A HIERARCHY OF DIFFUSIVE HIGHER-ORDER MOMENT EQUATIONS FOR SEMICONDUCTORS*

ANSGAR JÜNGEL[‡,†], STEFAN KRAUSE[‡], AND PAOLA PIETRA[§]

Abstract. A hierarchy of diffusive partial differential equations is derived by a moment method and a Chapman-Enskog expansion from the semiconductor Boltzmann equation assuming dominant elastic collisions. The moment equations are closed by employing the entropy maximization principle of Levermore. The new hierarchy contains the well-known drift-diffusion model, the energy-transport equations, and the six-moments model of Grasser et al. It is shown that the diffusive models are of parabolic type. Two different formulations of the models are derived: a drift-diffusion formulation, allowing for a numerical decoupling, and a symmetric formulation in generalized dual entropy variables, inspired by nonequilibrium thermodynamics. An entropy inequality (or H-theorem) follows from the latter formulation.

Key words. Semiconductor Boltzmann equation, moment method, Chapman-Enskog expansion, entropy maximization, energy-transport model, higher-order moments.

AMS subject classifications. 35Q35, 76P05, 82C35, 82D37.

1. Introduction. The semiconductor Boltzmann equation is of fundamental importance for the modeling of classical transport of charged carriers in solids. Its solution is the microscopic distribution function $f(x,p,t)$ depending on the spatial variable x, the (crystal) momentum p, and the time t. Macroscopic quantities, such as the particle density, current density, and energy density, can be computed from certain integrals over the momentum space, which are called moments. Since the numerical solution of the Boltzmann equation, by direct or Monte-Carlo methods, is extremely time-consuming and not suitable to simulate real problems in semiconductor production mode, approximate models have been derived, consisting of evolution equations for a certain number of moments of the distribution function.

The idea of the moment method is to multiply the Boltzmann equation by certain weight functions depending only on the momentum variable and to integrate over the momentum space. This leads (for a finite number of weight functions) to the so-called moment equations which are generally not closed, i.e., there are more moments than equations. This is called the closure problem. In order to obtain a closed set of equations, additional information are needed. Here, we use a diffusion scaling and follow the approach of Levermore [37] who closed the set of equations (essentially) by taking that distribution function in the definition of the moments, which maximizes the kinetic entropy under the constraints of given moments. This approach has been used also in [12]. In the context of semiconductor problems, entropy maximization

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†Institut für Analysis und Scientific Computing, Technische Universität Wien, Wiedner Hauptstr. 8-10, 1040 Wien, Austria (juengel@anum.tuwien.ac.at)

‡Institut für Mathematik, Universität Mainz, Staudingerweg 9, 55099 Mainz, Germany (krause@mathematik.uni-mainz.de)

§Istituto di Matematica Applicata e Tecnologie Informatiche, C.N.R., Via Ferrata 1, 27100 Pavia, Italy (pietra@dragon.ian.pv.cnr.it).

has been introduced in [3] (see also [2] for a complete list of references). We derive for the first time diffusive moment models of arbitrary order and for general collision operators.

Depending on the number of moments, one obtains a hierarchy of macroscopic equations. The lowest-order model is the standard drift-diffusion model, consisting of the mass conservation equation and a constitutive equation for the current density [40]. This model is often used in device simulations at an industrial level, but it cannot cope with hot-electron or high-field phenomena, occurring in modern ultrasmall devices. Hence, higher-order moments of the distribution function need to be included leading to hydrodynamic or diffusive systems of equations.

First we review the hydrodynamic-type models which are mathematically hyperbolic conservation laws [37]. These models are derived from the Boltzmann equation in the hydrodynamic scaling. As closure condition, an expansion of the distribution function around a heated Maxwellian using Hermite polynomials [21, 41] or using Grad's expansion [38] has been employed, which gives the so-called hydrodynamic equations [8], consisting of conservation laws for mass, momentum, and energy. The equations may be also closed by using the entropy maximization principle. When 13 moments are taken into account, the so-called extended hydrodynamic models have been derived [1, 4]. Hydrodynamic models of arbitrary order have been obtained in [44, 48]. Finally, we mention that recently, this approach has been generalized to (extended) quantum hydrodynamic models, which are obtained starting from the Wigner equation [16, 33].

Performing the diffusion limit in the Boltzmann equation, combined with the moment method, leads to diffusion-type moment equations. With the moments 1 and $\varepsilon(p)$, where $\varepsilon(p)$ is the carrier kinetic energy, energy-transport models [47] can be derived [6, 7]. These models consist of conservation laws of mass and energy and constitutive relations for particle and energy fluxes. They have been widely studied in the engineering as well as in the mathematical literature (see, e.g., [5, 11, 26, 39, 43, 49] for some engineering and [6, 13, 15, 19, 27, 28, 30] for some mathematical references). Energy-transport equations allow for the modeling of hot-electron effects. However, for ultrasmall devices, the numerical results are not sufficiently accurate compared to Monte-Carlo simulations of the Boltzmann equation.

Improved accuracy has been obtained by including further moments of the distribution function leading, for instance, to the six-moments model of Grasser et al. [23] (also see [46]). The six-moments model consists of conservation laws for mass, energy, and the so-called kurtosis and constitutive equations for the corresponding three fluxes. Compared to the extended hydrodynamic models, the advantage of this model is that it constitutes a system of parabolic equations instead of hyperbolic ones, which simplifies the numerical discretization and solution considerably. Up to now, the employed closure in the literature is only heuristic, and the determination of the flux relations is based on approximations [26]. Our approach does not need any approximation and works for general collision operators and general nonparabolic band structures.

