)$ of electrons in the conduction band of a semiconductor. For the sake of simplicity, we shall not consider boundary conditions and let the position variable x belong to $\mathbb{R}^3$. The pseudo wavevector k belongs to the Brillouin zone B associated with the underlying crystal lattice.(3) Since B is the elementary cell of the dual lattice L^*, it will be identified with the three-dimensional torus $\mathbb{T}^3 = \mathbb{R}^3/\mathbb{L}^* \cong B$. Here, f, like any other function of k appearing in this paper, will be identified with the periodic function on $\mathbb{R}^3$ with period $\mathbb{L}^*$, in an obvious way. The equations of motion of the individual electrons in an electric potential $V(x)$ are given in the semiclassical picture by(3)

$$\dot{x} = \frac{1}{h}\nabla_k \varepsilon(k), \qquad \dot{k} = \frac{q}{h}\cdot \nabla_x V(x) \tag{2.1}$$

where $(x(t), k(t))$ is the electron trajectory in phase space, h is the reduced Planck constant, q is the positive elementary charge, and ε is the kinetic energy.

For an ensemble of electrons subject to collisions with lattice defects or to binary collisions, the Boltzmann transport equation governs the evolution of the distribution function f according to(9)

$$\frac{\partial f}{\partial t} + \frac{1}{h}\nabla_k \varepsilon(k)\cdot\nabla_x f + \frac{q}{h}\nabla_x V(x, t)\cdot\nabla_k f = Q_{ld}(f) + Q_e(f) \tag{2.2}$$

where $Q_{ld}(f)$ stands for the collision operator modeling lattice-defect collisions and $Q_e(f)$ stands for electron–electron binary collisions.

The two main classes of lattice defects that we shall consider are impurities and phonons,(3)

$$Q_{ld}(f) = Q_{\text{imp}}(f) + Q_{\text{ph}}(f) \tag{2.3}$$

Because of the elastic character of impurity scattering, Pauli's exclusion terms in the gain and loss terms cancel and we get

$$Q_{\mathrm{imp}}(f)(k) = \int_B \Phi_{\mathrm{imp}}(k, k')\, \delta(\varepsilon' - \varepsilon)(f' - f)\, dk' \tag{2.4}$$

where $\varepsilon = \varepsilon(k)$, $\varepsilon' = \varepsilon(k')$, $f = f(k)$, $f' = f(k')$, δ is the delta measure, and the dependence on x and t of both f and $Q_{\mathrm{imp}}(f)$ have been omitted, to stress the fact that the collision operator operates only on the k variable. Finally, $\Phi_{\mathrm{imp}}(k, k') = \Phi_{\mathrm{imp}}(k', k)$.

For the sake of simplicity, we shall consider only one electron–phonon collision operator, but the analysis can be straightforwardly extended to a sum of such operators. Therefore, we consider, with the same notations as for (2.4),(25)

$$\begin{aligned} Q_{\mathrm{ph}}(f)(k) = \int_B & \Phi_{\mathrm{ph}}(k, k') \\ & \times \{ [(N_{\mathrm{ph}} + 1)\, \delta(\varepsilon - \varepsilon' + \varepsilon_{\mathrm{ph}}) + N_{\mathrm{ph}} \delta(\varepsilon - \varepsilon' - \varepsilon_{\mathrm{ph}})] f'(1 - f) \\ & - [(N_{\mathrm{ph}} + 1)\, \delta(\varepsilon' - \varepsilon + \varepsilon_{\mathrm{ph}}) + N_{\mathrm{ph}} \delta(\varepsilon' - \varepsilon - \varepsilon_{\mathrm{ph}})] f(1 - f') \}\, dk' \end{aligned} \tag{2.5}$$

where again $\Phi_{\mathrm{ph}}(k, k') = \Phi_{\mathrm{ph}}(k', k)$, $\varepsilon_{\mathrm{ph}}$ is the phonon energy, and N_{ph} is the phonon occupation number given by the Bose–Einstein statistics

$$N_{\mathrm{ph}} = (e^{\varepsilon_{\mathrm{ph}}/k_B T_L} - 1)^{-1} \tag{2.6}$$

where T_L is the lattice temperature and k_B is the Boltzmann constant. In general, $\varepsilon_{\mathrm{ph}}$ is a function of $k - k'$.

Finally, the electron–electron binary collision integral is considered in ref. 25 for nondegenerate gases and non-umklapp processes. Its extension to degenerate gases and the allowance of umklapp processes in the scattering lead to

$$\begin{aligned} & Q_e(f)(k) \\ & \quad = \int_{B^3} \Phi_e(k, k', k_1, k_1')\, \delta(\varepsilon' + \varepsilon_1' - \varepsilon - \varepsilon_1)\, \delta_p(k' + k_1' - k - k_1) \\ & \qquad \times [f' f_1' (1 - f)(1 - f_1) - f f_1 (1 - f')(1 - f_1')]\, dk_1\, dk'\, dk_1' \end{aligned} \tag{2.7}$$

where the delta function $\delta_p(k'+k'_1-k-k_1)$ is to be understood as periodized, which means that its support is

$$\begin{aligned}\operatorname{Supp}\delta_p(k'+k'_1-k-k_1)&\\ =\{(k,k_1,k',k'_1)\in B^4,\ \exists g\in \mathbb{L}^*,\ k+k_1-k'-k'_1=g\}&\end{aligned}\tag{2.8}$$

Obviously, $g=0$ stands for a non-umklapp process, while $g\neq 0$ implies an umklapp process. Note that the number of g's involved in (2.8) is finite. Owing to the indistinguishability of the particles and to the detailed-balance property, Φ_e satisfies

$$\Phi_e(k,k',k_1,k'_1)=\Phi_e(k',k,k_1,k'_1)=\Phi_e(k_1,k'_1,k,k')\tag{2.9}$$

In all these equations, the normalizing factors $1/4\pi^3$ coming from the momentum density of states have been transferred to the Φ's, and will be ignored in the remainder of the paper. The potential $V(x)$ is coupled with f via the Poisson equation. This point will not have any effect on the subsequent analysis and will be ignored.

3. EXPANSION OF THE PHONON COLLISION OPERATOR

We now introduce a set of units from which an appropriate scaling of Eq. (2.2) will be derived. Let n_0 and T_0 be the typical density and temperature, respectively of the electron gas in the semiconductor. Since we have in mind the derivation of a macroscopic model suitable for high-field or hot-electron transport, we choose $k_B T_0/q$ of the order of the applied voltage V_A, while n_0 can be larger than the doping density if high injection effects are to be expected. A time scale t_0 will be specified later.

