Diffusive semiconductor moment equations using Fermi-Dirac statistics

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Abstract. Diffusive moment equations with an arbitrary number of moments are formally derived from the semiconductor Boltzmann equation employing a moment method and a Chapman-Enskog expansion. The moment equations are closed by employing a generalized Fermi-Dirac distribution function obtained from entropy maximization. The current densities allow for a drift-diffusion-type formulation or a "symmetrized" formulation, using dual entropy variables from nonequilibrium thermodynamics. Furthermore, drift-diffusion and new energy-transport equations based on Fermi-Dirac statistics are obtained and their degeneracy limit is studied.

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1. Introduction

In semiconductor device modeling, macroscopic equations are derived from the semiconductor Boltzmann equation with the aim to obtain simpler and numerically cheaper models which still contain the important physical phenomena. One idea consists in multiplying the Boltzmann equation by a finite number of certain weight functions, depending on the momentum variable only, and to integrate over the momentum space. This leads to evolution equations for averaged quantities of the Boltzmann distribution function, the so-called moments. The moment equations can be closed by (essentially) taking that distribution function in the

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definition of the moments, which maximizes the kinetic entropy under the constraints of given moments. This approach was first used by Dreyer [11] and later carried out by Levermore [26]. The entropy-maximizing distribution function turns out to be a generalization of the Maxwell-Boltzmann distribution. In the context of semiconductor modeling, entropy maximization has been introduced by Anile and coworkers in a hydrodynamic scaling [2]. Moments models for one or two moments have been derived by Ben Abdallah and Degond in a diffusive scaling [3], leading to drift-diffusion equations (one moment) or energy-transport equations (two moments). Combining entropy maximization and a diffusive scaling, diffusive moment models with an arbitrary number of moments have been proposed recently in [23].

Most of these works are based on a moment closure using Maxwell-Boltzmann-type distribution functions. In degenerate semiconductor materials, it is known that the equilibrium situation is described by a Fermi-Dirac distribution. In this paper, we are concerned with the derivation of diffusive moment equations employing Fermi-Dirac statistics. Drift-diffusion models based on Fermi-Dirac statistics, under various assumptions on the collision operator, have been derived in [5, 14, 15]. Albinus et al. suggested a thermodynamics-based energy-transport model including Fermi-Dirac statistics [1]. Degond and Ben Abdallah derived energy-transport models using Fermi-Dirac distributions with general (nonexplicit) diffusion matrices [3]. Instead of the Maxwell distribution $M(p) = e^{-\varepsilon(p)/k_BT}$, where $\varepsilon(p)$ denotes the carrier energy, k_B the Boltzmann constant, and T the carrier temperature, Chen et al. [9] employed the equilibrium function $(1+\gamma/k_BT)M(p)$, where $\gamma \geq 0$, to derive a non-Maxwellian energy-transport model. Here, we derive diffusive moment models of arbitrary order, based on Fermi-Dirac statistics, and for collision operators under abstract hypotheses, continuing our work [23].

Our main results are as follows. Under suitable assumptions on the scattering operators (see (H1)-(H3) below), we derive the higher-order moment equations

$$\partial_t m_i + \mathrm{div} J_i - iJ_{i-1}\cdot\nabla V = W_i, \quad i = 0,\dots,N, \tag{1}$$

where $m = (m_0,\dots,m_N)$ is the moment vector (m_0 being the particle density and m_1 the energy density), J_i are the fluxes, V is the electric potential, and W_i are certain averaged scattering terms (with $W_0 = 0$). The fluxes are given by

$$J_i = -\sum_{j=0}^{N}\big(D_{ij}\nabla\lambda_j + j\lambda_j D_{i,j-1}\nabla V\big), \tag{2}$$

where D_{ij} are the (matrix-valued) diffusion coefficients, coming from the dominant scattering processes, and $\lambda = (\lambda_0,\dots,\lambda_N)$ is the Lagrange multiplier vector, coming from the constrained entropy maximization problem. The moments m_i depend nonlinearly on the Lagrange multipliers λ:

$$m_i(x,t) = \int_B \frac{\varepsilon(p)^i dp}{\eta + \exp(-\lambda(x,t)\cdot\kappa(p))}, \quad \kappa(p) = (1,\varepsilon(p),\dots,\varepsilon(p)^N),$$

where $\eta \geq 0$ is the degeneracy parameter. When $\eta = 0$, we recover the generalized Maxwell-Boltzmann case of [23]; $\eta = 1$ corresponds to Fermi-Dirac statistics. We observe that the moment balance equations (1) and the constitutive relations (2) are the same as in the generalized Maxwell-Boltzmann case. Fermi-Dirac statistics enters only in the relation between m and λ. Therefore, it is not surprising that the properties, which are valid for the generalized Maxwell-Boltzmann model, also hold here:

- Under some conditions on the collision operator (see Proposition 3), the diffusion matrix $\mathcal{D} = (D_{ij}) \in \mathbb{R}^{3(N+1)\times 3(N+1)}$ is symmetric and positive definite.
- If the dominant scattering mechanism is described by a BGK-type (Bhatnagar-Gross-Krook) operator (see Remark 6), the current equations can be written in the drift-diffusion form
$$J_i = -\nabla g_i - R_i(g) g_i \nabla V, \quad i = 0, \ldots, N,$$
where $g = (g_0, \ldots, g_N)$ are the new independent variables. For more general collision operators, we obtain the formulation
$$J_{ik} = -\mathrm{div} g_i^k - R_i^k(g) g_i^k \cdot \nabla V, \quad i = 0, \ldots, N, \ k = 1, 2, 3. \tag{3}$$
We refer to Proposition 7 for details.
- The convective parts including the electric field $-\nabla V$ in (1) and (2) can be eliminated by introducing so-called dual entropy variables $\bar{\lambda}_i$, depending on the Lagrange multipliers and the electric potential, such that
$$\partial_t \bar{m}_i + \mathrm{div}\, \bar{J}_i = \bar{W}_i, \quad \bar{J}_i = -\sum_{j=0}^{N} C_{ij} \nabla \bar{\lambda}_j, \tag{4}$$
where the new diffusion matrix (C_{ij}) is again symmetric and positive definite. This formulation extends the dual-entropy concept from nonequilibrium thermodynamics and it allows us to derive an entropy–entropy dissipation inequality (see Proposition 5).

We notice that the drift-diffusion formulation is less obvious, and the arguments leading to (3) are different from those in [23]. Also the entropy–entropy dissipation inequality is new. Compared to our previous work [23], the main novelties include (i) new alternative formulations of the model equations and a new entropy–entropy dissipation inequality; (ii) the derivation of the degenerate drift-diffusion model; and (iii) the derivation of a new energy-transport model based on Fermi-Dirac statistics.

Our derivation is formal since a rigorous proof in a general setting seems to be out of reach. Rigorous mathematical results for low-order moment models can be found, e.g., in [4, 14].

For BGK-type collision operators and a parabolic band structure, we are able to make the above model explicit. (Also more general scattering integrals and nonparabolic bands can be assumed, but the corresponding models would be less explicit.) Supposing a constant relaxation time τ, the *drift-diffusion model* becomes

$$\partial_t n + \operatorname{div} J = 0, \quad J = -\tau n \nabla(\lambda_0 - V), \quad n = (2\pi)^{3/2}\eta^{-1}F_{1/2}(\lambda_0 + \log\eta),$$

where $F_{1/2}$ is the Fermi integral with index 1/2 defined in (20) below. This model was first formulated by Bonch-Bruevich and Kalashnikov [6] and has been analyzed by Gajewski and Gröger [13]. A numerical treatment can be found in [29]. We present here the first derivation of this model from the Boltzmann equation. In the Maxwell-Boltzmann limit $\eta \to 0$, we recover the standard drift-diffusion equations, whereas in the degeneracy limit $\eta \to \infty$ (after a rescaling), the so-called degenerate drift-diffusion model

$$\partial_t n + \operatorname{div} J = 0, \quad J = -\tau\big(N_0 \nabla(n^{5/3}) + n\nabla V\big), \tag{5}$$

where $N_0 > 0$ is a number, is obtained. Such a limit was made rigorous in [20]. The initial-value problem was analyzed first in [18, 21], the stationary problem in [27]. A numerical discretization in one and two space dimensions has been presented in [19, 24] employing mixed finite elements and in [7, 8] using a finite-volume approximation. The model (5) coupled to a heat equation with power dissipation was studied by Guan and Wu [17]. Equations (5) may be employed in degenerate semiconductors in which the particle density is very large. We mention that Poupaud and Schmeiser [28] rigorously derived a high-density model from the Boltzmann equation, but their model differs from the above equations.