More precisely, we derive, under suitable assumptions (see (H1)-(H4) below), diffusive higher-order moment models of the form

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

where m_i are the moments (m_0 being the particle density and m_1 the energy density), J_i are the fluxes, V the electric potential, and W_i are the averaged inelastic scattering

terms (with $W_0 = 0$). The fluxes are given by

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

where D_{ij} are the diffusion coefficients (coming from the elastic scattering processes) and λ_i are the Lagrange multipliers (coming from the constrained entropy maximization problem). The moments m_i depend nonlinearly on the Lagrange multipliers λ_j. Besides of our derivation, the main results of this paper are as follows:

- The diffusion matrix (D_{ij}) is symmetric and positive definite under some topological assumptions on the semiconductor band structure and the dependence of the moments m_i on λ_j is monotone in the sense of operators. Thus, the evolution problem is of parabolic type.
- The flux equations can be written equivalently in the drift-diffusion form

  $$J_i = -\nabla d_i - F_i(d) d_i \nabla V, \quad i = 0, \ldots, N,$$

  where $d_i = D_{i0}$ and $F_i(d)$ are nonlinear functions of $d = (d_0, \ldots, d_N)$ (see section 4.1 for details). This formulation allows for a numerical decoupling and the use of local Slotboom variables for designing a discretization scheme (see [15] and Remark 4.2 below).
- The convective parts including the electric field $-\nabla V$ can be eliminated by introducing generalized dual entropy variables $\nu = (\nu_0, \ldots, \nu_N)$, depending on the Lagrange multipliers and the electric potential, such that

  $$\partial_t \rho_i(\nu) + \mathrm{div} F_i = g_i, \quad F_i = -\sum_{j=0}^{N} C_{ij} \nabla \nu_j,$$

  where ρ_i depends on ν, g_i depends on W_j and $\partial_t V$, and the new diffusion matrix (C_{ij}) is symmetric and positive definite (see section 4.2 for details). This formulation is useful for the numerical discretization of the equations employing standard (mixed) finite elements [20]. Moreover, it extends the dual entropy notation known in nonequilibrium thermodynamics [17, 36].
- We are able to recover many well-known diffusion models, like the drift-diffusion, energy-transport, and six-moments models of Grasser et al. Compared to [25], no approximation of the highest-order moment is needed.

The originality of this paper consists in the facts (i) that we present for the first time a complete hierarchy of diffusion moment models for general collision operators, (ii) that we present a unifying approach of the derivation of these models, and (iii) that the derived models have very pleasant features useful for the mathematical analysis and the numerical discretization of the equations.

The paper is organized as follows. In section 2 we state our assumptions on the band structure and the collision operator and we derive the model equations by a Chapman-Enskog expansion. Furthermore, some properties and several examples of the diffusion matrix are given. In section 3 we show that the drift-diffusion, energy-transport, and six-moments models can be recovered from the general theory. Finally, section 4 is devoted to the drift-diffusion and dual-entropy formulation.

2. Derivation of the model equations. Let $B \subset \mathbb{R}^3$ be the first Brillouin zone of the semiconductor crystal under consideration. The set B is symmetric with

respect to the origin; hence, we can identify it with the three-dimensional torus. We assume throughout this paper that all variables and functions are scaled. The evolution of the charged particles in the semiconductor is described by a distribution function $f(x,p,t) \geq 0$ depending on time $t > 0$ and space–crystal momentum variables $(x,p) \in \Omega \times B$, where $\Omega \subset \mathbb{R}^3$ is the semiconductor domain. The distribution function $f = f_\alpha$ is assumed to satisfy the (dimensionless) semiconductor Boltzmann equation in diffusion scaling,

$$\alpha^2 \partial_t f_\alpha + \alpha\big(u \cdot \nabla_x f_\alpha + \nabla_x V \cdot \nabla_p f_\alpha\big) = Q(f_\alpha). \tag{2.1}$$

The group velocity $u = u(p)$ is defined by $u = \nabla_p \varepsilon(p)$, where $\varepsilon(p)$ is the kinetic carrier energy given by the band structure of the semiconductor crystal. The function $V = V(x,t)$ denotes the electric potential which is assumed to be given or to be determined from the Poisson equation

$$\lambda^2 \Delta V = \int_B f dp - C(x),$$

where $\lambda > 0$ is the (scaled) Debye length and $C(x)$ the doping profile, modeling fixed charged background ions in the semiconductor crystal.

We assume that the inelastic collisions are weak compared to the elastic collisions in the sense that the collision operator $Q(f)$ can be decomposed into two parts according to

$$Q(f) = Q_{\rm el}(f) + \alpha^2 Q_{\rm in}(f),$$

where $Q_{\rm el}(f)$ and $Q_{\rm in}(f)$ denote the elastic and inelastic collision operators, respectively.

The Knudsen number $\alpha = \tau_0 v_0 / x_0$ represents the mean free path $\tau_0 v_0$ relative to the device dimension x_0, where τ_0 is the characterictic time between elastic scattering events, v_0 denotes a characteristic velocity, and x_0 is the diameter of the semiconductor crystal. Diffusion scaling assumes the time scale to be given by τ_0/α^2 [7].

In order to specify our assumptions on the collision operator, we need the so-called generalized Maxwellian introduced in the following subsection.

2.1. Entropy maximization. We define the (scaled) relative entropy for $f(x, p, t)$ by

$$H(f)(x,t) = -\int_B f(\log f - 1 + \varepsilon(p)) dp.$$

Here and in the following, we consider only scaled quantities. The generalized Maxwellian is defined as the maximizer of a certain constrained extremal problem. In order to define this problem, 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 impose the following assumptions on κ_i and ε:

(H1) Let $N \geq 1$. The weight functions $\kappa_i(p)$ $(i = 0, \ldots, N)$ and the kinetic energy $\varepsilon(p)$ are smooth and even in p. Moreover, $\kappa_0 = 1$ and $\kappa_1 = \varepsilon$.

The case $N = 0$ is treated in section 3.

EXAMPLE 2.1. Examples for the weight functions are

$$\kappa^{(1)} = (1, \varepsilon, \varepsilon^2, \varepsilon^3 \ldots), \quad \kappa^{(2)} = (1, \varepsilon, |u|^2, \varepsilon|u|^2, |u|^4, \varepsilon|u|^4, \ldots). \tag{2.2}$$

The kinetic energy may be given, for instance, in the parabolic band approximation, by $\varepsilon(p) = \frac{1}{2}|p|^2$. Clearly, in this case $\kappa^{(1)}$ and $\kappa^{(2)}$ coincide (up to multiplicative factors). 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 $\delta > 0$ is the nonparabolicity parameter. In terms of ε, we have

$$\varepsilon(p) = \frac{|p|^2}{1+\sqrt{1+2\delta|p|^2}} = \frac{1}{2\delta}\big(\sqrt{1+2\delta|p|^2}-1\big). \tag{2.3}$$

If $\delta = 0$, we recover the parabolic band approximation. The above examples for $\kappa^{(i)}$ and ε satisfy (H1).