Let $F_{\mu,T}(k)$ be the Fermi–Dirac distribution function associated with the chemical potential μ and temperature T:

$$F_{\mu,T}(k)=(e^{(\varepsilon(k)-\mu)/k_B T}+1)^{-1}\tag{3.1}$$

and let $n(\mu,T)$ and $n\mathscr{E}(\mu,T)$ be the associated density and internal energy, respectively,

$$\begin{pmatrix} n(\mu,T)\\ n\mathscr{E}(\mu,T)\end{pmatrix}=\int_B \begin{pmatrix}1\\ \varepsilon(k)\end{pmatrix} F_{\mu,T}(k)\,\frac{dk}{4\pi^3}\tag{3.2}$$

We specify units for the chemical potential μ_0 and the internal energy $\mathscr{E}_0$ such that

$$n(\mu_0,T_0)=n_0,\qquad n\mathscr{E}(\mu_0,T_0)=n_0\mathscr{E}_0\tag{3.3}$$

holds. The kinetic energy scale ε_0 is defined according to $\varepsilon_0 = 2\mathscr{E}_0/3$. For the wavevector scale k_0, we choose the "typical" norm of wavevectors k satisfying $\varepsilon(k) = \varepsilon_0$. The distribution function scale follows immediately,

$$f_0 = \frac{4\pi^3 n_0}{k_0^3} = \eta \tag{3.4}$$

The dimensionless parameter η measures the level of degeneracy of the electron gas, that is, if $\eta \to 0$, a classical nondegenerate statistics applies. The velocity scale is given by $v_0 = \varepsilon_0/\hbar k_0$, and the space scale x_0 is linked to the time scale through $x_0 = v_0 t_0$. Finally, the potential scale V_0 is connected with the energy scale ε_0 by $qV_0 = \varepsilon_0$.

In a parabolic band model $\varepsilon(k) = \hbar^2 k^2/2m_*$, where m_* is the effective mass, and if the relations (3.2) can be approximated by a Boltzmann statistics with $B = \mathbb{R}^3$, we get

$$\mu_0 = k_B T_0 \ln\left(\sqrt{2}\,\pi^{3/2}\frac{n_0}{k_0^3}\right) \tag{3.5}$$

$$k_0 = \left(\frac{m_* k_B T_0}{\hbar^2}\right)^{1/2}, \qquad v_0 = \left(\frac{k_B T_0}{m_*}\right)^{1/2} \tag{3.6}$$

$$n_0\mathscr{E}_0 = \tfrac{3}{2} n_0 k_B T_0, \qquad \varepsilon_0 = k_B T_0 \tag{3.7}$$

$$V_0 = k_B T_0/q \tag{3.8}$$

It is important to note that the potential scale V_0 is a thermal potential, not associated with the lattice temperature T_L, but with the typical electron temperature T_0. In view of the introduction to the present section, one would choose $V_0 = V_A$, that is, the applied voltage. Therefore, the forthcoming macroscopic limit will be valid for large applied potential differences.

To scale the collision operators, we introduce dimensionless numbers $\Phi_{\text{imp},0}$, $\Phi_{\text{ph},0}$, and $\Phi_{e,0}$, which are "typical values" of the transition rates $\Phi_{\text{imp}}(k, k')$, $\Phi_{\text{ph}}(k, k')$, and $\Phi_e(k, k_1, k', k_1')$, respectively. We introduce the following dimensionless parameters:

$$\nu_{\text{imp}} = \frac{\Phi_{\text{imp},0} k_0^3}{\varepsilon_0} t_0, \qquad \nu_{\text{ph}} = \frac{\Phi_{\text{ph},0} k_0^3}{\varepsilon_0} t_0 \tag{3.9}$$

$$\nu_e = \frac{\Phi_{e,0} 4\pi^3 n_0 k_0^3}{\varepsilon_0} t_0 \tag{3.10}$$

ν_{imp}, ν_{ph}, and ν_e are measures of the collision frequencies in units of t_0^{-1}. Let also $\varepsilon_{\text{ph},0}$ be the order of magnitude of the phonon energy and introduce the dimensionless parameters

$$\alpha^2 = \frac{\varepsilon_{\text{ph},0}}{\varepsilon_0}, \qquad \beta^2 = \frac{\varepsilon_{\text{ph},0}}{k_B T_L} \tag{3.11}$$

where the lattice temperature T_L is supposed constant, although this assumption can be easily waived. α is a measure of the inelasticity of phonon collisions acting on a "hot" electron of energy $k_B T_0$, while β is a similar measure, but for "thermal" electrons of energy $k_B T_L$. The present paper is concerned with the ordering

$$\alpha^2 \ll 1, \qquad \beta^2 = O(1) \tag{3.12}$$

In this case, the electrons are considered so hot that the energy loss per phonon collision is a small fraction of their total energy. A similar fact applies in a plasma for collisions against ions.(11,12)

We perform a change of variables and unknowns

$$t = t_0 \bar{t}, \qquad x = x_0 \bar{x}, \qquad k = k_0 \bar{k}, \qquad f = f_0 \bar{f},... \tag{3.13}$$

which leads to the following Boltzmann equation (the bars are omitted for the sake of simplicity):

$$\frac{\partial f}{\partial t} + \nabla_k \varepsilon(k) \cdot \nabla_x f + \nabla_x V \cdot \nabla_k f = Q_{\text{imp}}(f) + Q_{\text{ph}}(f) + Q_e(f) \tag{3.14}$$

with

$$Q_{\text{imp}}(f) = \nu_{\text{imp}} \int_B \Phi_{\text{imp}}(k, k')\, \delta(\varepsilon' - \varepsilon)(f' - f)\, dk' \tag{3.15}$$

$$\begin{aligned} Q_{\text{ph}}(f) = \nu_{\text{ph}} \int_B \Phi_{\text{ph}}(k, k') & \\ \times \{ [& (N_{\text{ph}} + 1)\, \delta(\varepsilon - \varepsilon' + \alpha^2 \varepsilon_{\text{ph}}) \\ & + N_{\text{ph}} \delta(\varepsilon - \varepsilon' - \alpha^2 \varepsilon_{\text{ph}})]\, f'(1 - \eta f) \\ & - [(N_{\text{ph}} + 1)\, \delta(\varepsilon' - \varepsilon + \alpha^2 \varepsilon_{\text{ph}}) \\ & + N_{\text{ph}} \delta(\varepsilon' - \varepsilon - \alpha^2 \varepsilon_{\text{ph}})]\, f(1 - \eta f')\}\, dk' \end{aligned} \tag{3.16}$$

$$
\begin{aligned}
Q_e(f) = \nu_e \int_{B^3} & \Phi_e(k, k', k_1, k_1') \\
& \times \delta(\varepsilon' + \varepsilon_1' - \varepsilon - \varepsilon_1)\, \delta_p(k' + k_1' - k - k_1) \\
& \times [f' f_1' (1 - \eta f)(1 - \eta f_1) \\
& - f f_1 (1 - \eta f')(1 - \eta f_1')]\, dk_1\, dk'\, dk_1'
\end{aligned}
\tag{3.17}
$$

with

$$
N_{\mathrm{ph}} = \frac{1}{e^{\beta^2 \varepsilon_{\mathrm{ph}}} - 1}
\tag{3.18}
$$

and B is the original Brillouin zone dilated by the factor k_0^{-1}.