Under the same assumptions as above, the diffusive moment model with two moments becomes the *Fermi-Dirac energy-transport model*:

$$\partial_t n + \operatorname{div} J_0 = 0, \quad J_0 = -\nabla g_0 + \frac{F_{1/2}(z)}{F_{3/2}(z)}\frac{g_0}{T}\nabla V,$$
$$\partial_t(ne) + \operatorname{div} J_1 - J_0 \cdot \nabla V = W, \quad J_1 = -\nabla g_1 + \frac{F_{3/2}(z)}{F_{5/2}(z)}\frac{g_1}{T}\nabla V,$$

where $z = \lambda_0 + \log\eta$, $T = -1/\lambda_1$, and the variables (g_0, g_1) are related to (n, ne) by

$$g_0 = \frac{2\tau}{3}ne, \quad g_1 = \frac{5\tau}{3}(ne)T\frac{F_{5/2}(z)}{F_{3/2}(z)}.$$

We remark that the mapping $(n, ne) \mapsto (\lambda_0, \lambda_1)$ is invertible. This model seems to be new in the literature. In the limit $\eta \to 0$, we recover the energy-transport model with diffusion matrix (8.21) from [22]; in the limit $\eta \to \infty$, we obtain again the degenerate model (5).

The paper is organized as follows. The model equations (1)-(2) are derived in Section 2, and some properties on the diffusion coefficients are proved. The drift-diffusion and dual-entropy formulations (3) and (4), respectively, are derived in Section 3. Finally, Section 4 is concerned with the computation of some explicit models, also including an extension of the six-moments model of Grasser et al. [16].

2. Derivation of the moment model

Let $B \subset \mathbb{R}^3$ be the first Brillouin zone, either being the periodic cube $B = (-\pi, \pi)^3$ or (for parabolic band structures) $B = \mathbb{R}^3$ [22]. The evolution of the charged particles in the semiconductor domain $\Omega \subset \mathbb{R}^3$ is described by a distribution function $f(x, p, t)$ depending on time $t \geq 0$ and space-crystal momentum variables $(x, p) \in \Omega \times B$. The distribution function $f = f_\alpha$ satisfies the (dimensionless) semiconductor Boltzmann equation in diffusion scaling:

$$\alpha^2 \partial_t f_\alpha + \alpha\big(u \cdot \nabla_x f_\alpha + \nabla_x V \cdot \nabla_p f_\alpha\big) = Q(f_\alpha). \tag{6}$$

Here, $\alpha > 0$ is the Knudsen number (the ratio between the optical phonon energy and the typical energy of an electron; see [3] for details). We assume that the kinetic electron energy is much larger than the phonon energy, i.e. $\alpha \ll 1$, and we are looking for limiting diffusive equations as $\alpha \to 0$. The group velocity u is defined by $u(p) = \nabla_p \varepsilon(p)$, where $\varepsilon(p)$ is the kinetic carrier energy given by the semiconductor band structure. The electric potential $V = V(x, t)$ is a given function or self-consistently determined from the Poisson equation

$$\lambda_D^2 \Delta V = \int_B f_\alpha dp - C(x),$$

where $\lambda_D > 0$ is the (scaled) Debye length and $C(x)$ the doping profile, modeling fixed charged background ions in the semiconductor crystal. The collision operator is supposed to consist of two parts: a dominant part and a small part,

$$Q(f) = Q_1(f) + \alpha^2 Q_2(f).$$

This decomposition has been justified, for particular scattering processes, in [3, 10], for instance. Below, we will specify our assumptions on the first operator Q_1, whereas the second one Q_2 will remain unspecified. To this end, we need to introduce generalized Fermi-Dirac equilibrium distributions.

2.1. Entropy maximization

We define the entropy (or free energy) functional

$$H(f)(x, t) = -\int_B \Big(f \log f + \frac{1}{\eta}(1 - \eta f)\log(1 - \eta f) + \varepsilon(p) f\Big) dp$$

for a given function $f(x, p, t)$, where $\eta > 0$ is a parameter. When $\eta = 1$, we obtain the Fermi-Dirac entropy. In the limit $\eta \to 0$, we recover the Maxwell-Boltzmann entropy density $f(\log f - 1 + \varepsilon(p))$. Let weight functions $\kappa(p) = (\kappa_0(p), \ldots, \kappa_N(p))$ and moments $m(x, t) = (m_0(x, t), \ldots, m_N(x, t))$ be given. We set $\langle g \rangle = \int_B g(p) dp$ for a function $g(p)$, and we call the expression $\langle \kappa_i f \rangle$ the *i-th moment* of f. The *generalized Fermi-Dirac distribution* is that function f^* which maximizes the entropy $H(f)$ under the constraints $\langle \kappa_i f \rangle(x, t) = m_i(x, t)$ for $i = 0, \ldots, N$, $x \in \Omega$, $t > 0$. The solution of this problem, if it exists, is given by

$$f^*(x, p, t) = \frac{1}{\eta + \exp(-\widetilde{\lambda}(x, t) \cdot \kappa(p) + \varepsilon(p))},$$

where $\widetilde{\lambda} = (\widetilde{\lambda}_0, \ldots, \widetilde{\lambda}_N)$ are the Lagrange multipliers. This representation simplifies under the following hypothesis:

(H1) The energy ε is even in p and the weight functions are given by $\kappa_i(p) = \varepsilon(p)^i$, $i = 0, \ldots, N$.

Then, setting $\lambda_1 = \widetilde{\lambda}_1 - 1$ and $\lambda_i = \widetilde{\lambda}_i$ for $i \neq 1$,

$$f^* = \big(\eta + \exp(-\lambda_0 + \varepsilon)\big)^{-1} \quad \text{for } N = 0,$$
$$f^* = \big(\eta + \exp(-\lambda \cdot \kappa)\big)^{-1} \quad \text{for } N > 0.$$

Furthermore, for given f with moments $m_i = \langle \kappa_i f \rangle$, we denote by $\mathcal{F}_f$ that function which maximizes the entropy under the constraints $\langle \kappa_i \mathcal{F}_f \rangle = m_i$ for $i = 0, \ldots, N$.

Hypothesis (H1) on the weight functions is imposed for simplicity only; the subsequent results are also valid if the functions $\kappa_i(p)$ are arbitrary but even in p (see [23]). The carrier energy may be given by the parabolic band approximation, $\varepsilon(p) = \frac{1}{2}|p|^2$. A more refined model is the Kane dispersion relation, which takes into account the nonparabolicity at higher energies, $\varepsilon(1+\delta\varepsilon) = \frac{1}{2}|p|^2$, where $\delta > 0$ measures the nonparabolicity. In terms of ε, we have

$$\varepsilon(p) = \frac{1}{2\delta}\big(\sqrt{1 + 2\delta|p|^2} - 1\big). \tag{7}$$

If $\delta = 0$, we recover the parabolic band approximation.

We point out that the mathematical solution of the constrained maximization problem may be delicate. The problem is uniquely solvable if, for instance, the Brillouin zone B is a bounded domain and $\varepsilon(p)$ is a general band structure; or if $B = \mathbb{R}^3$, $\kappa = (1, \varepsilon, \varepsilon^2)$, and $\varepsilon(p)$ is given by (7); or if $B = \mathbb{R}^3$, $\kappa = (1, \varepsilon)$, and $\varepsilon(p) = \frac{1}{2}|p|^2$. However, when the momentum space B is unbounded and the polynomial weight functions have superquadratic growth at infinity, the maximization problem may be unsolvable [12].