We recall that, instead of Kane's dispersion relation, also the approximation $a\varepsilon(p)^b = |p|^2/2$ has been suggested, where the parameters a and b are fitted for different energy ranges [9] (see the discussion in [26, Sec. IV]). □

We set $\langle g\rangle = \int_B g(p)dp$ for a function $g(p)$ and we call the expressions $\langle\kappa_i f\rangle$ the *i-th moment* of f. Then we consider the constrained maximization problem

$$H(f^*) = \max\Big\{H(f) : \langle\kappa f(x,\cdot,t)\rangle = m(x,t) \text{ for } x\in\Omega,\ t>0\Big\}. \tag{2.4}$$

The solution of this problem, if it exists, is given by

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

where $\widetilde{\lambda} = (\widetilde{\lambda}_0,\ldots,\widetilde{\lambda}_N)$ are the Lagrange multipliers. Defining $\lambda_1 = \widetilde{\lambda}_1 - 1$ and $\lambda_i = \widetilde{\lambda}_i$ for all $i\neq 1$, we have the more compact formulation

$$f^*(x,p,t) = e^{\lambda(x,t)\cdot\kappa(p)}.$$

Remark 2.2. We notice that the mathematical solution of (2.4) is quite delicate. In [29], it has been shown that (2.4) can be uniquely solved whenever the multipliers $\widetilde{\lambda} = \widetilde{\lambda}(m)$ can be found. However, there are situations for which problem (2.4) has no solution. This is the case if the momentum space is unbounded and if the polynomial weight functions have super-quadratic growth at infinity [18, 31]. When the constraint of the highest degree is relaxed (as an inequality instead of an equality), the constrained maximization problem is always uniquely solvable [45]. In particular, the maximization problem can be uniquely solved if one of the following conditions holds:

1. General band structure: B is a bounded set and $\kappa = (1,\varepsilon,\varepsilon^2,\ldots)$.
2. Kane's nonparabolic band approximation: $B=\mathbb{R}^3$ and $\kappa = (1,\varepsilon,\varepsilon^2)$, where ε is given by (2.3). Notice that $\varepsilon(p)$ grows linearly with p at infinity such that $\kappa_i(p)$ is at most quadratic.
3. Kane's nonparabolic band approximation: $B=\mathbb{R}^3$ and $\kappa = (1,\varepsilon,|u|^2,\varepsilon|u|^2, |u|^4,\varepsilon|u|^4,\ldots)$, where ε is given by (2.3) [34]. Notice that the velocity $u=\nabla_p\varepsilon$ is bounded, and therefore, $\kappa_i(p)$ is at most quadratic.
4. Parabolic band approximation: $B=\mathbb{R}^3$ and $\kappa = (1,|p|^2/2)$. □

Given a function $f(x,p,t)$ with moments $m_i = \langle\kappa_i f\rangle = \int_B \kappa_i f dp$, we call the maximizer of (2.4) the *generalized Maxwellian* with respect to f, $f^* = M_f$. In view of the above comments, there are Lagrange multipliers λ_i such that

$$M_f = e^{\lambda\cdot\kappa}. \tag{2.5}$$

By definition, M_f and f have the same moments, i.e. $\langle \kappa_i M_f \rangle = \langle \kappa_i f \rangle = m_i$.

Below, we employ M_f to close the moment equations. This closure implicitly assumes nondegenerate Boltzmann statistics. For degenerate Fermi-Dirac statistics in the context of the energy-transport model, we refer to [6, 7]. Furthermore, it has been found that in certain semiconductor devices a mixture of hot and cold electrons exists and a superposition of two (Maxwellian-type) distribution functions has been proposed as a closure [24].

2.2. Assumptions on the collision operators. With the above definition of the generalized Maxwellian, we can state the following hypotheses on the elastic and inelastic collision operators.

(H2) For all functions $f(p)$ and all $i = 0, \ldots, N$, $\langle \kappa_i Q_{\rm el}(f) \rangle = 0$. Furthermore, the null space $N(Q_{\rm el})$ of $Q_{\rm el}$ consists of generalized Maxwellians, $N(Q_{\rm el}) = \{f : f = M_f\}$.

(H3) For all functions $f(p)$, it holds $\langle Q_{\rm in}(f) \rangle = 0$.

These hypotheses express the collisional invariants. For instance, for elastic collisions, since $\kappa_0 = 1$ and $\kappa_1 = \varepsilon$ by (H1), we have mass and energy conservation,

$$\langle Q_{\rm el}(f) \rangle = 0, \quad \langle \varepsilon Q_{\rm el}(f) \rangle = 0.$$

Additionally, we suppose conservation properties for all moments with respect to the chosen weight functions. Hypothesis (H3) simply expresses mass conservation for the inelastic collisions, which is physically reasonable. However, inelastic collisions generally do not conserve energy.

EXAMPLE 2.3. (i) Consider the relaxation-time operator

$$Q_{\rm el}(f) = \frac{1}{\tau}(M_f - f), \tag{2.6}$$

where $\tau > 0$ is the (possibly space- and time-dependent) relaxation time. This collision operator satisfies $\langle \kappa_i Q_{\rm el}(f) \rangle = 0$ for all f (since f and M_f have the same moments), and its null space consists of the functions $f = M_f$.

(ii) Let $N = 1$, $\kappa = (1, \varepsilon)$, and define the elastic collision operator

$$Q_{\rm el}(f) = Q_{\rm imp}(f) + Q_{\rm ee}(f)$$

as the sum of the impurity scattering operator $Q_{\rm imp}$ and the electron-electron binary collision operator $Q_{\rm ee}$,

$$\begin{aligned} Q_{\rm imp}(f)(p) &= \int_B \phi_{\rm imp}(p,p')\delta(\varepsilon' - \varepsilon)(f' - f)dp', \\ Q_{\rm ee}(f)(p) &= \int_B \phi_{\rm ee}(p,p',p_1,p_1')\delta(\varepsilon' + \varepsilon_1' - \varepsilon - \varepsilon_1)\delta_p(p' + p_1' - p - p_1) \\ &\quad \times (f'f_1' - ff_1)dp_1dp'dp_1', \end{aligned}$$

where $\phi_{\rm imp}$, $\phi_{\rm ee} > 0$ are transition rates, δ_p is the periodized delta distribution, and $f' = f(p')$, $f_1 = f(p_1)$, $f_1' = f(p_1')$ (see [7]). It has been shown in [7] that $\langle \kappa_i Q_{\rm el}(f) \rangle = 0$ and that the kernel of $Q_{\rm el}$ consists of the functions $M_f = e^{\lambda_0 + \lambda_1 \varepsilon}$, i.e. $Q_{\rm el}$ satisfies (H2).