Six dimensionless parameters are thus involved in this model: η, α^2, β^2, ν_{imp}, ν_{ph}, and ν_e. Table I gives the numerical values of these parameters for silicon and gallium arsenide when the typical electron temperature is 1 eV, the lattice temperature is 300 K, and the typical electron density n_0 is 10^{22} or $10^{24}\ \mathrm{m}^{-3}$. The numerical parameters are taken from ref. 25. For α^2 and β^2, the value of the optical phonon energy has been taken. ν_{imp} is evaluated from (3.9) with k_0 given by (3.6). It is very small because of the very rapid falloff of the impurity scattering cross section as the electron energy increases. Therefore Q_{imp} can be neglected for the subsequent analysis. ν_{ph} is evaluated for the Δ–Δ intervalley scattering in silicon, and the L–L or L–Γ or Δ–Γ intervalley scattering in GaAs, for which the coupling constants are the largest ones among the various phonon scattering mchanisms. For ν_e, the value of (3.10) varies dramatically according to the value of (k, k_1, k', k_1') at which Φ_e is evaluated. We have indicated a range which corresponds to values from $|k - k'| = \lambda_D^{-1}$ to $|k - k'| = k_0$, where λ_D is the screening length. Electron–electron collisions can be extremely strong for small relative wavevectors, and there is a whole range of values of relative wavevectors for which the interaction is stronger and takes over the electron–phonon collision.

Table I. Dimensionless Parameters ($T_0 = 1$ eV, $T_L = 300$ K)

	Si		GaAs	
	$n_0 = 10^{22}\ \mathrm{m}^{-3}$	$n_0 = 10^{24}\ \mathrm{m}^{-3}$	$n_0 = 10^{22}\ \mathrm{m}^{-3}$	$n_0 = 10^{24}\ \mathrm{m}^{-3}$
η^2	3×10^{-5}	3×10^{-3}	10^{-3}	10^{-1}
α^2	7×10^{-2}		4×10^{-2}	
β^2	2.4		1.4	
$\nu_{\mathrm{imp}}\ (\mathrm{sec}^{-1})$	10^6	10^8	10^7	10^9
$\nu_{\mathrm{ph}}\ (\mathrm{sec}^{-1})$	10^{12}		10^{12}	
$\nu_e\ (\mathrm{sec}^{-1})$	$10^6 \to 10^{17}$	$10^8 \to 10^{15}$	$10^6 \to 10^{17}$	$10^8 \to 10^{15}$

From the previous analysis we can choose the time scale t_0 such that $\nu_{\text{imp}} = \nu_{\text{ph}} = \nu_e = 1$, possibly by sending some constants inside the Φ's. Although ν_{imp} was shown to be very small, it does not change the forthcoming study to keep it in the order-1 terms.

Now, by formally expanding the phonon operator $Q_{\text{ph}} = Q^{\alpha}_{\text{ph}}(f)$ in powers of α^2, we get

$$Q^{\alpha}_{\text{ph}}(f) = Q_{\text{ph},0}(f) + \alpha^2 Q^{\alpha}_1(f) \tag{3.19}$$

where

$$Q_{\text{ph},0}(f) = \int_B \Phi_{\text{ph}}(k, k')(2N_{\text{ph}} + 1)\, \delta(\varepsilon' - \varepsilon)(f' - f)\, dk' \tag{3.20}$$

and $Q^{\alpha}_1(f)$ is easily shown to be of order 1 when $\alpha \to 0$.

Since $Q_{\text{ph},0}(f)$ is an elastic operator, it can be gathered with Q_{imp} by defining

$$\begin{aligned} Q_0(f) &= Q_{\text{imp}}(f) + Q_{\text{ph},0}(f) \\ &= \int_B \Phi_0(k, k')\, \delta(\varepsilon' - \varepsilon)(f' - f)\, dk' \end{aligned} \tag{3.21}$$

$$\Phi_0(k, k') = \Phi_{\text{imp}}(k, k') + (2N_{\text{ph}} + 1)\, \Phi_{\text{ph}}(k, k') \tag{3.22}$$

We now consider a diffusion scaling of Eq. (3.14) in which the scaling parameter is α:

$$t' = \alpha^2 t, \qquad x' = \alpha x \tag{3.23}$$

This leads to the following scaled Boltzmann equation:

$$\frac{\partial f^{\alpha}}{\partial t} + \frac{1}{\alpha}\left[\nabla_k \varepsilon(k) \cdot \nabla_x f + \nabla_x V \cdot \nabla_k f\right] = \frac{1}{\alpha^2}\left[Q_0(f) + Q_e(f)\right] + Q^{\alpha}_1(f) \tag{3.24}$$

The remainder of this paper is concerned with the limit of (3.24) when $\alpha \to 0$.

Here α is the scaled mean free path, while α^2 is the scaled mean time between collisions, in the new set of dilated space and time units. Since no rescaling of the potential has been done, this analysis allows typical values of the electric field equal to the applied bias V_A divided by the macroscopic distance. By comparison, the standard drift-diffusion model is valid for typical fields equal to the thermal voltage $U_{T_L} = k_B T_L / q$ associated with the lattice temperature T_L divided by the macroscopic distance. Since $U_{T_L} \ll V_A$, our analysis sustains much larger fields than the usual drift-diffusion model.

4. THE DIFFUSION LIMIT

Let f_α be a solution of the Boltzmann equation (3.24). As usual, for deriving the diffusion limit, we will perform a Hilbert expansion of f_α. We let

$$f_\alpha(x, k, t) = f_0 + \alpha f_1 + \alpha^2 f_2 + \cdots \tag{4.1}$$

Inserting this expansion in the Boltzmann equation (3.24), we find the following equations:

$$(Q_e + Q_0)(f_0) = 0 \tag{4.2}$$

$$[DQ_e(f_0) + Q_0](f_1) = \nabla_k \varepsilon(k) \cdot \nabla_x f_0 + \nabla_x V \cdot \nabla_k f_0 \tag{4.3}$$

$$\begin{aligned}[DQ_e(f_0) + Q_0](f_2) = {} & \frac{\partial f_0}{\partial t} + \nabla_k \varepsilon \cdot \nabla_x f_1 + \nabla_x V \cdot \nabla_k f_1 \\ & - Q_1(f_0) - \frac{1}{2} D^2 Q_e(f_0)(f_1, f_1)\end{aligned} \tag{4.4}$$

where $DQ_e(f_0)$ and $D^2Q_e(f_0)$ denote the first and second derivatives of Q_e with respect to f_0.

4.1. Order-α^{-2} Terms

In order to solve (4.2), we have to study the operator $Q_e + Q_0$ and especially to determine the collision invariants.

Because of umklapp processes, the collision invariants of Q_e are not easy to find. We will see below that it is easier to determine those of $Q_e + Q_0$.

Lemma 4.1. We have (i)

$$\int_B Q_0(f)\, g\, dk = -\tfrac{1}{2} \iint \Phi_0(k, k')\, \delta(\varepsilon' - \varepsilon)(f' - f)(g' - g)\, dk'\, dk$$

and (ii)

$$\begin{aligned}\int_B Q_e(f)\, g\, dk = -\tfrac{1}{4} \iiiint & \Phi_e \delta(\varepsilon + \varepsilon_1 - \varepsilon' - \varepsilon'_1) \\ & \times \delta_p(k' + k'_1 - k - k_1)[g' + g'_1 - g - g_1] \\ & \times [f' f'_1 (1 - \eta f)(1 - \eta f_1) - f f_1 (1 - \eta f') \\ & \times (1 - \eta f'_1)]\, dk\, dk_1\, dk'\, dk'_1\end{aligned}$$

Proof. These formulas are straightforward after noticing that

$$\Phi_0(k, k') = \Phi_0(k', k)$$
$$\Phi_e(k, k_1, k', k'_1) = \Phi_e(k_1, k, k', k'_1) = \Phi_e(k', k'_1, k, k_1) \quad \blacksquare$$

Corollary 4.2 (H Theorem). We have (i)

$$\int Q_0(f)\, H(f)\, dk = -\tfrac{1}{2} \iint \Phi_0 \delta_\varepsilon (f' - f)[H(f') - H(f)]\, d^2k \leqslant 0$$

for every increasing H, where δ_ε stand for $\delta(\varepsilon' - \varepsilon)$ and $d^2k = dk\, dk'$.

