High-Field Approximations of the Energy-Transport Model for Semiconductors with Non-Parabolic Band Structure

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Abstract. An asymptotic analysis of the energy-transport equations for semiconductors with the scaled energy relaxation time as small parameter is performed. Using a variant of the Chapman-Enskog method, high-field drift-diffusion models are derived. Furthermore, the dependence of the macroscopic parameters such as the diffusivity are investigated for parabolic and non-parabolic band approximations (in the sense of Kane). Explicit expressions of the physical parameters are obtained.

Keywords. High-field drift-diffusion models, Chapman-Enskog method, non-parabolic band, semiconductors.

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1 Introduction

The accurate modeling of high-field effects is an important task in the simulation of charge carrier flow in modern semiconductor devices. A standard and commonly used approach is the inclusion of field-dependent transport parameters in macroscopic models. Often field-dependent mobilities are employed in standard drift-diffusion models [15]. The detailed form of the field dependence is then obtained by heuristic arguments combined with fitting to experimental values or to results of Monte-Carlo simulations of the semiconductor Boltzmann equation [9].

Recently, also more rigorous approaches have been considered. A drift-diffusion model with field-dependent mobility has been derived by Poupaud in [13]. There the drift-diffusion model is a result of a two-step procedure. First, by a limit process starting from the semiconductor Boltzmann equation, an equation without diffusion term is derived. Then the diffusion term with a field-dependent diffusion constant is obtained as a higher-order correction by a variant of the Chapman-Enskop method (arrow 1 in Fig. 1). However, this result has the disadvantage that the assumptions on the scattering mechanisms are physically unrealistic.

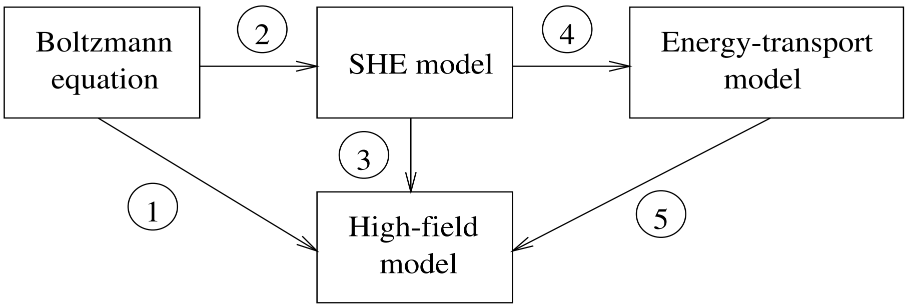

Figure 1: Derivation of high-field models.

Another approach has been employed by Ben Abdallah *et al.* [3]. They derive high-field models from the Spherical Harmonics Expansion (SHE) model. The SHE model can be obtained either by expansion of the distribution function in terms of spherical harmonics [16, 17], or by a Hilbert expansion assuming that elastic collisions are the dominating physical effect [1, 8, 14]. The latter approach seems more attractive since it can be easily applied to non-rotationally symmetric band structures (arrow 2). In a second limit with dominating inelastic scattering, Ben Abdallah *et al.* derive high-field drift-diffusion models (arrow 3). However, in this approach an operator equation (containing the collision operator) has to be inverted, and thus the field dependence is not always explicit.

In this paper we will derive high-field drift-diffusion equations with *explicit* field-dependent diffusivities. We derive these models from the energy-transport equations. The energy-transport equations can be obtained from the Boltzmann equation assuming dominating inelastic scattering mechanisms [2] or from the SHE model assuming dominant electron-electron collisions [1] (arrow 4). The advantage of the energy-transport model is that explicit expressions for the diffusion coefficients can be given even for non-parabolic band diagrams [7].

In Section 2 the energy-transport model is presented, the physical assumptions on the band structure and the relaxation mechanism are given, and a high-field scaling is introduced. The limiting equation is a (first order) convection equation for the macroscopic electron density with field-dependent mobility.

For the non-parabolic band approximation in the sense of Kane [11], we derive in Section 3 explicit expressions for the electron mean velocity and electron temperature. In the parabolic band approximation, we obtain the same field-dependent mobilities as in the literature.

By a variant of the Chapman-Enskog method, a (second order) correction is constructed in Section 4 which yields a high-field drift-diffusion equation (arrow 5). For general band diagrams, this model is of the form

$$\begin{aligned} \partial_t n - \operatorname{div}(D(n,E)\nabla n + G(n,E)) &= 0, \\ \operatorname{div} E &= n - C(x), \end{aligned}$$

where n is the electron density, E is the electric field, and $C(x)$ is the doping concentration characterizing the semiconductor device. The diffusion matrix $D(n,E)$ and the drift term $G(n,E)$ are given explicitely. We prove that the matrix $D(n,E)$ is positive definite for parabolic and non-parabolic band diagrams, i.e. the above equation for n is parabolic.

For parabolic bands in the Chen case [5] the above equation for n simplifies:

$$\partial_t n - \operatorname{div}\Big(d(|E|)\nabla n + \frac{n}{T(|E|)}E\Big) = 0,$$

where the diffusivity $d(|E|)$ and the temperature $T(|E|)$ are given by

$$d(|E|) = \frac{d_0}{2 - T_0/T(|E|)}, \quad T(|E|) = \frac{1}{2}\left(T_0 + \sqrt{T_0^2 + \frac{8}{3}d_0\tau_0|E|^2}\right),$$

d_0, τ_0 are diffusivity and relaxation time constants, respectively, defined in (3.6), and $T_0 = 1$ is the (scaled) ambient temperature. In the limit $|E| \to \infty$ the mobility $d(|E|)$ converges to $d_0/2$ which is half of the low-field diffusivity d_0.

We stress once more the fact that compared to the paper [3], we derive *explicit* expressions for the coefficients in the drift-diffusion equation. Therefore, the proposed models can be solved numerically (using, for instance, the methods in [4, 7]) and the results can be compared to Monte-Carlo simulations of the Boltzmann equation. The numerical simulation will be performed in a forthcoming publication.