2.2. Assumptions on the collision operators

For the dominant collisional part Q_1, we have in mind the simple BGK-type operator $Q_1(f) = (\mathcal{F}_f - f)/\tau$, where $\mathcal{F}_f$ is the Fermi-Dirac distribution defined in the previous subsection and $\tau > 0$ is the relaxation time, since this operator allows us to derive explicit models (see Section 4). Our results are also valid for more general operators satisfying the following hypothesis:

(H2) All moments of $Q_1(f)$ vanish, $\langle \kappa_i Q_1(f) \rangle = 0$ for all functions f and all $i = 0, \ldots, N$. Furthermore, $Q_1(f) = 0$ if and only if $f = \mathcal{F}_f$. Finally, $\langle Q_2(f) \rangle = 0$ for all functions f.

This assumption mainly expresses the collisional invariants. The conservation property for Q_1 with respect to *all* moments is rather strong but it is satisfied, for instance, by the BGK-type operator. In Sections 4.1 and 4.2, we only assume that mass and/or energy are conserved, which corresponds to elastic collisions, $\langle Q_1(f) \rangle = \langle \varepsilon Q_1(f) \rangle = 0$, since $\kappa_0 = 1$ and $\kappa_1 = \varepsilon$ by (H1). In Section 4.3, we discuss an extended energy-transport model based on conservation of the quantity $\langle \varepsilon^2 f \rangle$, which has no direct physical interpretation. Notice, however, that the moments of the *total* collision operator $Q = Q_1 + \alpha^2 Q_2$, $\langle \kappa_i Q(f) \rangle$, are of order α^2 and thus, we do not require complete conservation of the collision moments.

Another example for Q_1 is the electron-electron scattering operator

$$(Q_{\rm ee}(f))(p) = \int_{B^3} \sigma(p,p',p_1,p_1')\delta(\varepsilon' + \varepsilon_1' - \varepsilon - \varepsilon_1) \\ \times \big(f' f_1' (1-f)(1-f_1) - f f_1 (1-f')(1-f_1') \big) dp'\, dp_1\, dp_1',$$

where $f' = f(p')$, $f_1 = f(p_1)$, $f_1' = f(p_1')$ and the scattering rate σ is symmetric (see [22, formula (4.31)]). It is shown in [3] that this operator conserves mass and energy and that $Q_{\rm ee}(f) = 0$ if and only if f is a Fermi-Dirac distribution. An example for Q_2 is the inelastic phonon scattering operator

$$(Q_{\rm ph}(f))(p) = \int_B \big(s_{\rm ph}(p,p') f' - s_{\rm ph}(p',p) f \big) dp',$$

where $s_{\rm ph}(p,p') = \phi_{\rm ph}(p,p')[(N_{\rm ph}+1)\delta(\varepsilon - \varepsilon' + \varepsilon_{\rm ph}) + N_{\rm ph}\delta(\varepsilon - \varepsilon' - \varepsilon_{\rm ph})]$ and $\varepsilon' = \varepsilon(p')$ [3]. The number $N_{\rm ph}$ is the phonon occupation number, and $\varepsilon_{\rm ph}$ is the phonon energy. A computation shows that $\langle Q_{\rm ph}(f) \rangle = 0$, i.e., $Q_{\rm ph}$ conserves mass.

2.3. Moment equations and Chapman-Enskog expansion

First we derive the balance equations.

Proposition 1 (Balance equations). *Let (H1)-(H2) hold, and let f_α be a solution of the Boltzmann equation* (6)*. We assume that the formal limits $F = \lim_{\alpha\to 0} f_\alpha$, $G = \lim_{\alpha\to 0}(f_\alpha - \mathcal{F}_{f_\alpha})/\alpha$ exist. Then the moments $m_i = \langle \kappa_i \mathcal{F}_F \rangle$ and the current densities $J_i = \langle u\kappa_i G \rangle$ are solutions of*

$$\partial_t m_i + \operatorname{div} J_i - iJ_{i-1} \cdot \nabla V = W_i, \quad i = 0, \ldots, N, \tag{8}$$

where $W_i = \langle \kappa_i Q_2(F) \rangle$ are averaged collision integrals, $W_0 = 0$, and the differentiations are taken with respect to x.

Proof. We multiply the Boltzmann equation (6) by κ_i, integrate over B, integrate by parts in the electric force term, and observe that the moments of $Q_1(f_\alpha)$ vanish by (H2),

$$\partial_t \langle \kappa_i f_\alpha \rangle + \alpha^{-1}\big(\operatorname{div}_x \langle u\kappa_i f_\alpha \rangle - \nabla_x V \cdot \langle \nabla_p \kappa_i f_\alpha \rangle \big) = \langle \kappa_i Q_2(f_\alpha) \rangle.$$

Inserting the Chapman-Enskog expansion $f_\alpha = \mathcal{F}_{f_\alpha} + \alpha g_\alpha$ in this equation, taking into account that, by (H1), $p \mapsto u(p)\kappa_i(p)\mathcal{F}_{f_\alpha}(p)$ and $p \mapsto \nabla_p \kappa_i(p)\mathcal{F}_{f_\alpha}(p)$ are odd functions, and performing the formal limit $\alpha \to 0$, we infer that

$$\partial_t \langle \kappa_i \mathcal{F}_F \rangle + \operatorname{div}_x \langle u\kappa_i G \rangle - \nabla_x V \cdot \langle \nabla_p \kappa_i G \rangle = \langle \kappa_i Q_2(F) \rangle.$$

Since, by (H1), $\nabla_p \kappa_i = i\varepsilon^{i-1} u = i\kappa_{i-1} u$, we obtain (8). □

In order to specify the current densities J_i, we need a hypothesis on the linearization of Q_1 at $\mathcal{F}_F$, i.e. $L = DQ_1(\mathcal{F}_F)$. We introduce as in [3] the Hilbert space $L^2(B)$ with the scalar product

$$(g_1, g_2)_F = \int_B \frac{g_1 g_2}{\mathcal{F}_F(1-\eta\mathcal{F}_F)} dp$$

and the corresponding norm.

(H3) The linear operator $L = DQ_1(\mathcal{F}_F)$ is continuous, closed, and symmetric on $L^2(B)$, and $Lg = 0$ if and only if $g = \mathcal{F}_F$.

Hypothesis (H3) is needed to solve the equation $LG = H$. By the Fredholm alternative, this equation is solvable if and only if $H \in N(L^*)^\perp = N(L)^\perp$ and its solution is unique in $N(L)^\perp$, where $N(L)$ is the kernel of L. Since the kernel of L consists of the generalized Fermi-Dirac distributions, $LG = H$ is solvable if and only if $0 = (H, \mathcal{F}_F)_F$. In the case of the BGK-type operator $Q_1(f) = (\mathcal{F}_f - f)/\tau$, the limit function G can be explicitly determined (see Remark 6), and we do *not* need to impose (H3) in this situation.

Proposition 2 (Current equations). *Let (H1)-(H3) hold. Then the current densities can be written as*

$$J_0 = -D_{00}\nabla(\lambda_0 - V) \quad \textit{for } N = 0, \tag{9}$$

$$J_i = -\sum_{j=0}^{N} \big(D_{ij}\nabla\lambda_j + j\lambda_j D_{i,j-1}\nabla V\big) \quad \textit{for } N > 0, \tag{10}$$

where $i = 0, \ldots, N$, the diffusion coefficients $D_{ij} = (D_{ij}^{k\ell}) \in \mathbb{R}^{3\times 3}$ are defined by

$$D_{ij} = -\langle \kappa_i u \otimes \phi_j \rangle,$$

and $\phi_j = (\phi_{j1}, \phi_{j2}, \phi_{j3})$ is the unique solution in $N(L)^\perp$ of the operator equations

$$L\phi_{jk} = \kappa_j u_k \mathcal{F}_F(1-\eta\mathcal{F}_F), \quad j = 0, \ldots, N, \ k = 1,2,3. \tag{11}$$

Formula (10) has to be understood in the following way:

$$J_{ik} = -\sum_{j=0}^{N}\sum_{\ell=1}^{3} \Big(D_{ij}^{k\ell}\frac{\partial\lambda_j}{\partial x_\ell} + j\lambda_j D_{i,j-1}^{k\ell}\frac{\partial V}{\partial x_\ell}\Big), \quad k = 1,2,3.$$