(ii) Let $H(f) = \ln(f/1 - \eta f)$; then

$$\begin{aligned}\int Q_e(f)\, H(f)\, dk = -\tfrac{1}{4} \iiiint \Phi_e \delta_\varepsilon \delta_k & \\ \times [f' f'_1 (1 - \eta f)(1 - \eta f_1) - f f_1 (1 - \eta f')(1 - \eta f_1)] & \\ \times \{\ln[f' f'_1 (1 - \eta f)(1 - \eta f_1)] & \\ - \ln[f f_1 (1 - \eta f')(1 - \eta f'_1)]\}\, d^4k \leqslant 0 &\end{aligned}$$

where δ_ε and δ_k, respectively, stand for $\delta(\varepsilon' + \varepsilon'_1 - \varepsilon - \varepsilon_1)$ and $\delta_p(k' + k'_1 - k - k_1)$ and $d^4k = dk\, dk_1\, dk'\, dk'_1$.

Proof. The proof is a simple computation. $\blacksquare$

Corollary 4.3. (Collisional invariants):

(i) If $g = g(\varepsilon)$, then $\int Q_0((f)\, g\, dk = 0$.

(ii) $\int Q_e(f) \binom{1}{\varepsilon(k)}\, dk = 0$.

Proof. Again the proof follows directly from Lemma 4.1. $\blacksquare$

Proposition 4.4. Assume Φ_e, $\Phi_0 > 0$; then

$$Q_0(f) + Q_e(f) = 0 \Leftrightarrow \exists \mu, T \qquad \text{such that}$$

$$f(k) = F_{\mu, T}(k) \colon \overset{\text{def}}{=} \frac{1}{\eta + \exp\{[\varepsilon(k) - \mu]/T\}}$$

Hence if f_0 solves (4.2), then $f_0 = F_{\mu, T}$.

Proof. According to Corollary 4.2, if $Q_0(f) + Q_e(f) = 0$, then

$$\int Q_0(f)\, H(f)\, dk = \int Q_e(f)\, H(f)\, dk = 0$$

where $H(f) = \ln[f/(1 - \eta f)]$.

This implies that $H(f(k'))=H(f(k))$ when $\varepsilon(k)=\varepsilon(k')$, which can be rewritten

$$f=f(\varepsilon) \tag{4.5}$$

The condition $\int Q_e(f)\,H(f)\,dk=0$ implies

$$\ln[f'f_1'(1-\eta f)(1-\eta f_1)]=\ln[ff_1(1-\eta f')(1-\eta f_1')]$$

when $k+k_1=k_1'+k'$ (modulo B) and $\varepsilon'+\varepsilon_1'=\varepsilon+\varepsilon_1$, which can be rewritten

$$H(f)+H(f_1)=H(f')+H(f_1') \qquad \text{when} \quad \left\{\begin{matrix} k+k_1=k'+k_1'(B) \\ \varepsilon'+\varepsilon_1'=\varepsilon+\varepsilon_1 \end{matrix}\right\} \tag{4.6}$$

Now, we claim that for almost every value ε in $\varepsilon(B)$, the set $\{\varepsilon(k')\}$, where k' is an outgoing wavevector of a collision with incoming wavevectors k and k_1 of the same energy ε, contains an interval

$$[\varepsilon-\alpha_\varepsilon, \varepsilon+\alpha_\varepsilon]$$

This means that $\forall\alpha\in[-\alpha_\varepsilon,\alpha_\varepsilon]$ there exist k, k_1, k', k_1' such that

$$\varepsilon(k)=\varepsilon(k_1)=\varepsilon, \quad \varepsilon(k')=\varepsilon+\alpha, \quad \varepsilon(k_1')=\varepsilon-\alpha, \qquad k+k_1=k'+k_1'$$

Hence we have, as a consequence of (4.6) and from the fact that f is a function of the energy, that

$$2H(f(\varepsilon))=H(f(\varepsilon+\alpha))+H(f(\varepsilon-\alpha)) \qquad \forall\alpha\in[-\alpha_\varepsilon,\alpha_\varepsilon]$$

which implies that $H(f)$ is an affine function of ε and ends the proof. ∎

4.2. Order-α^{-1} Terms

To solve Eq. (4.6), we have to perform the spectral analysis of the linearized operator $DQ_e(F)+Q_0$.

Proposition 4.5. Let us denote $L_F=DQ_e(F)$; then, for every f, we have

$$L_F(f)=\iiint \Phi_e\delta_k\delta_\varepsilon F'F_1'(1-\eta F)(1-\eta F_1)$$
$$\times[h'+h_1'-h-h_1]\,dk_1\,dk'\,dk_1'$$

where $hF(1-\eta F)=f$; and

$$\int L_F(f)\, g\, dk = -\tfrac{1}{4}\iiiint \Phi_e \delta_k \delta_\varepsilon F' F'_1 (1-\eta F)(1-\eta F_1) \times [h'+h'_1-h-h_1][g'+g'_1-g-g_1]\, d^4k$$

Proof. The proof is a simple linearization of Q_e, where we note that

$$F=(1-\eta F)\, M \qquad \text{with} \quad M(k)=\exp\left(-\frac{\varepsilon(k)-\mu}{T}\right)$$

$$\delta(\varepsilon'+\varepsilon'_1-\varepsilon-\varepsilon_1)\, M' M'_1 = \delta(\varepsilon'+\varepsilon'_1-\varepsilon-\varepsilon_1)\, M M_1 \quad \blacksquare$$

Let us now introduce the scalar product

$$\langle f, g\rangle_F = \int_B fg \frac{dk}{F(1-\eta F)} \tag{4.7}$$

and the associated norm $\|\cdot\|_F$. Let

$$H_F = L^2(B) \qquad \text{with the scalar product } \langle\cdot\rangle_F \tag{4.8}$$

Then we have the following result.

Corollary 4.6. L_F and Q_0 are bounded, self-adjoint, nonpositive operators on H_F.

Lemma 4.7. The operator $\mathscr{L}_F = L_F + Q_0$ satisfies the following properties:

(i) $\operatorname{Ker}(\mathscr{L}_F) = \operatorname{span}(F(1-\eta F), F(1-\eta F)\,\varepsilon)$.

(ii) $\langle \mathscr{L}_F f, f\rangle_F \geqslant \mu \|f-Pf\|_F^2$, where P is the orthogonal projection on $\operatorname{Ker}(\mathscr{L}_F)$.