(iii) Inelastic scattering may come from phonon collisions modeled by, for instance,

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

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 $\varepsilon' = \varepsilon(p')$ [6]. The number $N_{\rm ph}$ is the phonon occupation number and $\varepsilon_{\rm ph}$ is the phonon energy. An elementary computation shows that $\langle Q_{\rm ph}(f)\rangle = 0$, i.e. $Q_{\rm ph}$ satisfies (H3). □

2.3. Chapman-Enskog expansion. First we derive the balance equations.

PROPOSITION 2.4. *Let (H1)-(H3) hold and let f_α be a solution to the Boltzmann equation (2.1). We assume that the formal limits $F = \lim_{\alpha\to 0} f_\alpha$ and $G = \lim_{\alpha\to 0}(f_\alpha - M_{f_\alpha})/\alpha$ exist. Then the moments $m_i = \langle \kappa_i M_F\rangle$ and the fluxes $J_i = \langle u\kappa_i G\rangle$ and $I_i = \langle \nabla_p \kappa_i G\rangle$ are solutions of*

$$\partial_t m_i + \mathrm{div} J_i - \nabla V \cdot I_i = W_i, \quad i = 0,\ldots,N, \tag{2.7}$$

where $W_i = \langle \kappa_i Q_{\rm in}(F)\rangle$ are the averaged inelastic collision terms, $W_0 = 0$, and the divergence and gradient are to be taken with respect to x.

We notice that the definition of the moments is consistent with the notations in section 2.1 since $\langle \kappa_i M_F\rangle = \langle \kappa_i F\rangle$.

Proof. We multiply the Boltzmann equation (2.1) by the weight functions κ_i, integrate over the Brillouin zone B, and integrate by parts in the term involving the electric potential,

$$\alpha^2\partial_t\langle\kappa_i f_\alpha\rangle + \alpha\big(\mathrm{div}_x\langle u\kappa_i f_\alpha\rangle - \nabla_x V\cdot\langle\nabla_p\kappa_i f_\alpha\rangle\big) = \langle\kappa_i Q_{\rm el}(f_\alpha)\rangle + \alpha^2\langle\kappa_i Q_{\rm in}(f_\alpha)\rangle, \tag{2.8}$$

for $i = 0,\ldots,N$. Next, we perform the following Chapman-Enskog expansion (see, e.g., [10]):

$$f_\alpha = M_{f_\alpha} + \alpha g_\alpha. \tag{2.9}$$

This equation in fact defines g_α and, by assumption, $G = \lim_{\alpha\to 0} g_\alpha$. The generalized Maxwellian M_{f_α} is an even function in p, by hypothesis (H1), whereas $p\mapsto u(p)\kappa_i(p)$ and $p\mapsto\nabla_p\kappa_i(p)$ are odd functions in p. Therefore, $\langle u\kappa_i M_{f_\alpha}\rangle = 0$, $\langle\nabla_p\kappa_i M_{f_\alpha}\rangle = 0$. Then, substituting (2.9) into the moment equations (2.8), observing that the moments of $Q_{\rm el}(f_\alpha)$ vanish by (H2), and dividing the resulting equation by α^2, we obtain

$$\partial_t\langle\kappa_i M_{f_\alpha}\rangle + \alpha\partial_t\langle\kappa_i g_\alpha\rangle + \mathrm{div}_x\langle u\kappa_i g_\alpha\rangle - \nabla_x V\cdot\langle\nabla_p\kappa_i g_\alpha\rangle = \langle\kappa_i Q_{\rm in}(f_\alpha)\rangle.$$

Performing the formal limit $\alpha\to 0$ in this equation leads to

$$\partial_t\langle\kappa_i M_F\rangle + \mathrm{div}_x\langle u\kappa_i G\rangle - \nabla_x V\cdot\langle\nabla_p\kappa_i G\rangle = \langle\kappa_i Q_{\rm in}(F)\rangle. \tag{2.10}$$

These are the balance equations (2.7). □

REMARK 2.5. For $i = 0$, we have $I_0 = 0$ and $W_0 = 0$ such that the first balance equation just expresses mass conservation:

$$\partial_t m_0 + \mathrm{div} J_0 = 0. \tag{2.11}$$

EXAMPLE 2.6. The integrals I_i can be expressed in terms of the fluxes J_i for special choices of the weight functions. For instance, if we choose $\kappa = (1,\varepsilon,\varepsilon^2,\ldots)$ (see (2.2)), we obtain $\nabla_p\kappa_i = iu\varepsilon^{i-1}$ for $i\ge 1$ and $\nabla_p\kappa_0 = 0$ and thus $I_i = iJ_{i-1}$ for all $i\ge 0$ (for $i = 0$, we have $I_0 = 0$). In this situation the balance equations become

$$\partial_t m_i + \mathrm{div} J_i - i\nabla V\cdot J_{i-1} = W_i. \tag{2.12}$$

If we choose $\kappa = \kappa^{(2)}$ in (2.2), we cannot express I_i in terms of the integrals $J_0, \ldots, J_N$ since, for instance, $\nabla_p \kappa_2 = \nabla_p |u|^2 = \varepsilon'' u$, where ε'' is the Hessian of $\varepsilon(p)$, and this cannot be written in general as a function of $|u|^{2j}$ and $\varepsilon|u|^{2j}$. $\square$

Next, we specify the flux equations J_i. For this, we need to determine G. We will see that this is equivalent to solve the operator equation $LG = H$, where $L = DQ_{\rm el}(M_F)$ is the Fréchet derivative of $Q_{\rm el}$ at $M_F = e^{\lambda\cdot\kappa} > 0$ and $H = u \cdot \nabla_x M_F + \nabla_x V \cdot \nabla_p M_F$. We introduce the Hilbert space $L^2(B)$ with the scalar product

$$(g_1, g_2)_F = \int_B g_1 g_2 M_F^{-1} dp$$

and the corresponding norm $\|\cdot\|_F$. In order to solve the equation $LG = H$, we impose the following hypothesis on the operator L.

(H4) The linear operator $L = DQ_{\rm el}(M_F)$ is continuous, closed, and symmetric on $L^2(B)$ and its null space is spanned by M_F.

By the Fredholm alternative, the linear, continuous, and closed operator L on the Hilbert space $L^2(B)$ satisfies the following property: The equation $LG = H$ is solvable if and only if $H \in N(L^*)^\perp$ and its solution is unique in $N(L^*)^\perp$. As L is assumed to be symmetric, $LG = H$ is solvable if and only if $H \in N(L)^\perp$ and the solution is unique in $N(L)^\perp$. Since the null space of L consists of the generalized Maxwellians, $LG = H$ is solvable if and only if $0 = (H, M_F)_F = \int_B H dp$.