2 Assumptions—scaling

Consider the dimensionless energy-transport equations in the entropy variables μ/T and $-1/T$ [1]:

$$\begin{aligned}
\partial_t n + \text{ div } j_n &= 0, &(2.1)\\
\partial_t W + \text{ div } j_W &= -E \cdot j_n + R, &(2.2)\\
j_n &= -L_{11}\left(\nabla \frac{\mu}{T} + \frac{E}{T}\right) - L_{12}\nabla\left(-\frac{1}{T}\right), &(2.3)\\
j_W &= -L_{21}\left(\nabla \frac{\mu}{T} + \frac{E}{T}\right) - L_{22}\nabla\left(-\frac{1}{T}\right), &(2.4)\\
\lambda^2 \text{div} E &= n - C(x). &(2.5)
\end{aligned}$$

These equations are solved in a bounded domain of $\mathbb{R}^N$ $(N \geq 1)$ and are supplemented with appropriate initial and boundary conditions (see [10]). The physical variables are the chemical potential μ, the electron temperature T, and the electric field $E = -\nabla\phi$ with the electrostatic potential ϕ. The electron density n, the density of the internal energy W, the energy relaxation term R and the diffusion coefficients L_{ij} depend on the entropy variables μ/T and $-1/T$. Furthermore, j_n and j_W are the particle and energy current densities, $\lambda > 0$ the scaled Debye length, and $C(x)$ the doping profile characterizing the device under consideration.

The existence of weak solutions of the system (2.1)-(2.5) with mixed Dirichlet-Neumann boundary conditions and initial conditions for the variables has been shown in [6] under some assumptions on the nonlinear functions. The equations have been numerically solved in, e.g., [7].

We impose the following physical assumptions:

(H1) The energy-band diagram ε of the semiconductor crystal is spherically symmetric, differentiable and a strictly monotone function of the modulus $k = |\vec{k}|$ of the wave vector $\vec{k}$. Therefore, the Brillouin zone equals $\mathbb{R}^3$ and $\varepsilon : \mathbb{R} \to \mathbb{R}, \;\; k \mapsto \varepsilon(k)$.

(H2) The momentum relaxation time is given by

$$\tau(\varepsilon) = \left(\phi_0(2N_0 + 1)\varepsilon^\beta N(\varepsilon)\right)^{-1}, \quad \beta \geq 0, \quad \phi_0 > 0, \qquad (2.6)$$

where $N(\varepsilon) = 4\pi k^2/|\varepsilon'(k)|$ is the density of states of energy $\varepsilon = \varepsilon(k)$ [1, (III.31)], ϕ_0 denotes the transition matrix constant, and N_0 is the phonon occupation number [3, Sect.4].

(H3) The electron density n and the internal energy W are given by non-degenerate Boltzmann statistics.

(H4) The energy relaxation is given by [1, (IV.18)]

$$R = \int_0^\infty S_1 \left(e^{(\mu-\varepsilon)/T} \right) \varepsilon d\varepsilon,$$

and the phonon collision operator S_1 reads in the Fokker-Planck approximation

$$S_1(e^{(\mu-\varepsilon)/T}) = \frac{\partial}{\partial \varepsilon} \left\{ \phi_0 \varepsilon^\beta N(\varepsilon)^2 \left[\left(1 + T_0 \frac{\partial}{\partial \varepsilon} \right) e^{(\mu-\varepsilon)/T} \right] \right\},$$

where $T_0 = 1$ is the (scaled) ambient temperature.

Under the hypothese (H1)-(H3), the diffusion coefficients are given by

$$L_{ij} = e^{\mu/T} \int_0^\infty \lambda_0(\varepsilon) \varepsilon^{i+j-2} e^{-\varepsilon/T} d\varepsilon,$$

where

$$\lambda_0(\varepsilon) = \frac{4\pi}{3} \tau(\varepsilon) |\varepsilon'(k)| k^2 \quad \text{and} \quad \varepsilon = \varepsilon(k)$$

(see [1, (IV.17)(III.33)]). We refer to [1] for more general expressions for the diffusion coefficients under weaker assumptions. From assumption (H3), we get for the electron density and internal energy the expressions [1, (IV.16)]

$$\begin{aligned} n &= e^{\mu/T} \int_0^\infty e^{-\varepsilon/T} N(\varepsilon) d\varepsilon, \\ W &= e^{\mu/T} \int_0^\infty e^{-\varepsilon/T} N(\varepsilon) \varepsilon d\varepsilon. \end{aligned}$$

The expression for the energy relaxation term can be simplified using (H4):

$$R = \phi_0 e^{\mu/T} (T_0 - T) \int_0^\infty \varepsilon^\beta N(\varepsilon)^2 e^{-\varepsilon/T} d\varepsilon.$$

Let $\gamma(\varepsilon) = k^2$ be the inverted $\varepsilon(k)$ relation. Then we can write the diffusion coefficients, the electron density, the internal energy and the energy relaxation term as follows (see [7] for details):

$$L_{ij} = e^{\mu/T} T^{i+j-\beta-1} P_\beta^{i+j}(T), \tag{2.7}$$
$$n = e^{\mu/T} T Q^0(T), \tag{2.8}$$
$$W = e^{\mu/T} T^2 Q^1(T), \tag{2.9}$$
$$R = e^{\mu/T} T^\beta R_\beta(T)(T_0 - T), \tag{2.10}$$

and the functions P_β^k, Q^l and R_β are defined by

$$\begin{aligned}
P_\beta^k(T) &= \frac{4}{3\phi_o(2N_0+1)}\int_0^\infty \frac{\gamma(Tu)}{\gamma'(Tu)^2}u^{k-\beta-2}e^{-u}du, && (2.11)\\
Q^l(T) &= 2\pi\int_0^\infty \gamma(Tu)^{1/2}\gamma'(Tu)u^l e^{-u}du, && (2.12)\\
R_\beta(T) &= 4\pi^2\phi_0\int_0^\infty \gamma(Tu)\gamma'(Tu)^2 u^\beta e^{-u}du, && (2.13)
\end{aligned}$$

where $k = 2, 3, 4$ and $l = 0, 1$.