Proof. Property (i) is the linearized version of Proposition 4.4 and is obtained in exactly the same manner. Now to prove (ii) we can put $L_F(f)$ in the form

$$L_F f = -\nu f + \int_B K(u,k) \frac{f(u)}{F(1-\eta F)}\, du$$

where

$$\nu(k) = \iiint \Phi_e \delta_p (k'_1 + k' - k - k_1)\, \delta(\varepsilon'+\varepsilon'_1-\varepsilon-\varepsilon_1) \times F' F'_1 (1-\eta F)(1-\eta F_1)\, d^3k$$

and

$$\begin{aligned}
K(u,k) &= \iint \Phi_c \delta(\varepsilon(u) + \varepsilon'_1 - \varepsilon - \varepsilon_1)\, \delta_p(u + k'_1 - k - k_1)\, dk'_1\, dk_1 \\
&\quad + \iint \Phi_c \delta(\varepsilon' + \varepsilon(u) - \varepsilon - \varepsilon_1)\, \delta_p(k' + u - k - k_1)\, dk'\, dk_1 \\
&\quad - \iint \Phi_c \delta(\varepsilon' + \varepsilon'_1 - \varepsilon - \varepsilon(u))\, \delta_p(k' + k'_1 - k - u)\, dk'\, dk_{11} \\
&= 2 \iint \Phi_c \delta(\varepsilon(u) + \varepsilon(k'_1) - \varepsilon(k) - \varepsilon(k_1))\, \delta_p(u + k'_1 - k - k_1)\, dk'_1\, dk_1 \\
&\quad - \iint \Phi_c \delta(\varepsilon(k') + \varepsilon(k'_1) - \varepsilon(k) - \varepsilon(u))\, \delta_p(k' + k'_1 - k - u)\, dk'\, dk'_1
\end{aligned}$$

If ε is smooth enough, then $\nu_1 \geqslant \nu \geqslant \nu_0 > 0$ and K is in L^∞, and then $L_F = -\nu f + Cf$, where C is compact. A consequence of this is that the spectrum $\mathrm{Sp}(L_F)$ of L_F is such that

$$\mathrm{Sp}(L_F) \subset \{0\} \cup \,]-\infty, -\mu_1[\qquad \text{with} \quad \mu_1 > 0$$

and

$$\dim(\mathrm{Ker}\, L_F) < \infty$$

This implies that

$$\langle -L_F f, f \rangle \geqslant \mu_1 \, \|f - P_1 f\|_F^2 \tag{4.9}$$

where P_1 is the projection on $\mathrm{Ker}\, L_F$. Since $\mathrm{Ker}\, \mathscr{L}_F = \mathrm{Ker}\, L_F \cap \mathrm{Ker}\, Q_0$, then $\mathrm{Ker}\, L_F = \mathrm{Ker}\, \mathscr{L}_F \oplus E$, $\dim E < +\infty$. Let $P_1 f = Pf + g$, where $g \in E$,

$$\|f - Pf\|_F^2 = \|f - P_1 f + g\|_F^2 = \|f - P_1 f\|_F^2 + \|g\|_F^2 \tag{4.10}$$

$$\begin{aligned}
\langle -\mathscr{L}_F f, f \rangle_F &= \langle -\mathscr{L}_F P_1 f, P_1 f \rangle_F + \langle -\mathscr{L}_F (f - P_1 f), (f - P_1 f) \rangle_F \\
&\quad - 2 \langle \mathscr{L}_F P_1 f, f - P_1 f \rangle_F \\
&\geqslant \langle -\mathscr{L}_F g, g \rangle_F - 2 \langle \mathscr{L}_F g, f - P_1 f \rangle_F \\
&\geqslant \langle -\mathscr{L}_F g, g \rangle_F - c \, \|g\|_F \, \|f - P_1 f\|_F
\end{aligned}$$

Now since $\langle -\mathscr{L}_F g, g\rangle_F > 0$ when $g \neq 0$ and g lies in a finite-dimensional space, we conclude that there exists $\mu_2 > 0$ such that $\langle -\mathscr{L}_F g, g\rangle_F \geqslant \mu_2 \|g\|_F^2$ and then

$$\langle -\mathscr{L}_F f, f\rangle_F \geqslant \mu_2 \|g\|_F^2 - c\|g\|_F \|f - P_1 f\|_F \tag{4.11}$$

We also have

$$\langle -\mathscr{L}_F f, f\rangle_F \geqslant \langle -L_F f, f\rangle_F \geqslant \mu_1 \|f - P_1 f\|_F^2 \tag{4.12}$$

Multiplying (4.12) by a constant large enough and adding (4.11), we end up with

$$\langle -\mathscr{L}_F f, f\rangle_F \geqslant \mu[\|f - P_1 f\|_F^2 + \|g\|_F^2]$$

which ends the proof in view of (4.10). ▮

Proposition 4.8. Let $g \in H_F$ be given. Then, the equation $\mathscr{L}_F(f) = g$ is solvable if and only if

$$\int_B g \begin{pmatrix} 1 \\ \varepsilon \end{pmatrix} dk = 0$$

and f is unique in the space

$$\left\{\int_B f \begin{pmatrix} 1 \\ \varepsilon \end{pmatrix} dk = 0\right\}$$

Proposition 4.9. Equation (4.3) admits a unique solution f_1 in $(1, \varepsilon)^\perp$ and

$$f_1(x, k, t) = -\left[\nabla_x\left(\frac{\mu}{T}\right) - \frac{\nabla_x V}{T}\right] \cdot \mathbf{\Psi}_1 + \nabla_x\left(\frac{1}{T}\right) \cdot \mathbf{\Psi}_2$$

where $\mathbf{\Psi}_1$ and $\mathbf{\Psi}_2$ are the unique solutions in $(1, \varepsilon)^\perp$ of

$$\mathscr{L}_F \mathbf{\Psi}_1 = -\nabla_k \varepsilon F(1 - \eta F)$$

$$\mathscr{L}_F \mathbf{\Psi}_2 = -\varepsilon\, \nabla_k \varepsilon F(1 - \eta F)$$

Proof. We recall that

$$\mathscr{L}_F(f_1) = \nabla_k \varepsilon \cdot \nabla_x F + \nabla_x V \cdot \nabla_k F \tag{4.13}$$

Noting that

$$\nabla_x F = -F(1-\eta F)\,\nabla_x\left(\frac{\varepsilon-\mu}{T}\right)$$

$$\nabla_k F = -F(1-\eta F)\,\nabla_k\left(\frac{\varepsilon-\mu}{T}\right)$$

and that $\varepsilon(k)$ is even, one can easily show that the solvability condition is satisfied. Also, we have

$$\nabla_k \varepsilon \cdot \nabla_x F + \nabla_x V \cdot \nabla_k F = \left[\nabla_x\left(\frac{\mu}{T}\right) - \frac{\nabla_x V}{T}\right] \cdot F(1-\eta F)\,\nabla_k \varepsilon$$
$$- \nabla_x\left(\frac{1}{T}\right) \cdot F(1-\eta F)\,\varepsilon\,\nabla_k \varepsilon$$

and then the form of f_1 comes from the fact that $\mathscr{L}_F$ acts only on the k variable. ▮

4.3. Order-α^0 Terms

Let us introduce the diffusion matrices

$$D_{1j} = \int_B \nabla\varepsilon(k) \otimes \psi_j \, dk$$

$$D_{2j} = \int_B \varepsilon\,\nabla\varepsilon(k) \otimes \psi_j \, dk, \qquad j = 1, 2$$

We have

$$D_{ij}^{lm} = -\langle \psi_i^l, \mathscr{L}_F \psi_j^m \rangle_F \tag{4.14}$$

where $\psi_j = (\psi_j^l)_{l=1,2,3}$, and therefore

$$D_{ij}^T = D_{ji} \tag{4.15}$$

which is the Onsager relation.(19)