PROPOSITION 2.7. *Let (H1)-(H4) hold. Then the fluxes of Proposition 2.4 can be written as*

$$J_i = -\sum_{j=0}^N \big(D_{ij}\nabla\lambda_j + E_{ij}\nabla V \lambda_j\big), \quad i = 0, \ldots, N, \tag{2.13}$$

where the diffusion matrices $D_{ij} \in \mathbb{R}^{3\times 3}$ and the matrices $E_{ij} \in \mathbb{R}^{3\times 3}$ are defined by

$$D_{ij} = -\langle \kappa_i u \otimes \phi_j\rangle, \quad E_{ij} = -\langle \kappa_i u \otimes \psi_j\rangle, \tag{2.14}$$

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

$$L\phi_{jk} = u_k \kappa_j M_F, \quad L\psi_{j\ell} = \frac{\partial \kappa_j}{\partial p_\ell} M_F, \quad j = 0, \ldots, N, \ k, \ell = 1, 2, 3. \tag{2.15}$$

Proof. Inserting the Chapman-Enskog expansion (2.9) into the Boltzmann equation (2.1), expanding formally the elastic collision operator

$$Q_{\rm el}(f_\alpha) = Q_{\rm el}(M_{f_\alpha}) + \alpha DQ_{\rm el}(M_{f_\alpha}) g_\alpha + O(\alpha^2),$$

and dividing the resulting equation by α, we obtain

$$\begin{aligned}&\alpha\partial_t(M_{f_\alpha} + \alpha g_\alpha) + u\cdot\nabla_x(M_{f_\alpha} + \alpha g_\alpha) + \nabla_x V\cdot\nabla_p(M_{f_\alpha} + \alpha g_\alpha)\\ &\quad = \alpha^{-1} Q_{\rm el}(M_{f_\alpha}) + DQ_{\rm el}(M_{f_\alpha}) g_\alpha + O(\alpha).\end{aligned}$$

By (H2), we have $Q_{\rm el}(M_{f_\alpha}) = 0$. Hence, the formal limit $\alpha \to 0$ gives

$$u\cdot\nabla_x M_F + \nabla_x V\cdot\nabla_p M_F = DQ_{\rm el}(M_F)G = LG. \tag{2.16}$$

Now, let $j \in \{0,\dots,N\}$ be fixed. The operator equations (2.15) are solvable in $L^2(B)$ since $u_k\kappa_j M_F$ and $(\partial\kappa_j/\partial p_\ell)M_F$ are odd functions in p, and hence, their integrals over B vanish. The unique solution G in $N(L)^\perp$ is given by

$$G = \sum_{j=0}^N \big(\phi_j \cdot \nabla_x\lambda_j + \nabla_x V \cdot \psi_j\lambda_j\big),$$

since, observing $\nabla_x M_F = \sum_j \nabla_x\lambda_j\kappa_j M_F$ and $\nabla_p M_F = \sum_j \lambda_j\nabla_p\kappa_j M_F$, we have

$$\begin{aligned} LG &= \sum_{j=0}^N \big(L\phi_j \cdot \nabla_x\lambda_j + \nabla_x V \cdot L\psi_j\lambda_j\big) = \sum_{j=0}^N \big(\kappa_j u\cdot\nabla_x\lambda_j + \nabla_x V\cdot\nabla_p\kappa_j\lambda_j\big)M_F \\ &= u\cdot\nabla_x M_F + \nabla_x V\cdot\nabla_p M_F. \end{aligned}$$

Hence, since $J_i = \langle u\kappa_i G\rangle$, we obtain (2.13). □

Example 2.8. In the case of the relaxation-time operator of Example 2.3 (i), the function G can be found explicitly. Indeed, from Chapman-Enskog expansion (2.9) and Boltzmann equation (2.1), we derive

$$\begin{aligned} g_\alpha &= \frac{1}{\alpha}(f_\alpha - M_{f_\alpha}) = -\frac{\tau}{\alpha}Q_{\rm el}(f_\alpha) \\ &= -\tau\alpha(\partial_t f_\alpha - Q_{\rm in}(f_\alpha)) - \tau(u\cdot\nabla_x f_\alpha + \nabla_x V\cdot\nabla_p f_\alpha), \end{aligned}$$

and the formal limit $\alpha\to 0$ gives

$$G = -\tau\big(u\cdot\nabla_x M_F + \nabla_x V\cdot\nabla_p M_F\big) = -\tau\sum_{j=0}^N \big(\kappa_j u\cdot\nabla_x\lambda_j + \nabla_x V\cdot\nabla_p\kappa_j\lambda_j\big)M_F.$$

Thus, the solutions ϕ_j and ψ_j of (2.15) are

$$\phi_j = -\tau u\kappa_j M_F, \quad \psi_j = -\tau\nabla_p\kappa_j M_F. \quad \square \tag{2.17}$$

Lemma 2.9. *Let $\kappa_i = \varepsilon^i$, $i = 0,\dots,N$. Then the coefficients E_{ij} in (2.14) can be expressed in terms of D_{ij},*

$$E_{ij} = jD_{i,j-1}, \quad E_{i0} = 0, \quad j = 1,\dots,N. \tag{2.18}$$

Proof. The assumption $\kappa_i = \varepsilon^i$ gives $\nabla_p\kappa_{i+1} = (i+1)\varepsilon^i\nabla_p\varepsilon = (i+1)u\varepsilon^i$ and hence $L\psi_{i+1} = \nabla_p\kappa_{i+1}M_F = (i+1)L\phi_i$. By the unique solvability in $N(L)^\perp$, $\psi_{i+1} = (i+1)\phi_i + cM_F$ for all $i\ge 0$ and $\psi_0 = cM_F$, where c is a constant vector. Therefore,

$$E_{ij} = -\int_B \kappa_i u\otimes\psi_j dp = -j\int_B \varepsilon^i u\otimes\phi_{j-1}dp = jD_{i,j-1},$$

proving the lemma. □

2.4. Properties of the diffusion matrix. The diffusion matrix $D = (D_{ij})$ defined in (2.14) is symmetric; this expresses the Onsager principle [36].