We introduce now the scaling

$$x \to \delta x, \quad t \to \delta t, \quad \phi \to \frac{1}{\delta}\phi,$$

for "small" $\delta > 0$. This scaling implies that the electric field $-\nabla\phi$ remains unchanged, which means that we assume the potential to have variations of order 1 over the microscopic scale. Then the rescaled equations (2.1)-(2.5) read

$$\begin{aligned}
\partial_t n + \operatorname{div} j_n &= 0, && (2.14)\\
\partial_t W + \operatorname{div} j_W &= \frac{1}{\delta}\Big(-E\cdot j_n + R\Big), && (2.15)\\
j_n &= -L_{11}\Big(\delta\nabla\frac{\mu}{T} + \frac{E}{T}\Big) - \delta L_{12}\nabla\Big(-\frac{1}{T}\Big), && (2.16)\\
j_W &= -L_{21}\Big(\delta\nabla\frac{\mu}{T} + \frac{E}{T}\Big) - \delta L_{22}\nabla\Big(-\frac{1}{T}\Big), && (2.17)\\
\delta\lambda^2 \operatorname{div} E &= n - C(x). && (2.18)
\end{aligned}$$

Assuming that in the limit $\delta \to 0$, $\delta\lambda^2$ is of order $O(1)$, we obtain (formally) the limit equations,

$$\partial_t n + \operatorname{div} j_n = 0, \quad -E\cdot j_n + R = 0, \tag{2.19}$$

$$j_n = -L_{11}\frac{E}{T}, \quad j_w = -L_{21}\frac{E}{T}, \quad \operatorname{div} E = n - C(x). \tag{2.20}$$

The second equation in (2.19) and the first equation in (2.20) imply that for given electric field E, the electron temperature T can be computed according to

$$|E|^2 = -T\frac{R(\mu/T, -1/T)}{L_{11}(\mu/T, -1/T)}. \tag{2.21}$$

Notice that for $E = 0$, $T = T_0$ solves (2.21) since $R = 0$ at $T = T_0$. We suppose that the nonlinear equation (2.21) for T can be solved uniquely:

(H5) For all $|E| \geq 0$ and $\mu \in \mathbb{R}$, there exists a unique solution $T = T(\mu, |E|)$ of (2.21).

If we only assume solvability of Eq. (2.21), this equation may have more than one solution T. The corresponding bifurcation problem will be studied in a future publication.

In view of the relations (2.7) and (2.10) for L_{11} and R, Eq. (2.21) can be reformulated as

$$|E|^2 = T^{2\beta}(T - T_0)\frac{R_\beta(T)}{P_\beta^2(T)} =: f(T), \tag{2.22}$$

i.e. in fact, T only depends on $|E|$ (and not on μ). A sufficient condition for (H5) is for instance the following assumption on f which is in fact an assumption on the energy band structure given by γ:

(H6) f is strictly increasing on $[T_0, \infty)$ and $\lim_{T\to\infty} f(T) = \infty$.

We show below that for parabolic bands and non-parabolic bands in the sense of Kane, the property (H6) on f is satisfied (see Lemma 3.1).

Let f be differentiable and let (H6) hold. Then the function $|E| \mapsto T(|E|)$ has the following properties:

$$T(0) = T_0, \quad T'(|E|) > 0 \text{ for all } |E| > 0, \quad \lim_{|E|\to\infty} T(|E|) = \infty.$$

We are also interested in the qualitive behavior of the mean electron velocity v_n depending on $|E|$. The velocity v_n is defined by

$$j_n = -nv_n,$$

which gives from (2.20) the expression

$$v_n = \frac{L_{11}}{n}\frac{E}{T},$$

or with (2.7) and (2.8):

$$v_n = v_n(E) = T(|E|)^{-1-\beta}\frac{P_\beta^2(T(|E|))}{Q^0(T(|E|))}E. \tag{2.23}$$

Then the mobility μ_n is given by $v_n(|E|) = \mu_n(|E|)E$. Without specifying the band structure, it is difficult to describe the qualitative behavior of the function $E \mapsto v_n(E)$. In particular, the limit $|v_n(E)|$ as $|E| \to \infty$ depends strongly on the assumptions on the band structure. In the general case, we can only conclude that

$$|v_n(E)| > 0 \text{ for } |E| > 0 \quad \text{and} \quad v_n(0) = 0.$$

3 High-field drift models

The high-field drift model for general band structure (assuming (H1)-(H5)) is given by Eqs. (2.19) and (2.23):

$$\begin{aligned} \partial_t n - \operatorname{div}(n v_n(E)) &= 0 && (3.1)\\ v_n(E) &= T(|E|)^{-1-\beta}\frac{P_\beta^2(T(|E|))}{Q^0(T(|E|))}E, && (3.2)\\ \operatorname{div}E &= n - C(x), && (3.3) \end{aligned}$$

and $T(|E|)$ is defined as the unique solution of $|E|^2 = f(T)$ (see (2.22)). In this section we will derive explicit expressions for $v_n(E)$ and $T(|E|)$ for more specific band diagrams, in particular for non-parabolic bands in the sense of Kane and for parabolic bands.

3.1 Non-parabolic band approximation

The non-parabolic band structure in the sense of Kane [11] is defined as follows:

(H7) Let the energy $\varepsilon(k)$ satisfy

$$\varepsilon(1+\alpha\varepsilon) = \frac{k^2}{2m^*}, \qquad \alpha > 0.$$

The constant m^* is the (scaled) effective electron mass given by $m^* = m_0 k_B T_0/\hbar^2 k_0^2$, where m_0 is the unscaled effective mass, k_B is the Boltzmann constant, $\hbar$ is the reduced Planck constant, k_0 is a typical wave vector, and $\alpha > 0$ is the (scaled) non-parabolicity parameter. When $\alpha = 0$, we get a parabolic band structure.