Proposition 4.10. Let f_0 and f_1 be given in Propositions 4.4 and 4.9, respectively. Then Eq. (4.7) is solvable if and only if $\mu(t, x)$ and $T(t, x)$ satisfy the following diffusion system:

$$\frac{\partial}{\partial t} n(\mu, T) - \nabla \cdot \left\{ D_{11} \left[\nabla_x \left(\frac{\mu}{T} \right) - \frac{\nabla_x V}{T} \right] + D_{12} \frac{\nabla_x T}{T^2} \right\} = 0 \tag{4.16}$$

$$\begin{aligned} &\frac{\partial}{\partial t} n\mathscr{E}(\mu, T) - \nabla \cdot \left\{ D_{21} \left[\nabla_x \left(\frac{\mu}{T} \right) - \frac{\nabla_x V}{T} \right] + D_{22} \frac{\nabla_x T}{T^2} \right\} \\ &\qquad + \nabla V \cdot \left\{ D_{11} \left[\nabla_x \left(\frac{\mu}{T} \right) - \frac{\nabla_x V}{T} \right] + D_{12} \frac{\nabla_x T}{T^2} \right\} = W^\alpha(\mu, T, T_2) \end{aligned} \tag{4.17}$$

where

$$W^\alpha(\mu, T, T_L) = \int_B Q_1^\alpha(F)\, \varepsilon \, dk \tag{4.18}$$

Proof. The solvability condition is

$$\begin{aligned} &\int \left(\frac{\partial f_0}{\partial t} + \nabla_k \varepsilon \cdot \nabla_x f_1 + \nabla_x V \cdot \nabla_k f_1 \right) \begin{pmatrix} 1 \\ \varepsilon \end{pmatrix} dk - \int Q_1^\alpha(f_0) \begin{pmatrix} 1 \\ \varepsilon \end{pmatrix} dk \\ &\qquad - \frac{1}{2} \int D^2 Q_e(f_0)(f_1, f_1) \begin{pmatrix} 1 \\ \varepsilon \end{pmatrix} dk = 0 \end{aligned}$$

Now since for every f we have $\int Q_e(f)\binom{1}{\varepsilon}\, dk = 0$, then differentiating twice at f_0, we easily end up with

$$\int D^2 Q_e(f_0)(f_1, f_1) \begin{pmatrix} 1 \\ \varepsilon \end{pmatrix} dk = 0$$

which now implies that

$$\int \left(\frac{\partial f_0}{\partial t} + \nabla_k \varepsilon \cdot \nabla_x f_1 + \nabla_x V \cdot \nabla_k f_1 \right) \begin{pmatrix} 1 \\ \varepsilon \end{pmatrix} dk = \begin{pmatrix} 0 \\ \int Q_1^\alpha(f_0)\, \varepsilon(k)\, dk \end{pmatrix}$$

Since $f_0 = F_{\mu, T}$ and f_1 is given by Proposition 4.9, the left-hand side gives the desired terms by straightforward computations. ▌

The following lemmas show, first, that $W^\alpha(\mu, T, T_L)$ is a temperature relaxation term which relaxes to the lattice temperature, and, second, that system (4.16), (4.17) is a nondegenerate parabolic system.

Lemma 4.11. We have

$$W^\alpha(\mu, T, T_L) \cdot (T - T_L) \leqslant 0$$

Lemma 4.12. Assume the six functions $(\partial_1 \varepsilon, \partial_2 \varepsilon, \partial_3 \varepsilon, \varepsilon \partial_1 \varepsilon, \varepsilon \partial_2 \varepsilon, \varepsilon \partial_3 \varepsilon)$ are linearly independent. Then the matrix

$$D = \begin{bmatrix} D_{11} & D_{12} \\ D_{21} & D_{22} \end{bmatrix}$$

is positive definite when $T > 0$, $-\infty < \mu < +\infty$.

Remark. The hypothesis of the above lemma is a geometric assumption on the band diagram and expresses that it has a real three-dimensional structure, which is natural. The hypothesis excludes, for example, the case of a band depending only on one or two space variables.

Proof of Lemma 4.11. We can write

$$\begin{aligned} \int Q_1^\alpha(f_0)\, \varepsilon\, dk = \frac{1}{\alpha^2} \iint & (1 - \eta F)(1 - \eta F')\, \Phi_{\text{ph}}(k, k^1) \\ & \times \{ [(N_{\text{ph}} + 1)\, \delta(\varepsilon - \varepsilon' + \alpha^2 \varepsilon_{\text{ph}}) + N_{\text{ph}} \delta(\varepsilon - \varepsilon' - \alpha^2 \varepsilon_{\text{ph}})]\, M' \varepsilon \\ & - [(N_{\text{ph}} + 1)\, \delta(\varepsilon' - \varepsilon + \alpha^2 \varepsilon_{\text{ph}}) \\ & + N_{\text{ph}} \delta(\varepsilon' - \varepsilon - \alpha^2 \varepsilon_{\text{ph}})]\, M\varepsilon \}\, dk\, dk' \end{aligned}$$

Hence

$$\begin{aligned} \int Q_1^\alpha(f_0)\, \varepsilon\, dk = \frac{1}{\alpha^2} \int & (1 - \eta F)(1 - \eta F')\, \Phi_{\text{ph}}(k, k') \\ & \times [\delta(\varepsilon - \varepsilon' + \alpha^2 \varepsilon_{\text{ph}}) [(N_{\text{ph}} + 1)\, M' - N_{\text{ph}} M]\, \varepsilon \\ & + \delta(\varepsilon - \varepsilon' - \alpha^2 \varepsilon_{\text{ph}}) [N_{\text{ph}} M' \\ & - (N_{\text{ph}} + 1)\, M] (\varepsilon' + \alpha^2 \varepsilon_{\text{ph}})]\, dk'\, dk \\ = \iint & \varepsilon_{\text{ph}} (1 - \eta F)(1 - \eta F')\, \Phi_{\text{ph}}(k, k')\, \delta(\varepsilon - \varepsilon' - \alpha^2 \varepsilon_{\text{ph}}) \\ & \times [N_{\text{ph}} M' - (N_{\text{ph}} + 1)\, M]\, dk\, dk' \end{aligned}$$

By noting that

$$(N_0 + 1) = N_0 e^{\alpha^2 \varepsilon_{\text{ph}} / T_L} \qquad \text{and} \qquad M' = M e^{\alpha^2 \varepsilon_{\text{ph}} / T}$$

we conclude

$$(T-T_L)\int Q_1^\alpha(f_0)\,\varepsilon\,dk=\iint \varepsilon_{\mathrm{ph}}(1-\eta F)(1-\eta F')\,\Phi_{\mathrm{ph}}(k,k')$$
$$\times\,\delta(\varepsilon-\varepsilon'-\alpha^2\varepsilon_{\mathrm{ph}})\,N_0 M(T-T_L)$$
$$\times\,[e^{\alpha^2\varepsilon_{\mathrm{ph}}/T}-e^{\alpha^2\varepsilon_{\mathrm{ph}}/T_L}]\,dk\,dk'$$
$$\leqslant 0 \quad \blacksquare$$