Lemma 2.10. *The matrices $D = (D_{ij})$, $E = (E_{ij}) \in \mathbb{R}^{3(N+1)\times 3(N+1)}$ are symmetric in the sense*

$$D_{ij}^\top = D_{ji}, \quad E_{ij}^\top = E_{ji} \quad \textit{for all } i,j = 0,\dots,N.$$

Proof. We write $D_{ij} = (D_{ij}^{k\ell}) \in \mathbb{R}^{3\times 3}$. Since L is symmetric on $L^2(B)$, we have

$$\begin{aligned} D_{ij}^{k\ell} &= -(u_k\kappa_i M_F, \phi_{j\ell})_F = -(L\phi_{ik}, \phi_{j\ell})_F = -(\phi_{ik}, L\phi_{j\ell})_F \\ &= -(\phi_{ik}, u_\ell\kappa_j M_F)_F = D_{ji}^{\ell k}. \end{aligned}$$

The symmetry of E is proven in a similar way. □

Under additional assumptions on the derivative of the elastic collision operator and on the band structure, we can show that the diffusion matrix is positive definite.

(H5) Let the operator $-L = -DQ_{\rm el}(M_F)$ be coercive on $N(L)^\perp$, i.e., there exists a constant $\mu > 0$ such that for all $g \in N(L)^\perp$,

$$(-Lg, g)_F \geq \mu\|g\|_F^2.$$

Example 2.11. We claim that the relaxation-time operator (2.6) satisfies (H5) if the weight functions $\kappa_0, \ldots, \kappa_N$ are linearly independent. Let $g \in N(L)^\perp$. We show first that $M_g \in N(L)$. It is sufficient to prove that $M_{M_g} = M_g$. For this, let $M_g = e^{\lambda\cdot\kappa}$ and $M_{M_g} = e^{\widetilde{\lambda}\cdot\kappa}$. Since the moments of M_g and M_{M_g} coincide by construction, we have

$$\int_B \kappa(e^{\lambda\cdot\kappa} - e^{\widetilde{\lambda}\cdot\kappa})dp = 0 \quad \text{and} \quad \int_B (\lambda\cdot\kappa - \widetilde{\lambda}\cdot\kappa)(e^{\lambda\cdot\kappa} - e^{\widetilde{\lambda}\cdot\kappa})dp = 0.$$

By the strict monotonicity of $x \mapsto e^x$, the integrand vanishes and therefore, $(\lambda - \widetilde{\lambda})\cdot\kappa = 0$. Since $\kappa_0, \ldots, \kappa_N$ are linearly independent, $\lambda = \widetilde{\lambda}$. Hence, $M_{M_g} = M_g$ which proves that $M_g \in N(L)$. This property gives

$$(-Lg, g)_F = -\frac{1}{\tau}(M_g - g, g)_F = -\frac{1}{\tau}(M_g, g)_F + \frac{1}{\tau}\|g\|_F^2 = \frac{1}{\tau}\|g\|_F^2. \quad \square$$

Lemma 2.12. *Let (H5) hold and let $\{u_k\kappa_i : k = 1, 2, 3, i = 0, \ldots, N\}$ be linearly independent functions in p. Then the diffusion matrix $D = (D_{ij})$ is positive definite, i.e. for all $\xi_0, \ldots, \xi_N \in \mathbb{R}^{N+1}$, $(\xi_0, \ldots, \xi_N) \neq 0$,*

$$\sum_{i,j=0}^N \xi_i^\top D_{ij}\xi_j > 0.$$

Proof. The proof is inspired from the proof of Proposition IV.6 in [6]. We write as above $D_{ij} = (D_{ij}^{k\ell})$ and $\xi_i = (\xi_{ik})$. Let $(\xi_0, \ldots, \xi_N) \neq 0$. Then, by the definition of the matrices D_{ij},

$$\sum_{i,j=0}^N \xi_i^\top D_{ij}\xi_j = \sum_{i,j=0}^N \sum_{k,\ell=1}^3 \xi_{ik} D_{ij}^{k\ell}\xi_{j\ell} = -\sum_{i,j=0}^N \sum_{k,\ell=1}^3 \int_B \xi_{ik}\kappa_i u_k \phi_{j\ell}\xi_{j\ell} dp.$$

Since $\kappa_i u_k M_F = L\phi_{ik}$, we obtain

$$\begin{aligned}\sum_{i,j=0}^N \xi_i^\top D_{ij}\xi_j &= -\sum_{i,j=0}^N\sum_{k,\ell=1}^3 \int_B \xi_{ik} L\phi_{ik}\phi_{j\ell}\xi_{j\ell}M_F^{-1}dp \\ &= \sum_{i,j=0}^N\sum_{k,\ell=1}^3 \big(-L(\xi_{ik}\phi_{ik}),\xi_{j\ell}\phi_{j\ell}\big)_F \\ &= \Big(-L\Big(\sum_{i=0}^N\sum_{k=1}^3\xi_{ik}\phi_{ik}\Big),\sum_{i=0}^N\sum_{k=1}^3\xi_{ik}\phi_{ik}\Big)_F.\end{aligned}$$

As $\phi_{ik}\in N(L)^\perp$, assumption (H5) and the boundedness of L (with constant $c_L>0$) give

$$\begin{aligned}\sum_{i,j=0}^N \xi_i^\top D_{ij}\xi_j &\ge \mu\Big\|\sum_{i=0}^N\sum_{k=1}^3\xi_{ik}\phi_{ik}\Big\|_F^2 \ge \frac{\mu}{c_L^2}\Big\|L\Big(\sum_{i=0}^N\sum_{k=1}^3\xi_{ik}\phi_{ik}\Big)\Big\|_F^2 \\ &= \frac{\mu}{c_L^2}\Big\|\sum_{i=0}^N\sum_{k=1}^3\xi_{ik}u_k\kappa_i M_F\Big\|_F^2 = \frac{\mu}{c_L^2}\int_B\Big|\sum_{i=0}^N\sum_{k=1}^3\xi_{ik}u_k\kappa_i\Big|^2 M_F dp > 0,\end{aligned}$$

since the functions $u_k\kappa_i$ are linearly independent. □

The diffusion matrices D_{ij} can be simplified under additional assumptions.

PROPOSITION 2.13. *Let $\kappa_i=\varepsilon^i$, $i=0,\ldots,N$ and $Q_{\rm el}(f)=(M_f-f)/\tau$. Then the diffusion coefficients can be written as*

$$D_{ij}=\frac{\tau}{3}\int_B e(\tfrac12|p|^2)^{i+j}e'(\tfrac12|p|^2)^2|p|^2\exp\Big(\sum_{k=0}^N\lambda_k e(\tfrac12|p|^2)^k\Big)dp\,I,$$

where $\varepsilon(p)=e(\frac12|p|^2)$ and I is the unit matrix in $\mathbb{R}^{3\times3}$.