Under the assumption (H7), Eqs. (2.22) and (2.23) become

$$\begin{aligned} |E|^2 &= (d_0\tau_0)^{-1}T^{2\beta}(T-T_0)\frac{r_\beta(\alpha T)}{P_\beta(\alpha T)} = f(T), && (3.4)\\ v_n(E) &= d_0 T^{-1/2-\beta}\frac{P_\beta(\alpha T)}{q(\alpha T)}E, && (3.5) \end{aligned}$$

where

$$\tau_0 = \left(2\pi\phi_0(2m^*)^{3/2}\right)^{-1}, \quad d_0 = \left(3\pi\phi_0(2N_0+1)m^*(2m^*)^{3/2}\right)^{-1/2} \qquad (3.6)$$

and

$$\begin{aligned} P_\beta(\alpha T) &= \int_0^\infty \frac{1+\alpha T u}{(1+2\alpha T u)^2}u^{1-\beta}e^{-u}du,\\ q(\alpha T) &= \int_0^\infty (1+\alpha T u)^{1/2}(1+2\alpha T u)u^{1/2}e^{-u}du,\\ r_\beta(\alpha T) &= \Gamma(2+\beta) + 5\Gamma(3+\beta)\alpha T + 8\Gamma(4+\beta)(\alpha T)^2 + 4\Gamma(5+\beta)(\alpha T)^3, \end{aligned}$$

and Γ is the Gamma function defined by

$$\Gamma(s) = \int_0^\infty u^{s-1} e^{-u} du \quad \text{for } s > 0.$$

These formulas follow from Eqs. (2.11)-(2.13) and $\gamma(Tu) = 2m^* Tu(1 + \alpha Tu)$.

First we show that Hypothesis (H5) is satisfied for non-parabolic and parabolic band approximations:

Lemma 3.1 *Let (H1)-(H4) and (H7) for $\alpha \geq 0$ hold and let $\beta < 2$. Then for any $|E| \geq 0$, Eq. (3.4) has a unique solution $T = T(|E|)$, i.e. Hypothesis (H5) is satisfied.*

Proof. We show that the function f defined in (2.22) satisfies (H6). Since

$$P_\beta(\alpha T) \leq \int_0^\infty (1 + \alpha Tu) u^{1-\beta} e^{-u} du = \Gamma(2 - \beta) + \Gamma(3 - \beta)\alpha T$$

(here we need the condition $\beta < 2$), we get

$$f(T) \geq (d_0 \tau_0)^{-1} T^{2\beta}(T - T_0) \frac{r_\beta(\alpha T)}{\Gamma(2 - \beta) + \Gamma(3 - \beta)\alpha T}.$$

The term $r_\beta(\alpha T)$ is of order $O(T^3)$ as $T \to \infty$, therefore $f(T) \to \infty$ as $T \to \infty$.

In order to show that f is strictly increasing, it is sufficient to prove that both $T \mapsto T^{2\beta}(T - T_0)$ and $T \mapsto r_\beta(\alpha T)/P_\beta(\alpha T)$ are strictly increasing. For the first function, this is clear. For the second function we compute its derivative:

$$\frac{d}{dT} \frac{r_\beta(\alpha T)}{P_\beta(\alpha T)} = \frac{\alpha}{P_\beta(\alpha T)^2} \left(r'_\beta(\alpha T) P_\beta(\alpha T) - r_\beta(\alpha T) P'_\beta(\alpha T) \right) > 0$$

since $r'_\beta(\alpha T) \geq 5\Gamma(3 + \beta) > 0$ and

$$P'_\beta(\alpha T) = -\int_0^\infty \frac{3 + 2\alpha Tu}{(1 + 2\alpha Tu)^3} u^{2-\beta} e^{-u} du < 0.$$

Hence, f satisfies (H6) and therefore (H5). $\square$

Lemma 3.2 *Let (H1)-(H4) and (H7) hold. Then, as $|E| \to \infty$,*

$$T(|E|) = O(|E|^{2/(5+2\beta)}), \qquad |v_n(E)| = O(|E|^{-1/(5+2\beta)}).$$

Proof. The definitions of $P_\beta(\alpha T)$, $r_\beta(\alpha T)$ and $q(\alpha T)$ imply

$$P_\beta(\alpha T) = O(T^{-1}), \quad r_\beta(\alpha T) = O(T^3), \quad q(\alpha T) = O(T^{-3/2}) \quad \text{as } T \to \infty,$$

and hence, from (3.4),

$$|E|^2 = O(T^{5+2\beta}) \quad \text{as } T \to \infty.$$

Since $|E| \to \infty$ implies $T \to \infty$, we get

$$T = O(|E|^{2/(5+2\beta)}) \quad \text{as } |E| \to \infty.$$

Furthermore, by (3.5),

$$|v_n(E)| = \sqrt{\frac{d_0}{\tau_0}\Big(1 - \frac{T_0}{T}\Big)} \frac{\sqrt{P_\beta(\alpha T) r_\beta(\alpha T)}}{q(\alpha T)} = O(T^{-1/2}) \quad \text{as } T \to \infty, \tag{3.7}$$

and

$$|v_n(E)| = O(|E|^{-1/(5+2\beta)}) \quad \text{as } |E| \to \infty.$$

The lemma is proved. □

Remark 3.3 The mean velocity derived from the SHE model in the mean-free path limit for the cases $\beta = 0$ and $\beta = \frac{1}{2}$ has the same qualitative behavior as above (see [3, Ex. 4.3 and 4.4]).

3.2 Parabolic band approximation

In the parabolic band case $\varepsilon(k) = k^2/2m^*$ for $\beta = 0$ and $\beta = \frac{1}{2}$, we can give explicit formulas for $T(|E|)$ and $v_n(E)$.