Proof. First, we notice that the operator equations (11) are solvable in $L^2(B)$, by the Fredholm alternative, since $\kappa_j u_k \mathcal{F}_F(1-\eta\mathcal{F}_F)$ is odd in p, and hence, $(\mathcal{F}_F, \kappa_j u_k \mathcal{F}_F(1-\eta\mathcal{F}_F))_F = 0$. Next, we expand the collision operator $Q_1(f_\alpha) = Q_1(\mathcal{F}_{f_\alpha}) + \alpha DQ_1(\mathcal{F}_{f_\alpha})g_\alpha + O(\alpha^2)$. Inserting the Chapman-Enskog expansion $f_\alpha = \mathcal{F}_{f_\alpha} + \alpha g_\alpha$ into the Boltzmann equation (6), dividing the equation by α, and performing the formal limit $\alpha \to 0$ gives

$$u \cdot \nabla_x \mathcal{F}_F + \nabla_x V \cdot \nabla_p \mathcal{F}_F = LG,$$

where we recall that $G = \lim_{\alpha\to 0} g_\alpha$. We claim that

$$G = \phi_0 \cdot \nabla_x(\lambda_0 - V) \quad \text{for } N = 0,$$
$$G = \sum_{j=0}^{N} \big(\nabla_x\lambda_j \cdot \phi_j + j\lambda_j \nabla_x V \cdot \phi_{j-1}\big) \quad \text{for } N > 0. \tag{12}$$

Indeed, observing that

$$\nabla_x \mathcal{F}_F = \mathcal{F}_F(1-\eta\mathcal{F}_F)\sum_{j=0}^{N}\kappa_j \nabla_x\lambda_j, \quad \nabla_p \mathcal{F}_F = \mathcal{F}_F(1-\eta\mathcal{F}_F)\sum_{j=0}^{N} j\kappa_{j-1}u\lambda_j$$

(if $N = 0$, $\nabla_p\mathcal{F}_F = -\mathcal{F}_F(1-\eta\mathcal{F}_F)u$), we compute for $N > 0$

$$\begin{aligned} LG &= \sum_{j=0}^{N}\big(\nabla_x\lambda_j \cdot L\phi_j + j\lambda_j\nabla_x V \cdot L\phi_{j-1}\big) \\ &= \mathcal{F}_F(1-\eta\mathcal{F}_F)\sum_{j=0}^{N}\big(\kappa_j\nabla_x\lambda_j \cdot u + j\kappa_{j-1}\lambda_j\nabla_x V\cdot u\big) \\ &= \nabla_x\mathcal{F}_F \cdot u + \nabla_x V \cdot \nabla_p \mathcal{F}_F. \end{aligned}$$

The conclusion now follows from $J_i = \langle u\kappa_i G\rangle$. The proof for $N = 0$ is similar. □

2.4. Properties of the diffusion matrix

We show that the diffusion matrix $\mathcal{D} = (D_{ij})$ is symmetric and, under an additional condition on the operator L and the band structure, positive definite. Notice that the symmetry of $\mathcal{D}$ expresses the Onsager principle of thermodynamics [25], whereas the positive definiteness shows that the balance equations (8) together with the current relations (9)-(10) are of diffusive type. The condition on L reads as follows.

> **(H4)** The operator $-L = -DQ_1(\mathcal{F}_F)$ is bounded and coercive on the space $N(L)^\perp$, i.e., there exist μ_0, $\mu_1 > 0$ such that for all $g \in N(L)^\perp$, $(-Lg, g)_F \geq \mu_0\|g\|_F^2$ and $\|-Lg\|_F \leq \mu_1\|g\|_F$.

Proposition 3. *The diffusion matrix $\mathcal{D} = (\mathcal{D}_{\alpha\beta}) \in \mathbb{R}^{3(N+1)\times 3(N+1)}$ is symmetric and positive semi-definite. Moreover, if (H4) holds and $\{\kappa_i u_k : i = 0,\ldots,\ k = 1,2,3\}$ is linearly independent, $\mathcal{D}$ is positive definite.*

The explicit expression of $\mathcal{D}$ for BGK-type collision operators (see Remark 6 below) shows that the proposition also holds in this situation.

Proof. First, we prove the symmetry of $\mathcal{D}$. Let α, $\beta \in \{1,\ldots,3(N+1)\}$. There exist unique indices i, $j \in \{0,\ldots,N\}$ and k, $\ell \in \{1,2,3\}$ such that $\alpha = 3i + k$ and $\beta = 3j + \ell$. By (H3), L is symmetric on $L^2(B)$. Hence,

$$\begin{aligned} \mathcal{D}_{\alpha\beta} &= D_{ij}^{k\ell} = -\langle\kappa_i u_k\phi_{j\ell}\rangle = -(L\phi_{ik}, \phi_{j\ell})_F = -(\phi_{ik}, L\phi_{j\ell})_F = -\langle\kappa_j u_\ell \phi_{ik}\rangle \\ &= D_{ji}^{\ell k} = \mathcal{D}_{\beta\alpha}. \end{aligned}$$

Next, we compute, for $\xi \in \mathbb{R}^{3(N+1)}$, $\xi \neq 0$:

$$\xi^\top \mathcal{D}\xi = \sum_{i,j=0}^{N}\sum_{k,\ell=1}^{3} \xi_{3i+k}\xi_{3j+\ell}D_{ij}^{k\ell} = \Big(-L\Big(\sum_{i=0}^{N}\sum_{k=1}^{3}\xi_{3i+k}\phi_{ik}\Big), \sum_{j=0}^{N}\sum_{\ell=1}^{3}\xi_{3j+\ell}\phi_{j\ell}\Big)_F$$
$$\geq \frac{\mu_0}{\mu_1^2}\Big\|L\Big(\sum_{i=0}^{N}\sum_{k=1}^{3}\xi_{3i+k}\phi_{ik}\Big)\Big\|_F^2 = \frac{\mu_0}{\mu_1^2}\int_B \Big|\sum_{i=0}^{N}\sum_{k=1}^{3}\xi_{3i+k}\kappa_i u_k\Big|^2 dp.$$

In view of the linear independence of $\kappa_i u_k$, the sum and hence the integral are positive. □

3. Alternative formulations

Similarly as in the Maxwell-Boltzmann case of [23], the moment model (8)-(10) can be rewritten either in a dual-entropy variable or in a drift-diffusion formulation. In the case $N = 0$, we do not need to rewrite the model. Therefore, let in the following $N > 0$. We suppose that (H1)-(H4) hold.

The dual-entropy formulation is similar to the corresponding one in the Maxwell-Boltzmann case [23]. Indeed, let the transformation matrix $P = (P_{ij}) \in \mathbb{R}^{(N+1)\times(N+1)}$ be defined by

$$Q_{ij} = \binom{j}{i} a_{ij} V^{j-i}, \quad P_{ij} = (-1)^{i+j} Q_{ij} \quad \text{with} \quad a_{ij} = \begin{cases} 1 & \text{if } i \leq j, \\ 0 & \text{if } i > j, \end{cases}$$

where i, $j = 0, \ldots, N$. Notice that $Q = (Q_{ij})$ is the inverse matrix of P. Define the dual-entropy variables $\bar\lambda = (\bar\lambda_0, \ldots, \bar\lambda_N)^\top$, the transformed moments $\bar m = (\bar m_0, \ldots, \bar m_N)^\top$, and the thermodynamic fluxes $\bar J = (\bar J_0, \ldots, \bar J_N)^\top$ by, respectively,

$$\bar\lambda = Q\lambda, \quad \bar m = P^\top m, \quad \text{and} \quad \bar J = P^\top J.$$

Proposition 4 (Dual-entropy formulation). *The model equations* (8)-(10) *can be equivalently written as*

$$\partial_t \bar m_i + \operatorname{div}\bar J_i = (P^\top W)_i - i\partial_t V \bar m_{i-1}, \quad \bar J_i = -\sum_{j=0}^{N} C_{ij}\nabla\bar\lambda_i, \tag{13}$$

where $i = 0, \ldots, N$, $W = (0, W_1, \ldots, W_N)^\top$ *and the new diffusion matrix* $\mathcal{C} = (C_{ij}^{k\ell})$ *is defined by* $C^{k\ell} = P^\top D^{k\ell} P$ *or, more precisely, by*

$$C_{ij}^{k\ell} = \sum_{m,n=0}^{N} P_{mi} D_{mn}^{k\ell} P_{nj}, \quad i,j = 0, \ldots, N, \ k,\ell = 1,2,3.$$