Proof of Lemma 4.12. Let us recall that

$$D_{ij}^{lm}=-\langle \psi_i^l,\mathscr{L}_F\psi_j^m\rangle_F$$

As a consequence of the linear independence of $(\varepsilon\partial_1\varepsilon, \varepsilon\partial_2\varepsilon, \varepsilon\partial_3\varepsilon, \partial_1\varepsilon, \partial_2\varepsilon, \partial_3\varepsilon)$ we easily deduce from Proposition 4.9 that the family (Ψ_j^l) is independent. Since ψ_j^l lies in a finite-dimensional subspace of $(\mathrm{Ker}\,\mathscr{L}_F)^\perp$, we deduce that $-\mathscr{L}_F$ is coercive on $\mathrm{span}(\Psi_j^l)$. This means that there exists $\mu>0$ such that

$$\left\langle -\mathscr{L}_F\left(\sum_{j,l}a_j^l\psi_j^l\right),\left(\sum_{j,l}a_j^l\psi_j^l\right)\right\rangle_F\geqslant \mu\sum(a_i^l)^2$$

But the left-hand side of this inequality is exactly equal to A^TDA, where A is the vector

$$A=(a_1^1,a_1^2,a_1^3,a_2^1,a_2^2,a_2^3)^T$$

Hence

$$A^TDA\geqslant\mu A^TA$$

which ends the proof. $\blacksquare$

5. A HYDRODYNAMIC MODEL FOR DEGENERATE ELECTRON GAS IN A SEMICONDUCTOR

The aim of this section is to show that the diffusion system (4.16), (4.17) can be rewritten as a hydrodynamic system in which some of the transport terms are neglected. We first begin by recalling the hydrodynamic system for a degenerate gas with an arbitrary kinetic energy relation $\varepsilon(k)$. For that purpose, we consider a Boltzmann equation (2.2) in which (for simplicity, we take $\eta=1$)

$$\int Q_e(f) \begin{pmatrix} 1 \\ k \\ \varepsilon \end{pmatrix} dk = 0, \qquad \int Q_e(f) \ln \frac{f}{1-f}\, dk \leqslant 0 \tag{5.1}$$

and

$$Q_e(f) = 0 \Leftrightarrow \exists \mu \in \mathbb{R}, \quad u \in \mathbb{R}^3, \quad T > 0 \tag{5.2}$$

such that

$$f = F_{\mu,\, u,\, T} = (e^{\varepsilon(k) - u.k - \mu)/T} + 1)^{-1}$$

This means that $Q_e(f)$ is of the form (2.7) where the umklapp collisions $(g \neq 0)$ are disregarded. We also assume that $R(\mu, u, T)$ and $W(\mu, u, T)$ are such that

$$\int Q_{ld}(F) \begin{pmatrix} 1 \\ k \\ \varepsilon \end{pmatrix} dk = \begin{pmatrix} 0 \\ R(\mu, u, T) \\ W(\mu, u, T) \end{pmatrix} \tag{5.3}$$

Then we introduce the mean density n, momentum K, energy $\mathscr{E}$, velocity u, pressure tensor $\mathbb{P}$, and heat flux vector $\mathbb{Q}$ by

$$\begin{pmatrix} n \\ nK \\ n\mathscr{E} \end{pmatrix} = \int f(k) \begin{pmatrix} 1 \\ k \\ \varepsilon(k) \end{pmatrix} dk \tag{5.4}$$

$$\begin{cases} nu = \int f(k)\, \nabla_k \varepsilon(k)\, dk \\ \mathbb{P} = \int (k - K) \otimes (\nabla_k \varepsilon(k) - u) f(k)\, dk \\ \mathbb{Q} = \int \varepsilon (\nabla_k \varepsilon - u) f(k)\, dk \end{cases} \tag{5.5}$$

Then, multiplying Eq. (2.2) by $(1, k, \varepsilon(k))^T$ and integrating over k leads to the following system:

$$\begin{cases} \dfrac{\partial n}{\partial t} + \nabla \cdot (nu) = 0 \\ \dfrac{\partial}{\partial t}(nK) + \nabla \cdot (nK \otimes u) + \nabla \cdot \mathbb{P} - n \nabla V = R \\ \dfrac{\partial}{\partial t}(n\mathscr{E}) + \nabla \cdot (n\mathscr{E} u + \mathbb{Q}) - nu \nabla V = W \end{cases} \tag{5.6}$$

The closure relations obtained by taking $f = F_{\mu,u,T}$ give

$$\begin{pmatrix} n \\ nk \\ n\mathscr{E} \end{pmatrix} = \begin{pmatrix} n(\mu, u, T) \\ nK(\mu, u, T) \\ n\mathscr{E}(\mu, u, T) \end{pmatrix} = \int F_{\mu,u,T}(k) \begin{pmatrix} 1 \\ k \\ \varepsilon \end{pmatrix} dk \tag{5.7}$$

$$\begin{cases} nu = \int F_{\mu,u,T}(k)\, \nabla_k \varepsilon \, dk \\ \mathbb{P} = pId, \qquad p = -T \int \ln(1 - F_{\mu,u,T})\, dk \\ \mathbb{Q} = pu \end{cases} \tag{5.8}$$

Finally, let S, G be the entropy–entropy flux pair defined by

$$\begin{cases} S = \int [F \ln F + (1 - F) \ln(1 - F)]\, dk \\ G = \int [F \ln F + (1 - F) \ln(1 - F)]\, \nabla_k \varepsilon \, dk \end{cases} \tag{5.9}$$

The entropy identity is given by

$$\frac{\partial S}{\partial t} + \nabla \cdot G = -\frac{1}{T}(W - u \cdot R) \tag{5.10}$$

We now have the following result.

Proposition 5.1. System (4.16), (4.17) can be written

$$\begin{cases} \dfrac{\partial n}{\partial t} + \nabla \cdot (nu) = 0 \\ \nabla p - n \nabla V = R \\ \dfrac{\partial}{\partial t}(n\mathscr{E}) + \nabla \cdot (n\mathscr{E} u) + \nabla \cdot (pu) - nu \cdot \nabla V + \nabla \cdot q = W^{\alpha} \end{cases} \tag{5.11}$$

where

$$\begin{pmatrix} n \\ n\mathscr{E} \end{pmatrix} = \int F_{\mu,0,T}(k) \begin{pmatrix} 1 \\ \varepsilon \end{pmatrix} dk \tag{5.12}$$

$$\begin{cases} p = -T \int \ln(1 - F_{\mu,0,T})\, dk \\ R = -(nTD_{11}^{-1})\, nu - (nD_{11}^{-1} D_{12} - (p + n\mathcal{E})) \dfrac{\nabla T}{T} \\ q = (nD_{21} D_{11}^{-1} - (p + n\mathcal{E}))\, u - (D_{22} - D_{21} D_{11}^{-1} D_{12}) \dfrac{\nabla T}{T^2} \end{cases} \tag{5.13}$$

and W^{α} given by (4.18).