Lemma 3.4 *Let (H1)-(H4) hold and let $\varepsilon = k^2/2m^*$ and $\beta < 2$. Then $T = T(|E|)$ is unique solution of the nonlinear equation*

$$|E|^2 = \frac{\Gamma(2+\beta)}{d_0 \tau_0 \Gamma(2-\beta)} T^{2\beta}(T - T_0) \tag{3.8}$$

and

$$v_n(E) = \sqrt{\frac{d_0}{\tau_0}\Gamma(2-\beta)\Gamma(2+\beta)\Big(1 - \frac{T_0}{T(|E|)}\Big)} \frac{E}{|E|}. \tag{3.9}$$

The velocity satisfies, as $|E| \to \infty$,

$$|v_n(E)| \to v_\infty := \frac{2}{\sqrt{\pi}} \sqrt{\Gamma(2-\beta)\Gamma(2+\beta)} \sqrt{\frac{d_0}{\tau_0}}.$$

Moreover, in the Chen case $\beta = \frac{1}{2}$ [5], it holds

$$T(|E|) = \frac{1}{2}\left(T_0 + \sqrt{T_0^2 + \frac{8}{3} d_0 \tau_0 |E|^2}\right), \tag{3.10}$$

$$v_n(E) = \frac{2 d_0 E}{T_0 + \sqrt{T_0^2 + \frac{8}{3} d_0 \tau_0 |E|^2}} \tag{3.11}$$

with $v_\infty = \sqrt{3d_0/2\tau_0}$, *and in the Lyumkis case* $\beta = 0$ *[12] we have*

$$\begin{aligned} T(|E|) &= T_0 + \frac{1}{C_T}|E|^2, && (3.12) \\ v_n(E) &= \frac{4d_0}{\sqrt{\pi}} \frac{E}{\sqrt{T_0 + d_0\tau_0|E|^2}}, && (3.13) \end{aligned}$$

with $v_\infty = 4\sqrt{d_0/\pi\tau_0}$.

Proof. Eqs. (3.8) and (3.9) follow from (3.4) and (3.7) since $r_\beta(0) = \Gamma(2+\beta)$, $P_\beta(0) = \Gamma(2-\beta)$ and $q(0) = \Gamma(3/2) = \sqrt{\pi}/2$. Furthermore,

$$|v_n(E)|^2 = \frac{4}{\pi}\frac{d_0}{\tau_0}\Gamma(2-\beta)\Gamma(2+\beta)\Big(1 - \frac{T_0}{T}\Big) \to v_\infty^2$$

as $|E| \to \infty$ or, equivalently, $T \to \infty$. In the Chen case $\beta = \frac{1}{2}$ we have to solve the equation

$$|E|^2 = \frac{3}{2d_0\tau_0}T(T - T_0)$$

(using $\Gamma(5/2) = 3\sqrt{\pi}/4$), which gives (3.10) and (3.11). Finally, if $\beta = 0$, we have to solve

$$|E|^2 = \frac{1}{d_0\tau_0}(T - T_0),$$

from which we immediately conclude (3.12) and (3.13). □

Remark 3.5 Notice that we have velocity saturation both in the parabolic and non-parabolic case (see Lemma 3.2). In the non-parabolic case however, the limit velocity vanishes. This behavior has already been observed in [3].

4 High-field drift-diffusion models

In Section 3 we have derived high-field models with no diffusion terms. Diffusion can be obtained as a higher-order correction by using a variant of the Chapman-Enskog method.

4.1 General band structure

Let the assumptions (H1)-(H5) hold and let (n^δ, T^δ) be a solution to (2.14) - (2.17), defining the chemical potential μ and the internal energy W (uniquely) via

$$\mu^\delta = \mu(n^\delta, T^\delta), \quad W^\delta = W(n^\delta, T^\delta).$$

More precisely, we obtain from (2.8), (2.9) the relations

$$\mu^\delta = T^\delta \ln \frac{n^\delta}{T^\delta Q^0(T^\delta)}, \quad W^\delta = \frac{Q^1(T^\delta)}{Q^0(T^\delta)}T^\delta n^\delta. \qquad (4.1)$$

We approximate n^δ and T^δ as follows:

$$\begin{aligned} n^\delta &= n^0 + O(\delta), \\ T^\delta &= T^0 + \delta T^\perp + O(\delta^2) \quad \text{as } \delta \to 0. \end{aligned}$$

Then we can decompose μ^δ, W^δ and $R^\delta = R(W(n^\delta, T^\delta))$ as

$$\begin{aligned} \mu^\delta &= \overline{\mu} + \delta \overline{\frac{\partial \mu}{\partial T}} T^\perp + O(\delta^2), \\ W^\delta &= \overline{W} + \delta \overline{\frac{\partial W}{\partial T}} T^\perp + O(\delta^2), \\ R^\delta &= \overline{R} + \delta \overline{\frac{\partial R}{\partial T}} T^\perp + O(\delta^2), \end{aligned}$$

where the overlined functions are evaluated at (n^δ, T^0), for instance

$$\overline{\mu} \stackrel{\text{def}}{=} \mu(n^\delta, T^0), \quad \overline{W} \stackrel{\text{def}}{=} W(n^\delta, T^0), \quad \overline{R} \stackrel{\text{def}}{=} R(n^\delta, T^0).$$

Similarly, using Eqs. (2.16) and (2.17), we can write the current densities as follows:

$$\begin{aligned} j_n^\delta &= -\overline{L_{11}} \frac{E}{T^0} + \delta \left(-\overline{L_{11}} \nabla \frac{\overline{\mu}}{T^0} - \frac{\partial}{\partial T} \left(\overline{\frac{L_{11}}{T}} \right) T^\perp E - \overline{L_{12}} \nabla \left(-\frac{1}{T^0} \right) \right) + O(\delta^2) \\ &= \overline{j_n} + \delta j_n^\perp + O(\delta^2), \\ j_W^\delta &= -\overline{L_{21}} \frac{E}{T^0} + \delta \left(-\overline{L_{21}} \nabla \frac{\overline{\mu}}{T^0} - \frac{\partial}{\partial T} \left(\overline{\frac{L_{21}}{T}} \right) T^\perp E - \overline{L_{22}} \nabla \left(-\frac{1}{T^0} \right) \right) + O(\delta^2) \\ &= \overline{j_w} + \delta j_w^\perp + O(\delta^2). \end{aligned}$$