The current relation has to be understood in the following way:

$$\bar J_{ik} = -\sum_{j=0}^{N}\sum_{\ell=1}^{3} C_{ij}^{k\ell}\frac{\partial\bar\lambda_j}{\partial x_\ell}, \quad i = 0, \ldots, N, \ k = 1,2,3.$$

The proof of the above result is exactly as the proof of Proposition 4.6 in [23] and is therefore omitted. One advantage of the "symmetrized" formulation is that it allows us to derive an entropy–entropy dissipation inequality. Here, the (relative) entropy is defined by

$$\begin{aligned} H(t) &= \int_{\mathbb{R}^3} h(\lambda)dx \\ &= -\int_{\mathbb{R}^3} \big(m\cdot(\lambda-\lambda_{\rm eq}) - \eta^{-1}\langle\log(1+\eta e^{\lambda\cdot\kappa})\rangle + \eta^{-1}\langle\log(1+\eta e^{\lambda_{\rm eq}\cdot\kappa})\rangle\big)dx, \end{aligned}$$

where $h(\lambda)$ is the entropy density and $\lambda_{\rm eq} = (V,-1,0,\ldots,0)$ the equilibrium value. Notice that in the Maxwell-Boltzmann limit $\eta\to 0$, we recover the entropy suggested in [23] since

$$\eta^{-1}\log(1+\eta e^{\lambda\cdot\kappa}) = \log\big((1+\eta e^{\lambda\cdot\kappa})^{1/\eta}\big) \to e^{\lambda\cdot\kappa} \quad \text{as } \eta\to 0.$$

Proposition 5 (Entropy–entropy dissipation inequality). *Let the electric potential be time-independent and let W in* (13) *be monotone in the sense of $\int_{\mathbb{R}^3} W\cdot(\lambda-\lambda_{\rm eq})dx \le 0$. Then any (smooth) solution of* (13) *satisfies*

$$-\frac{dH}{dt} + \int_{\mathbb{R}^3}\sum_{i,j=0}^{N} (\nabla\bar\lambda_i)^\top C_{ij}(\nabla\bar\lambda_j)dx \le 0.$$

The second integral is called the entropy dissipation. If $\mathcal{D}$ is symmetric positive definite (see Proposition 3 for sufficient conditions), so does $\mathcal{C}$, and hence, the entropy is nondecreasing in time.

Proof. A simple computation shows that

$$\frac{\partial}{\partial\lambda_i}\langle\eta^{-1}\log(1+\eta e^{-\lambda\cdot\kappa})\rangle = \big\langle\kappa_i(\eta+e^{\lambda\cdot\kappa})^{-1}\big\rangle = m_i, \quad i=0,\ldots,N.$$

Therefore, the derivative of the entropy density $h(\lambda)$ becomes

$$\frac{\partial h}{\partial\lambda_i} = -\frac{\partial m}{\partial\lambda_i}\cdot(\lambda-\lambda_{\rm eq}) - m_i + \frac{\partial}{\partial\lambda_i}\langle\eta^{-1}\log(1+\eta e^{\lambda\cdot\kappa})\rangle = -\frac{\partial m}{\partial\lambda_i}\cdot(\lambda-\lambda_{\rm eq}).$$

Moreover, we have

$$\partial_t m\cdot(\lambda-\lambda_{\rm eq}) = \sum_{i=0}^N \frac{\partial m}{\partial\lambda_i}\cdot(\lambda-\lambda_{\rm eq})\partial_t\lambda_i = -\sum_{i=0}^N\frac{\partial h}{\partial\lambda_i}\partial_t\lambda_i = -\partial_t h(\lambda). \tag{14}$$

Hence, multiplying (13) by $\bar\lambda-\bar\lambda_{\rm eq}$, where $\bar\lambda_{\rm eq} = Q\lambda_{\rm eq} = (0,-1,0,\ldots,0)^\top$, integrating over $\mathbb{R}^3$, and summing over $i=0,\ldots,N$, it follows that

$$\int_{\mathbb{R}^3}(P^\top\partial_t m)^\top(\bar\lambda-\bar\lambda_{\rm eq})dx + \int_{\mathbb{R}^3}(\operatorname{div}\bar J)^\top(\bar\lambda-\bar\lambda_{\rm eq})dx = \int_{\mathbb{R}^3}(P^\top W)^\top(\bar\lambda-\bar\lambda_{\rm eq})dx.$$

The integrand of the right-hand side equals $W^\top PQ(\lambda-\lambda_{\rm eq}) = W^\top(\lambda-\lambda_{\rm eq})$, and thus, its integral is nonpositive, by assumption. Because of (14), the first integrand of the left-hand side is equal to $\partial_t m^\top PQ(\lambda - \lambda_{\rm eq}) = -\partial_t h(\lambda)$. Then, integrating by parts in the second integral, we conclude that

$$-\int_{\mathbb{R}^3} \partial_t h(\lambda) dx + \int_{\mathbb{R}^3} \sum_{i,j=0}^N (\nabla\bar\lambda_i)^\top C_{ij}(\nabla\bar\lambda_j)dx \le 0,$$

proving the proposition. □

Remark 6. The expressions for the diffusion coefficients can be simplified if the collision operator Q_1 is of BGK type and the band energy $\varepsilon(p)$ only depends on $|p|$. We will use this fact in Section 4.1 for the drift-diffusion case. Indeed, let $Q_1(f) = (\mathcal{F}_f - f)/\tau$ and $\varepsilon(p) = E(\frac12|p|^2)$ for $p \in B = \mathbb{R}^3$ and for some function E. Inserting the Chapman-Enskog expansion $f_\alpha = \mathcal{F}_{f_\alpha} + \alpha g_\alpha$ into the Boltzmann equation (6) and letting $\alpha \to 0$, we obtain an explicit expression for the limit function $G = \lim_{\alpha\to 0} g_\alpha$:

$$\begin{aligned} G &= -\tau\big(u\cdot\nabla_x\mathcal{F}_F + \nabla_x V\cdot\nabla_p\mathcal{F}_F\big) \\ &= -\tau\sum_{j=0}^N \Big(\kappa_j u\cdot\nabla_x\lambda_j + j\kappa_{j-1}\lambda_j u\cdot\nabla_x V\Big)\mathcal{F}_F(1-\eta\mathcal{F}_F). \end{aligned}$$

Comparing this relation with (12), we see that

$$D_{ij}^{k\ell} = -\langle\kappa_i u_k \phi_{j\ell}\rangle, \quad \text{where } \phi_{j\ell} = -\tau\kappa_j u_\ell \mathcal{F}_F(1-\eta\mathcal{F}_F).$$

Using the radial symmetry of $\varepsilon(p)$, we compute

$$\begin{aligned} D_{ij} &= \tau\langle\varepsilon(p)^{i+j}u\otimes u\mathcal{F}_F(1-\eta\mathcal{F}_F)\rangle = \tau\int_{\mathbb{R}^3} E^{i+j}(E')^2 p\otimes p\mathcal{F}_F(1-\eta\mathcal{F}_F)dp \\ &= \frac{\tau}{3}\int_{\mathbb{R}^3} E^{i+j}(E')^2|p|^2\mathcal{F}_F(1-\eta\mathcal{F}_F)dp\,\mathbb{I}, \end{aligned} \tag{15}$$

where $\mathbb{I}$ is the identity matrix in $\mathbb{R}^{3\times 3}$. Thus, we can identify the matrix D_{ij} by the above scalar value. □

We are able to write the current densities in a drift-diffusion-type formulation which may be convenient for a numerical decoupling of the equations.