Clearly, we may identify the matrix D_{ij} with its diagonal elements and obtain the $(N\times N)$ matrix $D=(D_{ij})$.

Proof. Since the elastic collision operator is assumed to be a relaxation-time operator, the solution of the operator equation (2.15) is equal to $\phi_j=-\tau u\kappa_j M_F=-\tau\varepsilon^j\nabla_p\varepsilon M_F$ (see (2.17)). Thus, by definition (2.14),

$$D_{ij}=-\int_B\varepsilon^i\nabla_p\varepsilon\otimes\phi_j dp=\tau\int_B\varepsilon^{i+j}\nabla_p\varepsilon\otimes\nabla_p\varepsilon M_F dp.$$

Since $\nabla_p\varepsilon(p)=pe'(\frac12|p|^2)$, we obtain

$$D_{ij}=\tau\int_B e(\tfrac12|p|^2)^{i+j}e'(\tfrac12|p|^2)^2p\otimes pM_F dp.$$

The function $p\mapsto p\otimes p$ is odd in every off-diagonal element such that the above integral vanishes except for the diagonal elements. Since each diagonal element has the same value and $M_F=e^{\lambda\cdot\kappa}$, the expression for D_{ij} is proven. □

The diffusion coefficients can be further simplified under additional assumptions on the energy band structure. We consider three examples.

EXAMPLE 2.14. (Monotone energy band) Let the assumption of Proposition 2.13 hold. We suppose additionally that $e(\frac12|p|^2)$ is strictly monotone in $|p|$ and that

$e(0) = 0$ and $e(\infty) = \infty$. This allows to choose $B = \mathbb{R}^3$. Then, with spherical coordinates (ρ, θ, ϕ), for $i, j = 0, \ldots, N$,

$$D_{ij} = \frac{\tau}{3}\int_0^{2\pi}\int_0^{\pi}\int_0^{\infty} e(\tfrac{1}{2}\rho^2)^{i+j} e'(\tfrac{1}{2}\rho^2)^2\rho^4 \exp\Big(\sum_{k=0}^N \lambda_k e(\tfrac{1}{2}\rho^2)^k\Big)\sin\theta d\rho d\theta d\phi.$$

Now we perform the change of variables $\varepsilon = e(\frac{1}{2}\rho^2)$, setting $\gamma(\varepsilon) = \rho^2$. Then $d\rho = (\gamma'(\varepsilon)/2\sqrt{\gamma(\varepsilon)})d\varepsilon$ such that

$$D_{ij} = \frac{8\pi\tau}{3}\int_0^{\infty} \varepsilon^{i+j}\frac{\gamma(\varepsilon)^{3/2}}{\gamma'(\varepsilon)}\exp\Big(\sum_{k=0}^N \lambda_k\varepsilon^k\Big)d\varepsilon. \tag{2.19}$$

In the special case $N = 1$, the same diffusion coefficients have been derived in [6, (3.36), (4.17)]. Notice that the above transformation allows to simplify the expression for the moments:

$$\begin{aligned} m_i &= \int_B e(\tfrac{1}{2}|p|^2)^i \exp\Big(\sum_{k=0}^N \lambda_k e(\tfrac{1}{2}|p|^2)^k\Big)dp \\ &= 4\pi\int_0^{\infty} e(\tfrac{1}{2}\rho^2)^i \exp\Big(\sum_{k=0}^N \lambda_k e(\tfrac{1}{2}|p|^2)^k\Big)\rho^2 d\rho \\ &= 2\pi\int_0^{\infty} \varepsilon^i\sqrt{\gamma(\varepsilon)}\gamma'(\varepsilon)\exp\Big(\sum_{k=0}^N \lambda_k\varepsilon^k\Big)d\varepsilon, \end{aligned} \tag{2.20}$$

where $i = 0, \ldots, N$. □

EXAMPLE 2.15. (Nonparabolic band approximation) In the case of Kane's nonparabolic band approximation (2.3), we can further simplify the integrals (2.19) and (2.20). Since $\gamma(\varepsilon) = |p|^2 = 2\varepsilon(1 + \delta\varepsilon)$ and $\gamma'(\varepsilon) = 2(1 + 2\delta\varepsilon)$, we compute

$$D_{ij} = \frac{8\sqrt{2}\pi}{3}\tau\int_0^{\infty}\varepsilon^{i+j+3/2}\frac{(1+\delta\varepsilon)^{3/2}}{1+2\delta\varepsilon}\exp\Big(\sum_{k=0}^N\lambda_k\varepsilon^k\Big)d\varepsilon,$$

$$m_i = 4\sqrt{2}\pi\int_0^{\infty}\varepsilon^{i+1/2}(1+\delta\varepsilon)^{1/2}(1+2\delta\varepsilon)\exp\Big(\sum_{k=0}^N\lambda_k\varepsilon^k\Big)d\varepsilon, \quad i, j = 0, \ldots, N. \quad \square$$

EXAMPLE 2.16. (Parabolic band approximation) Setting $\delta = 0$ in the formulas of Example 2.15, we obtain

$$D_{ij} = \frac{8\sqrt{2}\pi}{3}\tau\int_0^{\infty}\varepsilon^{i+j+3/2}\exp\Big(\sum_{k=0}^N\lambda_k\varepsilon^k\Big)d\varepsilon,$$

$$m_i = 4\sqrt{2}\pi\int_0^{\infty}\varepsilon^{i+1/2}\exp\Big(\sum_{k=0}^N\lambda_k\varepsilon^k\Big)d\varepsilon, \quad i, j = 0, \ldots, N. \quad \square$$

3. Examples. In this section we derive the diffusive models for $N = 0$, leading to the drift-diffusion equations, the case $N = 1$, leading to the energy-transport model, and $N = 2$, leading to a higher-order model.