Substitution of the decomposition for j_n^δ into (2.14) yields

$$\partial_t n^\delta + \text{ div } (\overline{j_n} + \delta j_n^\perp) = O(\delta^2). \tag{4.2}$$

In the similar way, we obtain for (2.15):

$$\partial_t W^\delta + \text{ div } \overline{j_W} = \frac{1}{\delta}(-E \cdot \overline{j_n} + \overline{R}) - E \cdot j_n^\perp + \overline{\frac{\partial R}{\partial T}} T^\perp + O(\delta). \tag{4.3}$$

The $O(\delta^{-1})$-term gives

$$E \cdot \overline{j_n} = \overline{R}$$

such that with the definition $\overline{j_n} = -\overline{L_{11}} E / T_0$ we get

$$|E|^2 = -\frac{\overline{R}}{\overline{L_{11}}} T^0 = -\frac{R(n^\delta, T^0)}{L_{11}(n^\delta, T^0)} T^0. \tag{4.4}$$

Therefore, T^0 is the (unique) solution to (4.4) which exists due to (H5). Notice that in view of assumptions (H1)-(H4), the quotient R/L_{11} and hence T^0 do not depend on n^δ (see (2.22)), i.e. $T^0 = T(|E|)$.

From the $O(1)$-terms in (4.3) we obtain an expression for $T^\perp$. Indeed, substitution of the definition of $j_n^\perp$ in the $O(1)$-terms of (4.3) leads to

$$\begin{aligned} \partial_t W^\delta + \operatorname{div} \overline{j_W} &= -E \cdot j_n^\perp + \overline{\frac{\partial R}{\partial T}} T^\perp \\ &= \left(\frac{\partial}{\partial T} \left(\overline{\frac{L_{11}}{T}} \right) |E|^2 + \overline{\frac{\partial R}{\partial T}} \right) T^\perp \\ &\quad + E \cdot \left(\overline{L_{11}} \nabla \frac{\overline{\mu}}{T^0} + \overline{L_{12}} \nabla \left(-\frac{1}{T^0} \right) \right). \end{aligned} \tag{4.5}$$

Now, the unique solvability of (4.4) with respect to T implies that

$$\frac{\partial}{\partial T} \left(\overline{\frac{L_{11}}{T}} \right) |E|^2 + \overline{\frac{\partial R}{\partial T}} = \frac{\partial}{\partial T} \left(\frac{L_{11}}{T} |E|^2 + R \right) (n^\delta, T^0) \neq 0.$$

Therefore,

$$\Lambda \stackrel{\text{def}}{=} \left[\frac{\partial}{\partial T} \left(\overline{\frac{L_{11}}{T}} \right) |E|^2 + \overline{\frac{\partial R}{\partial T}} \right]^{-1}$$

is well defined and we obtain from (4.5)

$$T^\perp = \Lambda \left[\frac{\partial W^\delta}{\partial t} + \operatorname{div} \overline{j_W} - E \cdot \left(\overline{L_{11}} \nabla \frac{\overline{\mu}}{T^0} + \overline{L_{12}} \nabla \left(-\frac{1}{T^0} \right) \right) \right].$$

The term $\partial W^\delta / \partial t$ equals, by the chain rule and (4.2),

$$\left(\frac{\partial W^\delta}{\partial n} + \frac{\partial W^\delta}{\partial T} \frac{\partial T}{\partial n} \right) (n^\delta, T^0) \frac{\partial n^\delta}{\partial t} = -\overline{\frac{\partial W}{\partial n}} \operatorname{div} \overline{j_n} + O(\delta),$$

since $T = T^0$ does not depend on n^δ. Hence, we can substitute $T^\perp$ in $j_n^\perp$ by the above expression to obtain up to order $O(\delta)$

$$\begin{aligned} j_n^\perp &= -\Big[1 - \frac{\partial}{\partial T} \Big(\overline{\frac{L_{11}}{T}} \Big) \Lambda |E|^2 \Big] \Big[\overline{L_{11}} \nabla \frac{\overline{\mu}}{T^0} + \overline{L_{12}} \nabla \Big(-\frac{1}{T^0} \Big) \Big] \\ &\quad - \frac{\partial}{\partial T} \Big(\overline{\frac{L_{11}}{T}} \Big) \Lambda E \Big[\overline{\frac{\partial W}{\partial n}} \operatorname{div} \Big(\overline{L_{11}} \frac{E}{T^0} \Big) - \operatorname{div} \Big(\overline{L_{21}} \frac{E}{T^0} \Big) \Big]. \end{aligned} \tag{4.6}$$

The function $j_n^\perp$ depends on n^δ, ∇n^δ, E, and $\operatorname{div} E$. Therefore we can rewrite (4.2) as

$$\partial_t n^\delta + \operatorname{div} \left(\delta j_n^\perp (n^\delta, \nabla n^\delta, E, \operatorname{div} E) + \overline{j_n}(E, n^\delta) \right) = 0,$$

where $\overline{j_n}(E, n^\delta)$ is given by

$$\overline{j_n}(E, n^\delta) = -L_{11}(n^\delta, T(|E|)) \frac{E}{T(|E|)}.$$

Using (4.1), we can rewrite (4.6) as

$$j_n^\perp = -D(n^\delta, E)\nabla n^\delta + F(n^\delta, E, \mathrm{div}E),$$

where the diffusion matrix is defined by

$$\begin{aligned} D(n,E) &= \left(1 - \frac{\partial}{\partial T}\left(\frac{L_{11}}{T}\right)\Lambda|E|^2\right)\frac{L_{11}}{n}I \\ &\quad + \frac{\partial}{\partial T}\left(\frac{L_{11}}{T}\right)\frac{\Lambda}{T}\left(\frac{\partial W}{\partial n}\frac{\partial L_{11}}{\partial n} - \frac{\partial L_{21}}{\partial n}\right)(E \otimes E), \end{aligned} \tag{4.7}$$