Proposition 7 (Drift-diffusion-type formulation). *Let $g_i \in \mathbb{R}^{3\times 3}$ be defined by $g_i = -\langle\kappa_i u\otimes\chi\rangle$, where $\chi = (\chi_j)$ are the unique solutions in $N(L)^\perp$ of $L\chi_j = u_j\mathcal{F}_F$, $j = 1,2,3$ (see (H3) for the definition of L). Then the current densities* (10) *can be written as*

$$J_{ik} = -\sum_{\ell=1}^3\Big(\frac{\partial g_i^{k\ell}}{\partial x_\ell} + R_i^{k\ell}(g)g_i^{k\ell}\frac{\partial V}{\partial x_\ell}\Big), \quad i = 0,\ldots,N,\ k = 1,2,3, \tag{16}$$

where $g = (g_0,\ldots,g_N)$ and

$$R_i^{k\ell}(g) = \sum_{j=0}^N j\frac{D_{i,j-1}^{k\ell}}{g_i^{k\ell}}\lambda_j, \quad i = 0,\ldots,N,\ k,\ell = 1,2,3.$$

Furthermore, if the assumptions of Remark 6 *hold and* $\{\kappa_0,\ldots,\kappa_N\}$ *is linearly independent, we may identify* g_i *by its scalar value, and the current equations* (16) *become*

$$J_i = -\nabla g_i - R_i(g) g_i \nabla V, \quad i = 0,\ldots,N, \tag{17}$$

where $R_i(g) = \sum_j j(D_{i,j-1}/g_i)\lambda_j$*, and* $\lambda = (\lambda_j)$ *is uniquely computed from* $g = g(\lambda) \in \mathbb{R}^{N+1}$*.*

In the Maxwell-Boltzmann case $\eta = 0$, the functions χ_j and ϕ_{0j} coincide (up to an element of $N(L)$), and we can choose $g_i = D_{i0}$.

Proof. The new variables g_i are different from those in [23], therefore we give a complete proof. From

$$L\Big(\frac{\partial \chi_k}{\partial x_\ell}\Big) = \frac{\partial}{\partial x_\ell}(u_k\mathcal{F}_F) = \sum_{j=0}^N \kappa_j u_k \frac{\partial \lambda_j}{\partial x_\ell}\mathcal{F}_F(1-\eta\mathcal{F}_F) = L\Big(\sum_{j=0}^N \frac{\partial \lambda_j}{\partial x_\ell}\phi_{jk}\Big)$$

and the unique solvability in $N(L)^\perp$, we obtain $\partial\chi_k/\partial x_\ell = \sum_j(\partial\lambda_j/\partial x_\ell)\phi_{jk} + c\mathcal{F}_F$, where c is a constant. Then

$$\sum_{\ell=1}^3 \frac{\partial g_i^{k\ell}}{\partial x_\ell} = -\sum_{\ell=1}^3\Big\langle \kappa_i u_k \frac{\partial \chi_\ell}{\partial x_\ell}\Big\rangle = -\sum_{j=0}^N\sum_{\ell=1}^3 \langle \kappa_i u_k \phi_{j\ell}\rangle \frac{\partial \lambda_j}{\partial x_\ell} = \sum_{j=0}^N\sum_{\ell=1}^3 D_{ij}^{k\ell}\frac{\partial\lambda_j}{\partial x_\ell}$$

corresponds to the first term in (10), and (16) follows.

Under the assumptions of Remark 6, we can write $D_{ij}^{k\ell} = D_{ij}\delta_{k\ell}$ and $g_i^{k\ell} = g_i\delta_{k\ell}$, where, similarly as in Remark 6,

$$g_i^{k\ell} = \frac{\tau}{3}\int_{\mathbb{R}^3} E^i(E')^2|p|^2\mathcal{F}_F dp\, \delta_{k\ell}. \tag{18}$$

The linear independency of (κ_i) implies, arguing similarly as in the proof of Proposition 3, that the matrix $\mathcal{D} = (D_{ij}) \in \mathbb{R}^{(N+1)\times(N+1)}$ is positive definite. It remains to prove that λ_j can be uniquely defined from the mapping $g = g(\lambda)$. We show that the mapping $\lambda \mapsto g(\lambda)$ is one-to-one. To emphasize the dependency of $\mathcal{F}_F$ on λ, we will write $\mathcal{F}_F(\lambda\cdot\kappa)$. Let $\lambda^{(1)}$, $\lambda^{(2)}$ be such that $g(\lambda^{(1)}) = g(\lambda^{(2)})$. By (18), identifying $g_i^{k\ell}$ with its scalar value g_i and summing over $i = 0,\ldots,N$,

$$\sum_{i=0}^N \lambda_i^{(j)}\int_{\mathbb{R}^3} E^i(E')^2|p|^2\big(\mathcal{F}_F(\lambda^{(1)}\cdot\kappa) - \mathcal{F}_F(\lambda^{(2)}\cdot\kappa)\big)dp = 0, \quad j = 1,2.$$

Taking the difference of the above equation for $j = 1$ and $j = 2$, we find that

$$\begin{aligned} 0 &= \sum_{i=0}^N \int_{\mathbb{R}^3} E^i(E')^2|p|^2\big(\mathcal{F}_F(\lambda^{(1)}\cdot\kappa) - \mathcal{F}_F(\lambda^{(2)}\cdot\kappa)\big)\big(\lambda_i^{(1)} - \lambda_i^{(2)}\big)dp \\ &= \int_{\mathbb{R}^3} (E')^2|p|^2\big(\mathcal{F}_F(\lambda^{(1)}\cdot\kappa) - \mathcal{F}_F(\lambda^{(2)}\cdot\kappa)\big)\big(\lambda^{(1)}\cdot\kappa - \lambda^{(2)}\cdot\kappa\big)dp, \end{aligned}$$

observing that $\kappa = (1, E, \ldots, E^N)$. Since $\mathcal{F}_F$ is increasing, the last integral is nonnegative and hence, its integrand vanishes:

$$\big(\mathcal{F}_F(\lambda^{(1)} \cdot \kappa) - \mathcal{F}_F(\lambda^{(2)} \cdot \kappa)\big)\big(\lambda^{(1)} \cdot \kappa - \lambda^{(2)} \cdot \kappa\big) = 0.$$

The same argument shows that $\lambda^{(1)} \cdot \kappa = \lambda^{(2)} \cdot \kappa$. By the linear independence of $\{\kappa_0, \ldots, \kappa_N\}$, it follows that $\lambda^{(1)} = \lambda^{(2)}$, proving the claim. □

4. Explicit models

The diffusive moment model (8)-(10) can be made explicit under additional conditions. We assume that the collision operator Q_1 is of BGK type and that the energy is given by the parabolic band approximation,

$$Q_1(f) = \frac{1}{\tau}(\mathcal{F}_f - f), \quad \varepsilon(p) = \frac{1}{2}|p|^2, \ p \in \mathbb{R}^3. \tag{19}$$

Below, we need the Fermi integrals

$$F_a(z) = \frac{1}{\Gamma(a+1)} \int_0^\infty \frac{t^a}{1 + e^{t-z}} dt, \quad z \in \mathbb{R}, \ a > -1, \tag{20}$$

where Γ is the Gamma function satisfying $\Gamma(\frac{1}{2}) = \sqrt{\pi}$ and $\Gamma(a+1) = a\Gamma(a)$. We recall the following properties:

$$F'_{a+1}(z) = F_a(z), \quad z \in \mathbb{R}, \ a > -1; \tag{21}$$

$$F_a(z) \sim e^z \quad \text{as } z \to -\infty; \tag{22}$$

$$F_a(z) \sim \frac{z^{a+1}}{\Gamma(a+2)} \quad \text{as } z \to \infty; \tag{23}$$

$$(a+2)F_{a-1}(z)F_{a+1}(z) - (a+1)F_a(z)^2 > 0, \quad z \in \mathbb{R}, \ a > 0. \tag{24}$$

Here $f(z) \sim g(z)$ as $z \to b$ signifies $\lim_{z \to b} f(z)/g(z) = 1$.

4.1. Drift-diffusion models

In the case $N = 0$, we obtain a drift-diffusion model based on Fermi-Dirac statistics.