Remark 5.2. (5.11) is just (5.6) without the transport term $\partial nK/\partial t + \nabla \cdot (nK \otimes u)$ in the momentum equation, which corresponds to neglecting all the terms in factor of the mass m (in physical units). Therefore, system (6.16), (6.17) can be viewed as a hydrodynamic model for an infinitely light particle. System (5.11) also provides a formula for the friction force R. It is the sum of the momentum relaxation term $-(nTD_{11}^{-1})\, nu$, which gives rise to a tensor mobility μ_n

$$\mu_n = \frac{1}{nT} D_{11} \tag{5.14}$$

and a term proportional to the gradient of the electron temperature (the thermopower). Although this term is absent from most semiconductor models, it is present in plasma models,(8, 12) where it is referred to as the "thermal force." The total energy flux $\mathbb{Q}$ is now the sum of the work of the pressure force pu and the heat flux q. The heat flux q is itself the sum of two terms: The first one is a friction heat flux proportional to u. The coefficient of u is minus the transpose of the coefficient of $\nabla T/T$ in the thermal force, which is a form of Onsager's reciprocity relation. The second one is a thermal heat flux associated with a positive-definite tensor heat conductivity

$$\kappa = \frac{1}{T^2} (D_{22} - D_{21} D_{11}^{-1} D_{12}) \tag{5.15}$$

The application of symmetry groups associated with particular lattice geometries may reduce some of the above-defined tensors to scalars. This question will not be investigated here.

Proof of Proposition 5.1. From (4.16) and the first equation of (5.11), it is clear that u should be defined by

$$nu = -D_{11} \left(\nabla \left(\frac{\mu}{T} \right) - \frac{\nabla V}{T} \right) - D_{12} \frac{\nabla T}{T^2} \tag{5.16}$$

or

$$-(nTD_{11}^{-1})\,nu = nT\nabla\left(\frac{\mu}{T}\right) - n\,\nabla V + \frac{n}{T} D_{11}^{-1} D_{12}\,\nabla T$$

But, with p given by the first equation of (5.13), we have

$$\nabla p = \frac{\nabla T}{T} p + nT\nabla\left(\frac{\mu}{T}\right) + n\mathscr{E}\,\frac{\nabla T}{T}$$

Replacing $\nabla(\mu/T)$ by its value computed from (5.16) gives the second equations of both (5.11) and (5.13). To get the third equation of (5.11) and (5.13), we just have to replace

$$\nabla\left(\frac{\mu}{T}\right) - \frac{\nabla_x V}{T}$$

in the second term of (4.17) by its value deduced from (5.16).

We now prove that the heat diffusivity tensor κ is positive definite. For this aim we recall that the matrix

$$D = \begin{bmatrix} D_{11} & D_{12} \\ D_{21} & D_{22} \end{bmatrix}$$

is positive definite. Then for every block vector

$$Z = \begin{pmatrix} -D_{11}^{-1} D_{12} X \\ X \end{pmatrix}$$

$$\langle DZ, Z\rangle \geqslant \lambda \cdot \langle Z, Z\rangle \geqslant \lambda\langle X, X\rangle$$

for some $\lambda > 0$. It is then easy to check that $\langle DZ, Z\rangle$ is nothing but $\langle T^2\kappa X, X\rangle$. ▮

6. THE NONDEGENERATE ELECTRON GAS WITH A PARABOLIC BAND STRUCTURE

In this section, we take $\eta \to 0$, $B \to \mathbb{R}^3$, $\mathscr{E}(k) = k^2/2$, and we now replace k by v. We also suppose that the transition function Φ_e only depends on $|v - v_1|$ and on the scattering angle θ and that Φ_0 only depends on $v \cdot v_1$. Then, by straightforward computations(12) we have the following result.

Proposition 6.1. The Hilbert expansion (4.1) is solvable for f_2 if and only if n and T satisfy the following diffusion system:

$$\begin{cases} \dfrac{\partial n}{\partial t} - \nabla \cdot \left[D_{11} \left(\dfrac{\nabla n}{n} - \dfrac{\nabla V}{T} \right) + \left(D_{12} - \dfrac{3}{2} T D_{11} \right) \dfrac{\nabla T}{T^2} \right] = 0 \\ \dfrac{\partial}{\partial t} \left(\dfrac{3}{2} nT \right) - \nabla \cdot \left[D_{21} \left(\dfrac{\nabla n}{n} - \dfrac{\nabla V}{T} \right) + \left(D_{22} - \dfrac{3}{2} T D_{21} \right) \dfrac{\nabla T}{T^2} \right] \\ \qquad + \nabla V \left[D_{11} \left(\dfrac{\nabla n}{n} - \dfrac{\nabla V}{T} \right) + \left(D_{12} - \dfrac{3}{2} T D_{11} \right) \dfrac{\nabla T}{T^2} \right] = W^\alpha \end{cases} \tag{6.1}$$

where

$$\begin{cases} D_{1j} = \frac{1}{3} \left(\displaystyle\int |v|^2 M_{n,T} \psi_j(|v|) \, dv \right) Id \\ D_{2j} = \frac{1}{6} \left(\displaystyle\int |v|^4 M_{n,T} \psi_j(|v|) \, dv \right) Id \end{cases} \tag{6.2}$$

$$M_{n,T}(v) = \frac{n}{(2\pi T)^{3/2}} e^{-|v|^2/2T}$$

$\psi_j(|v|)$, $j = 1, 2$, are solutions of

$$\begin{cases} \mathscr{L}_M(-\psi_1(|v|)\, v) + Q_0(-\psi_1(|v|)\, v) = vM(v) \\ \mathscr{L}_M(-\psi_2(|v|)\, v) + Q_0(-\psi_2(|v|)\, v) = \dfrac{|v|^2}{2} vM(v) \end{cases} \tag{6.3}$$

and where $\mathscr{L}_M$ is the linearized Boltzmann operator about M and

$$W^\alpha(n, T, T_L) = \int Q_1^\alpha(M) \frac{|v|^2}{2} \, dv \tag{6.4}$$

This system can also be put in the form of a hydrodynamic system, as follows.

Proposition 6.2. System (6.1) is equivalent to

$$\begin{cases} \dfrac{\partial n}{\partial t} + \nabla \cdot (nu) = 0 \\ \nabla(nT) - n \nabla V = R \\ \dfrac{\partial}{\partial t} \left(\dfrac{3}{2} nT \right) + \nabla \cdot \left(\dfrac{5}{2} nTu \right) - nu \cdot \nabla V + \nabla \cdot q = W^\alpha \end{cases} \tag{6.5}$$

with

$$\begin{cases} R = -\dfrac{nT}{D_{11}}(nu) - \left(\dfrac{1}{T}\dfrac{D_{12}}{D_{11}} - \dfrac{5}{2}\right) n\,\nabla T \\ q = \left(\dfrac{D_{12}}{TD_{11}} - \dfrac{5}{2}\right) nTu - \left(D_{22} - \dfrac{D_{21}D_{12}}{D_{11}}\right)\dfrac{\nabla T}{T^2} \end{cases} \tag{6.6}$$

Remark 6.3. The third equation of (6.5) is the usual energy equation, while the second one is just the momentum equation in which the terms $\partial nu/\partial t + \nabla\cdot(nu\otimes u)$ have been removed. This corresponds to the removal of all the terms which have the mass in the factor. Therefore, system (6.1) can be viewed as a hydrodynamic system for a massless particle. The significance of the terms appearing in R and q has been explained in Remark 5.2. Again, Onsager's reciprocity relation should be pointed out between the cross terms of R and q. Finally, an entropy identity for this system is given in ref. 12.

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