I is the unit matrix of $\mathbb{R}^{d\times d}$ and $(E\otimes E)_{ij} = E_iE_j$. The drift part $F(n, E, \mathrm{div}E)$ is given by:

$$\begin{aligned} F(n,E,\mathrm{div}E) &= \left(1 - \frac{\partial}{\partial T}\Big(\frac{L_{11}}{T}\Big)\Lambda|E|^2\right)\left(\frac{3}{2}TL_{11} - L_{12}\right)\frac{\nabla T}{T^2} \\ &\quad - \frac{\partial}{\partial T}\Big(\frac{L_{11}}{T}\Big)\frac{\Lambda}{T}\left(\frac{\partial W}{\partial n}\frac{\partial L_{11}}{\partial T} - \frac{\partial W}{\partial n}\frac{L_{11}}{T} + \frac{L_{21}}{T}\right)(E\otimes E)\nabla T \\ &\quad - \frac{\partial}{\partial T}\Big(\frac{L_{11}}{T}\Big)\frac{\Lambda}{T}\left(\frac{\partial W}{\partial n}L_{11} - L_{21}\right)E\mathrm{div}E. \end{aligned}$$

Hence, the *high-field drift-diffusion model* for general band diagrams reads (for $\delta = 1$)

$$\partial_t n - \mathrm{div}\left(D(n,E)\nabla n - F(n,E,\mathrm{div}E) + \frac{L_{11}(n,T(E|))}{T(|E|)}E\right) = 0, \tag{4.8}$$

$$\mathrm{div}E = n - C(x). \tag{4.9}$$

A necessary condition for the well-posedness of Eq. (4.8) is given by the positive definiteness of $D(n,E)$. A sufficient condition is proved in the following lemma.

Lemma 4.1 *The symmetric matrix $D(n,E)$ defined in (4.7) is positive definite if for all $|E| \geq 0$,*

$$\frac{\partial}{\partial T}\left(\frac{L_{11}}{T}\right)\frac{\Lambda}{T}\left(\frac{\partial W}{\partial n}\frac{\partial L_{11}}{\partial n} - \frac{\partial L_{21}}{\partial n}\right) \leq 0, \tag{4.10}$$

$$\frac{L_{11}}{n} + \frac{\partial}{\partial T}\left(\frac{L_{11}}{T}\right)|E|^2\frac{\Lambda}{T}\left(-\frac{TL_{11}}{n} + \frac{\partial W}{\partial n}\frac{\partial L_{11}}{\partial n} - \frac{\partial L_{21}}{\partial n}\right) > 0. \tag{4.11}$$

Proof. Let $\xi \in \mathbb{R}^d$. Then, using the inequality $|E\cdot\xi| \leq |E|\cdot|\xi|$ and the assumption (4.10),

$$\begin{aligned} \xi^T D(n,E)\xi &= \frac{L_{11}}{n}|\xi|^2 - \frac{\partial}{\partial T}\left(\frac{L_{11}}{T}\right)\Lambda\frac{L_{11}}{n}|E|^2|\xi|^2 \\ &\quad + \frac{\partial}{\partial T}\left(\frac{L_{11}}{T}\right)\frac{\Lambda}{T}\left(\frac{\partial W}{\partial n}\frac{L_{11}}{\partial n} - \frac{\partial L_{21}}{\partial n}\right)|E\cdot\xi|^2 \\ &\geq \delta(|E|)|\xi|^2, \end{aligned}$$

with

$$\delta(|E|) = \frac{L_{11}}{n} + \frac{\partial}{\partial T}\left(\frac{L_{11}}{T}\right)|E|^2\frac{\Lambda}{T}\left(-\frac{TL_{11}}{n} + \frac{\partial W}{\partial n}\frac{\partial L_{11}}{\partial n} - \frac{\partial L_{21}}{\partial n}\right). \tag{4.12}$$

Thus, by assumption (4.11), the assertion follows. □

4.2 Parabolic band approximation

In the parabolic band case, it holds (see [7, 10]):

$$\begin{aligned}
L_{11} &= \frac{2}{\sqrt{\pi}}\Gamma(2-\beta)d_0 n T^{1/2-\beta}, \\
L_{21} &= \frac{2}{\sqrt{\pi}}\Gamma(3-\beta)d_0 n T^{3/2-\beta}, \\
W &= \frac{3}{2}nT, \\
R &= \frac{2}{\sqrt{\pi}}\Gamma(2+\beta)nT^{-1/2+\beta}\frac{T_0 - T}{\tau_0}.
\end{aligned}$$

Lemma 4.2 *Let $\beta \leq \frac{1}{2}$. Then the diffusion matrix $D(n,E)$ is uniformly positive definite for all $T \geq T_0$.*

Proof. By Lemma 4.1, it is sufficient to prove (4.10) and (4.11). Elementary computations give

$$\begin{aligned}
\frac{\partial}{\partial T}\left(\frac{L_{11}}{T}\right) &= -\frac{2}{\sqrt{\pi}}\Gamma(2-\beta)\Big(\frac{1}{2}+\beta\Big)d_0 n T^{-3/2-\beta} \leq 0, \\
\frac{\partial}{\partial T}R &= \frac{2}{\sqrt{\pi}}\Gamma(2+\beta)\frac{nT^{-1/2+\beta}}{\tau_0}\left(\left(\beta - \frac{1}{2}\right)\frac{T_0}{T} - \left(\frac{1}{2}+\beta\right)\right) \leq 0,
\end{aligned}$$

and hence

$$\frac{\partial}{\partial T}\left(\frac{L_{11}}{T}\right)\Lambda = \frac{\frac{\partial}{\partial T}(L_{11}/T)|E|^2}{\frac{\partial}{\partial T}(L_{11}/T)|E|^2 + \frac{\partial}{\partial T}R}|E|^{-2} > 0.$$