Proposition 8 (Drift-diffusion model). *Let* (19) *hold. Then equations* (8) *and* (9) *specify for $N = 0$ to*

$$\partial_t n + \operatorname{div} J_0 = 0, \quad J_0 = -\tau n \nabla(\lambda_0 - V) = -\tau\Big(\frac{F_{1/2}(z)}{F_{-1/2}(z)}\nabla n - n\nabla V\Big), \tag{25}$$

where $z = \lambda_0 + \log \eta$ and the zeroth moment $n = m_0$ and the Lagrange multiplier λ_0 are related by

$$n = (2\pi)^{3/2}\eta^{-1}F_{1/2}(\lambda_0 + \log \eta).$$

Proof. The expression D_{00} in (15) becomes, using $\partial\mathcal{F}_F/\partial\lambda_0 = \mathcal{F}_F(1-\eta\mathcal{F}_F)$ and the substitution $\varepsilon = |p|^2/2$,

$$\begin{aligned}
D_{00} &= \tau\langle p\otimes p\mathcal{F}_F(1-\eta\mathcal{F}_F)\rangle = \frac{4\pi\tau}{3}\frac{\partial}{\partial\lambda_0}\int_0^\infty |p|^4\mathcal{F}_F d|p| \\
&= \frac{4\pi\tau}{3\eta}\frac{\partial}{\partial\lambda_0}\int_0^\infty \frac{(2\varepsilon)^{3/2}d\varepsilon}{1+\exp(-\lambda_0-\log\eta+\varepsilon)} = \frac{(2\pi)^{3/2}\tau}{\eta}\frac{\partial F_{3/2}}{\partial\lambda_0}(z) \\
&= \frac{(2\pi)^{3/2}\tau}{\eta}F_{1/2}(z),
\end{aligned}$$

where we have used (21) and $z = \lambda_0 + \log\eta$. Moreover,

$$n = \langle\mathcal{F}_F\rangle = \frac{4\pi}{\eta}\int_0^\infty \frac{\sqrt{2\varepsilon}d\varepsilon}{1+e^{-z+\varepsilon}} = \frac{(2\pi)^{3/2}}{\eta}F_{1/2}(z) = \tau^{-1}D_{00}.$$

Thus, by (9), $J_0 = -\tau n\nabla(\lambda_0 - V)$. The drift-diffusion formulation of the current density follows from $\nabla n = (2\pi)^{3/2}\eta^{-1}F_{-1/2}(z)\nabla\lambda_0$. □

The quantity $\phi = \lambda_0 - V$ is called the *Fermi potential* and the current equation can be written in terms of ϕ as

$$J_0 = -\tau n\nabla\phi, \quad n = (2\pi)^{3/2}\eta^{-1}F_{1/2}(\phi+V).$$

We recall that the corresponding drift-diffusion model was first formulated by Bonch-Bruevich and Kalashnikov [6] (see the introduction).

Remark 9 (Limits $\eta\to 0$ and $\eta\to\infty$). Notice that in the *Maxwell-Boltzmann limit* $\eta\to 0$, the second current relation in (25) reduces to $J_0 = -\tau(\nabla n - n\nabla V)$ (employing (22)), which is the current density of the standard drift-diffusion equations. In the *degeneracy limit* $\eta\to\infty$, we rescale the particle and current densities by setting $n_s = \eta n$ and $J_s = \eta J_0$. Then, by (23), as $\eta\to\infty$,

$$\frac{F_{1/2}(\lambda_0+\log\eta)}{F_{-1/2}(\lambda_0+\log\eta)} \sim \frac{2}{3}(\lambda_0+\log\eta), \quad n_s \sim \frac{8\sqrt{2}\pi}{3}(\lambda_0+\log\eta)^{3/2}.$$

This implies that

$$\frac{F_{1/2}(\lambda_0+\log\eta)}{F_{-1/2}(\lambda_0+\log\eta)} \sim \frac{n_s^{2/3}}{2(6\pi^2)^{1/3}} \quad \text{as } \eta\to\infty$$

and, using (25) and setting $N_0 = 3/(10(6\pi^2)^{1/3})$,

$$J_s \sim -\tau\big(N_0\nabla(n_s^{5/3}) - n_s\nabla V\big) \quad \text{as } \eta\to\infty. \tag{26}$$

This relation, together with the mass conservation equation, is the degenerate drift-diffusion model first analyzed in [18, 27]. □

4.2. Energy-transport models

Energy-transport models are obtained for $N = 1$. The balance equations are

$$\partial_t n + \operatorname{div} J_0 = 0, \quad \partial_t(ne) + \operatorname{div} J_1 - J_0 \cdot \nabla V = W, \tag{27}$$

where we have set $n = m_0$ and $m_1 = ne$ for the particle and energy densities. To simplify the notation, we define the (generalized) particle temperature T by $T = -1/\lambda_1$.

Proposition 10 (Energy-transport model). *Let* (19) *hold. The particle and energy densities simplify to*

$$n = (2\pi T)^{3/2}\eta^{-1}F_{1/2}(z), \quad ne = \frac{3}{2}\frac{F_{3/2}(z)}{F_{1/2}(z)}nT,$$

where $z = \lambda_0 + \log\eta$. The diffusion coefficients of the energy-transport model read as

$$D_{00} = \tau nT, \quad D_{01} = D_{10} = \frac{5\tau}{2}\frac{F_{3/2}(z)}{F_{1/2}(z)}nT^2, \quad D_{11} = \frac{35\tau}{4}\frac{F_{5/2}(z)}{F_{1/2}(z)}nT^3.$$

In the drift-diffusion formulation, the current densities can be written as

$$J_0 = -\nabla g_0 + \frac{F_{1/2}(z)}{F_{3/2}(z)}\frac{g_0}{T}\nabla V, \quad J_1 = -\nabla g_1 + \frac{F_{3/2}(z)}{F_{5/2}(z)}\frac{g_1}{T}\nabla V,$$

where the variables (g_0, g_1) are related to (n, ne) by

$$g_0 = \frac{2\tau}{3}ne, \quad g_1 = \frac{10\tau}{9}\frac{F_{1/2}(z)F_{5/2}(z)}{F_{3/2}(z)^2}\frac{(ne)^2}{n}.$$

We recall that, by Proposition 7, the mapping $(g_0, g_1) \mapsto (\lambda_0, \lambda_1)$ is invertible on its range.

Proof. The relation for the particle density follows after substituting $t = -\lambda_1\varepsilon$:

$$\begin{aligned} n = \langle \mathcal{F}_F \rangle &= \frac{4\pi}{\eta}\int_0^\infty \frac{\sqrt{2\varepsilon}d\varepsilon}{1 + \exp(-z - \lambda_1\varepsilon)} = \frac{4\sqrt{2}\pi}{\eta(-\lambda_1)^{3/2}}\int_0^\infty \frac{t^{1/2}dt}{1 + e^{-z+t}} \\ &= \frac{(2\pi)^{3/2}}{\eta(-\lambda_1)^{3/2}}F_{1/2}(z). \end{aligned}$$

The expression for ne is shown in a similar way. Because of $\partial\mathcal{F}_F/\partial\lambda_0 = \mathcal{F}_F(1 - \eta\mathcal{F}_F)$, formula (15) simplifies to

$$\begin{aligned} D_{ij} &= \frac{4\pi\tau}{3}\frac{\partial}{\partial\lambda_0}\int_0^\infty \varepsilon^{i+j}(2\varepsilon)^{3/2}\mathcal{F}_F d\varepsilon = \frac{8\sqrt{2}\pi\tau}{3\eta}\frac{\partial}{\partial\lambda_0}\int_0^\infty \frac{\varepsilon^{i+j+3/2}d\varepsilon}{1 + \exp(-z - \lambda_1\varepsilon)} \\ &= \frac{8\sqrt{2}\pi\tau\Gamma(i + j + \frac{5}{2})}{3\eta(-\lambda_1)^{i+j+5/2}}\frac{\partial}{\partial\lambda_0}F_{i+j+3/2}(z) = \frac{8\sqrt{2}\pi\tau\Gamma(i + j + \frac{5}{2})}{3\eta(-\lambda_1)^{i+j+5/2}}F_{i+j+1/2}(z), \end{aligned}$$

employing (21). Furthermore, we specify (18):

$$g_0 = \frac{\tau}{3}\langle |p|^2 \mathcal{F}_F\rangle = \frac{4\pi\tau}{3\eta}\int_0^\infty \frac{(2\varepsilon)^{3/2}d\varepsilon}{1+\exp(-z-\lambda_1\varepsilon)} = \frac{(2\pi)^{3/2}\tau}{\eta(-\lambda_1)^{5/2}}F_{3/2}(z) = \frac{2}{3}\tau ne,$$

$$g_1 = \frac{5\sqrt{2}\pi^{3/2}\tau}{\eta(-\lambda_1)^{7/2}}F_{5/2}(z) = \frac{5\tau}{3}\,\frac{ne}{-\lambda_1}\,\frac{F_{5/2}(z)}{F_{3/2}(z)} = \frac{10\tau}{9}\,\frac{F_{1/2}(z)F_{5/2}(z)}{F_{3/2}(z)^2}\,\frac{(ne)^2}{n}.$$