Furthermore, it holds

$$\frac{\partial W}{\partial n}\frac{\partial L_{11}}{\partial n} - \frac{\partial L_{21}}{\partial n} = \frac{2}{\sqrt{\pi}}\Gamma(2-\beta)\left(\beta - \frac{1}{2}\right)d_0 T^{3/2-\beta} \leq 0,$$

if $\beta \leq \frac{1}{2}$. This shows that the condition (4.10) is satisfied. It remains to estimate $\delta(|E|)$ defined in (4.12). Using

$$\frac{\partial}{\partial T}\left(\frac{L_{11}}{T}\right)|E|^2\Lambda$$

$$
\begin{aligned}
&= \frac{(\frac{1}{2}+\beta)\Gamma(2-\beta)d_0|E|^2}{(\frac{1}{2}+\beta)\Gamma(2-\beta)d_0|E|^2+\Gamma(2+\beta)\tau_0^{-1}\left(\left(\frac{1}{2}-\beta\right)T_0+(\frac{1}{2}+\beta)T\right)T^{2\beta}} \\
&= \frac{(\frac{1}{2}+\beta)(T-T_0)}{(\frac{1}{2}+\beta)(T-T_0)+\left((\frac{1}{2}-\beta)T_0+(\frac{1}{2}+\beta)T\right)} \\
&= \frac{(\frac{1}{2}+\beta)(T-T_0)}{(1+2\beta)T-2\beta T_0},
\end{aligned}
\tag{4.13}
$$

which follows from (3.8), and

$$
-\frac{TL_{11}}{n}+\frac{\partial W}{\partial n}\frac{\partial L_{11}}{\partial n}-\frac{\partial L_{21}}{\partial n}=\frac{2}{\sqrt{\pi}}\Gamma(2-\beta)\left(-\frac{3}{2}+\beta\right)d_0T^{3/2-\beta},
$$

we obtain for $T \geq T_0$,

$$
\begin{aligned}
\delta(|E|) &= \frac{2}{\sqrt{\pi}}\Gamma(2-\beta)d_0T^{1/2-\beta} \\
&\quad + \frac{(1+2\beta)(T-T_0)}{(1+2\beta)T-2\beta T_0}\frac{1}{\sqrt{\pi}}\Gamma(2-\beta)\Big(-\frac{3}{2}+\beta\Big)d_0T^{1/2-\beta} \\
&= \frac{1}{\sqrt{\pi}}\Gamma(2-\beta)d_0T^{1/2-\beta}\left(2-\left(\frac{3}{2}-\beta\right)\frac{(1+2\beta)T-(1+2\beta)T_0}{(1+2\beta)T-2\beta T_0}\right) \\
&\geq \frac{1}{\sqrt{\pi}}\Gamma(2-\beta)d_0T^{1/2-\beta}\left(2-\left(\frac{3}{2}-\beta\right)\right) \\
&= \frac{d_0}{\sqrt{\pi}}\Gamma(2-\beta)\left(\frac{1}{2}+\beta\right)T^{1/2-\beta} \\
&\geq \frac{d_0}{\sqrt{\pi}}\Gamma(2-\beta)\left(\frac{1}{2}+\beta\right)T_0^{1/2-\beta} \\
&> 0,
\end{aligned}
$$

using $\beta \leq \frac{1}{2}$ again. □

With the use of Eqs. (4.13) and (3.8) we obtain, after elementary but lengthy computations, the following expressions:

$$
\begin{aligned}
&D(n,E) \\
&= \frac{2}{\sqrt{\pi}}\frac{\Gamma(2-\beta)d_0T^{1/2-\beta}}{T+2\beta(T-T_0)}\Bigg[\Big(\Big(\frac{1}{2}+\beta\Big)T+\Big(\frac{1}{2}-\beta\Big)T_0\Big)I \\
&\quad - \frac{(\frac{1}{2}+\beta)(\frac{1}{2}-\beta)d_0\tau_0}{\Gamma(2+\beta)T^{2\beta}}(E\otimes E)\Bigg], \\
&F(n,E,\mathrm{div}E) \\
&= \frac{2}{\sqrt{\pi}}\frac{\Gamma(2-\beta)(\frac{1}{2}-\beta)d_0nT^{3/2-\beta}}{(1+2\beta)T-2\beta T_0}\Bigg[-\Big(\Big(\frac{1}{2}+\beta\Big)T+\Big(\frac{1}{2}-\beta\Big)T_0\Big)\frac{\nabla T}{T^2} \\
&\quad - \frac{5(\frac{1}{2}+\beta)\Gamma(2-\beta)d_0\tau_0}{2\Gamma(2+\beta)T^{2(\beta+1)}}(E\otimes E)\nabla T+\frac{(\frac{1}{2}+\beta)\Gamma(2-\beta)d_0\tau_0}{\Gamma(2+\beta)T^{2(\beta+1)}}(\mathrm{div}E)E\Bigg].
\end{aligned}
$$

In the Chen case $\beta = \frac{1}{2}$ the above formulas simplify to

$$\begin{aligned} D(n, E) &= \frac{d_0}{2 - T_0/T(|E|)}, \\ F(n, E, \mathrm{div}E) &= 0. \end{aligned}$$

Therefore, the high-field drift-diffusion model for parabolic bands in the Chen case reads (see (4.8)):

$$\partial_t n - \mathrm{div}\left(\frac{d_0}{2 - T_0/T(|E|)}\nabla n + \frac{n}{T(E|)}E\right) = 0,$$

and $T(|E|)$ is given by (3.10). Notice that for $|E| \to \infty$, the diffusivity converges to $d_0/2$:

$$\frac{d_0}{2 - T_0/T(|E|)} \to \frac{d_0}{2} \quad \text{as } |E| \to \infty,$$

whereas for $|E| \to 0$, we obtain:

$$\frac{d_0}{2 - T_0/T(|E|)} \to d_0 \quad \text{as } |E| \to 0.$$

For the drift term it holds

$$\frac{n}{T(|E|)}E \sim \frac{3}{8d_0\tau_0}\frac{E}{|E|} \quad \text{as } |E| \to \infty.$$

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