Since $D_{10} = (5/3)\tau(ne)T$, these formulas allow us to compute

$$F_0(g) = \frac{D_{00}}{g_0}\lambda_1 = -\frac{F_{1/2}(z)}{F_{3/2}(z)}\,\frac{1}{T}, \quad F_1(g) = \frac{D_{10}}{g_1}\lambda_1 = -\frac{F_{3/2}(z)}{F_{5/2}(z)}\,\frac{1}{T},$$

which proves the current relations. □

Remark 11 (Energy-dependent relaxation time). Above, we have assumed that the relaxation time in (19) is constant. Different energy-transport models can be derived by assuming that the relaxation time depends on the macroscopic energy,

$$\tau = \tau_0\Big(\frac{\langle \varepsilon\mathcal{F}_F\rangle}{\langle \mathcal{F}_F\rangle}\Big)^{-\beta},$$

or on the microscopic energy, $\tau = \tau(\varepsilon) = \tau_0\varepsilon^{-\beta}$, where $\beta \geq 0$. We refer to [22, Remark 8.9] and leave the details to the reader. □

Remark 12 (Limits $\eta \to 0$ and $\eta \to \infty$). In the *Maxwell-Boltzmann limit* $\eta \to 0$, the diffusion coefficients and the energy density become, using (22),

$$D_{00} = \tau nT, \quad D_{01} = D_{10} = \frac{5}{2}\tau nT^2, \quad D_{11} = \frac{35}{4}\tau nT^3, \quad ne = \frac{3}{2}nT,$$

which are exactly the expressions derived in [23, Example 3.4]. The current densities read as

$$J_0 = -\tau\big(\nabla(nT) - n\nabla V\big), \quad J_1 = -\frac{5}{2}\tau\big(\nabla(nT^2) - nT\nabla V\big).$$

For the *degeneracy limit* $\eta \to \infty$, we rescale the variables and introduce $n_s = \eta n$, $(ne)_s = \eta(ne)$, $T_s = (\log\eta)T$, $J_{i,s} = \eta J_i$, and $g_{i,s} = \eta g_i$ for $i = 0, 1$. Then, employing (23),

$$n \sim N_1T^{3/2}\eta^{-1}(\log\eta)^{3/2}, \quad ne \sim \frac{3}{5}N_1T^{5/2}\eta^{-1}(\log\eta)^{5/2} \quad \text{as } \eta \to \infty,$$

where $N_1 = 8\sqrt{2}\pi/3$, and we obtain in the limit $\eta \to \infty$ the relations $n_s = N_1T_s^{3/2}$ and $(ne)_s = \frac{3}{5}N_1T_s^{5/2} = \frac{3}{5}n_sT_s$. Notice that the limiting energy density differs from its Maxwell-Boltzmann limit $ne = \frac{3}{2}nT$ by a factor. Since

$$\frac{F_{1/2}(z)}{F_{3/2}(z)} \sim \frac{5}{2\log\eta},$$

the particle current density can be written in the limit $\eta \to \infty$ as

$$J_{0,s} = -\nabla g_{0,s} + \frac{5}{2}\,\frac{g_{0,s}}{T_s}\nabla V.$$

Furthermore, since $g_{0,s} = \frac{2}{3}\tau(ne)_s = \frac{2}{5}N_1^{-2/3}\tau n_s^{5/3}$ and $\frac{2}{5}N_1^{-2/3} = N_0$ (see Remark 9 for the definition of N_0), we conclude that

$$J_{0,s} = -\tau\big(N_0\nabla(n_s^{5/3}) - n_s\nabla V\big),$$

which equals the degeneracy limit (26). Since the temperature T_s is completely determined by the density n_s, the energy equation becomes obsolete, and the energy-transport model reduces to the degenerate drift-diffusion equations (26). $\square$

4.3. Extended energy-transport model

The balance equations (8) and current relations (17) for $N = 2$ read as

$$\begin{aligned}
&\partial_t m_0 + \operatorname{div} J_0 = 0,\\
&\partial_t m_1 + \operatorname{div} J_1 - J_0\cdot\nabla V = W_1,\\
&\partial_t m_2 + \operatorname{div} J_2 - 2J_1\cdot\nabla V = W_2,\\
&J_i = -\nabla g_i - \Big(\frac{D_{i0}}{g_i}\lambda_1 + 2\frac{D_{i1}}{g_i}\lambda_2\Big)g_i\nabla V, \quad i = 0,1,2.
\end{aligned}$$

The variables g_i and the diffusion coefficients D_{ij} are given by

$$g_i = \frac{8\sqrt{2}\pi\tau}{3\eta}\int_0^\infty \frac{\varepsilon^{i+3/2}d\varepsilon}{1+\exp(-\lambda_0-\log\eta-\lambda_1\varepsilon-\lambda_2\varepsilon^2)}, \quad D_{ij} = \frac{\partial g_{i+j}}{\partial\lambda_0}.$$

Interestingly, the current equations can be expressed in terms of m_i only. An integration by parts yields

$$\begin{aligned}
m_i &= \frac{4\sqrt{2}\pi}{\eta}\int_0^\infty \frac{\varepsilon^{i+1/2}d\varepsilon}{1+\exp(-\lambda_0-\log\eta-\lambda_1\varepsilon-\lambda_2\varepsilon^2)}\\
&= \frac{4\sqrt{2}\pi}{\eta}\int_0^\infty \frac{2}{2i+3}\,\frac{d}{d\varepsilon}(\varepsilon^{i+3/2})\frac{d\varepsilon}{1+\exp(-\lambda_0-\log\eta-\lambda_1\varepsilon-\lambda_2\varepsilon^2)}\\
&= -\frac{4\sqrt{2}\pi}{\eta}\int_0^\infty \frac{2}{2i+3}(\lambda_1+2\lambda_2\varepsilon)\,\frac{\partial}{\partial\lambda_0}\,\frac{\varepsilon^{i+3/2}}{1+\exp(-\lambda_0-\log\eta-\lambda_1\varepsilon-\lambda_2\varepsilon^2)}d\varepsilon\\
&= -\frac{3}{(2i+3)\tau}\big(D_{i0}\lambda_1 + 2D_{i1}\lambda_2\big),
\end{aligned}$$

and, since $g_i = (2\tau/3)m_{i+1}$,

$$J_i = -\frac{2\tau}{3}\Big(\nabla m_{i+1} - \frac{3(2i+3)}{4}m_i\nabla V\Big), \quad i = 0,1,2.$$

This is the same expression as in the Maxwell-Boltzmann case, see [23, formula (4.5)]. The Fermi-Dirac statistics enter only through the relation between m_3 and $(\lambda_0,\lambda_1,\lambda_2)$ or, alternatively, (m_0,m_1,m_2). This model extends the six-moments model of Grasser et al. [16] to the Fermi-Dirac case.

Notice that, according to Section 2.1, the entropy maximization problem with $N = 2$ is solvable if the Kane dispersion relation (7) is employed, but it may be unsolvable in the parabolic band approximation. In order to justify the above derivation for parabolic bands, we derive the extended energy-transport model first for the band structure (7) and perform then the limit $\delta \to 0$, which leads to the above model.

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