3.1. Drift-diffusion equations. We consider the case $N = 0$. Then $\kappa_0(p) = 1$ and the generalized Maxwellian reads $M_F = e^{\lambda_0 - \varepsilon(p)}$. The balance equation is given by (2.11). We need to compute the flux J_0 since in section 2.3, the case $N = 0$ was excluded. For this, we have to solve $LG = u \cdot \nabla_x \lambda_0 M_F + \nabla_x V \cdot \nabla_p M_F = u \cdot \nabla_x (\lambda_0 - V) M_F$. Let ϕ_0 be the unique solution in $N(L)^\perp$ of $L\phi_0 = uM_F$. It is not difficult to check that $G = \nabla_x(\lambda_0 - V) \cdot \phi_0$ solves the above operator equation. This shows that

$$J_0 = \langle uG \rangle = \langle u \otimes \phi_0 \rangle \nabla_x (\lambda_0 - V).$$

The flux can be written in terms of the particle density m_0. Indeed, since

$$m_0 = \int_B M_F dp = Ae^{\lambda_0}, \quad \text{where } A = \int_B e^{-\varepsilon(p)} dp > 0,$$

we obtain $\nabla_x \lambda_0 = (\nabla_x m_0)/m_0$ and hence,

$$J_0 = -D_0(\nabla_x m_0 - m_0 \nabla_x V), \quad \text{where } D_0 = -\frac{1}{m_0} \int_B u \otimes \phi_0 dp.$$

This gives the well-known drift-diffusion equations for the particle density $n = m_0$ and the current density $J = J_0$:

$$\partial_t n + \operatorname{div} J = 0, \quad J = D_0(\nabla n - n \nabla V).$$

We specify the diffusion matrix D_0 and the relation between m_0 and λ_0 in the following example.

Example 3.1. Under the assumptions of Example 2.14, we obtain for the expressions for $D_0 = D_{00}/m_0$ and m_0:

$$D_0 = \frac{8\pi}{3} \frac{\tau}{m_0} e^{\lambda_0} \int_0^\infty \varepsilon^{3/2} \frac{\gamma(\varepsilon)^{3/2}}{\gamma'(\varepsilon)} e^{-\varepsilon} d\varepsilon,$$
$$m_0 = 2\pi e^{\lambda_0} \int_0^\infty \sqrt{\gamma(\varepsilon)} \gamma'(\varepsilon) e^{-\varepsilon} d\varepsilon.$$

For nonparabolic bands $\gamma(\varepsilon) = 2\varepsilon(1 + \delta\varepsilon)$, this becomes

$$D_0 = \frac{8\sqrt{2}\pi}{3} \frac{\tau}{m_0} e^{\lambda_0} \int_0^\infty \varepsilon^{3/2} \frac{(1+\delta\varepsilon)^{3/2}}{1+2\delta\varepsilon} e^{-\varepsilon} d\varepsilon, \tag{3.1}$$
$$m_0 = 4\sqrt{2}\pi e^{\lambda_0} \int_0^\infty \varepsilon^{1/2} (1+\delta\varepsilon)^{1/2} (1+2\delta\varepsilon) e^{-\varepsilon} d\varepsilon, \tag{3.2}$$

and for parabolic bands, the formulas simplify to

$$m_0 = 4\sqrt{2}\pi e^{\lambda_0} \int_0^\infty \varepsilon^{1/2} e^{-\varepsilon} d\varepsilon = 4\sqrt{2}\pi e^{\lambda_0} \Gamma(\tfrac{3}{2}) = (2\pi)^{3/2} e^{\lambda_0}, \tag{3.3}$$
$$D_0 = \frac{8\sqrt{2}\pi}{3} \frac{\tau}{m_0} e^{\lambda_0} \int_0^\infty \varepsilon^{3/2} e^{-\varepsilon} d\varepsilon = \frac{4\tau}{3\sqrt{\pi}} \Gamma(\tfrac{5}{2}) = \tau, \tag{3.4}$$

where Γ is the Gamma function satisfying $\Gamma(\frac{1}{2}) = \sqrt{\pi}$ and $\Gamma(x+1) = x\Gamma(x)$. The expressions (3.3) and (3.4) coincide with the standard drift-diffusion model, see for instance [32, 40]. □

3.2. Energy-transport equations. We take $N = 1$ and $\kappa = (1, \varepsilon)$. Then $M_F = e^{\lambda_0 + \lambda_1 \varepsilon}$. The balance equations are, according to Proposition 2.4 and Example 2.6,

$$\partial_t m_0 + \mathrm{div} J_0 = 0, \quad \partial_t m_1 + \mathrm{div} J_1 - \nabla V \cdot J_0 = W_1. \tag{3.5}$$

The diffusion coefficients D_{ij} are, by (2.14),

$$D_{00} = -\langle u \otimes \phi_0 \rangle,\ D_{01} = -\langle u \otimes \phi_1 \rangle,\ D_{10} = -\langle \varepsilon u \otimes \phi_0 \rangle,\ D_{11} = -\langle \varepsilon u \otimes \phi_1 \rangle,$$

and the coefficients E_{ij} can be expressed in terms of D_{ij} according to (2.18),

$$E_{00} = E_{10} = 0, \quad E_{01} = D_{00}, \quad E_{11} = D_{01}.$$

Notice that $D_{01} = D_{10}$ since $\langle u \otimes \phi_1 \rangle = (L\phi_0, \phi_1)_F = (\phi_0, L\phi_1)_F = \langle \varepsilon u \otimes \phi_0 \rangle$. Then, the particle and energy current densities (2.13) can be written as follows:

$$J_0 = -D_{00}(\nabla \lambda_0 + \nabla V \lambda_1) - D_{01} \nabla \lambda_1, \tag{3.6}$$
$$J_1 = -D_{10}(\nabla \lambda_0 + \nabla V \lambda_1) - D_{11} \nabla \lambda_1, \tag{3.7}$$

and the moments are given by

$$m_0 = e^{\lambda_0} \int_B e^{\lambda_1 \varepsilon(p)} dp, \quad m_1 = e^{\lambda_0} \int_B \varepsilon(p) e^{\lambda_1 \varepsilon(p)} dp. \tag{3.8}$$

Equations (3.5)-(3.8) are called the energy-transport model.

Example 3.2. (Monotone energy band) In the situation of Example 2.14, we can make the above expressions more explicit. First, we remark that it must hold $\lambda_1 < 0$ in order to ensure the integrability of $M_F = e^{\lambda_0 + \lambda_1 \varepsilon(p)}$ in $B = \mathbb{R}^3$. Thus, we can define $T = -1/\lambda_1$ and we call $T > 0$ the particle temperature. Formulas (2.19) and (2.20) give

$$D_{ij} = \frac{8\pi}{3} \tau e^{\lambda_0} \int_0^\infty \varepsilon^{i+j} \frac{\gamma(\varepsilon)^{3/2}}{\gamma'(\varepsilon)} e^{-\varepsilon/T} d\varepsilon,$$
$$m_i = 2\pi e^{\lambda_0} \int_0^\infty \varepsilon^i \sqrt{\gamma(\varepsilon)} \gamma'(\varepsilon) e^{-\varepsilon/T} d\varepsilon, \quad i, j = 0, 1. \quad \square$$

Example 3.3. (Nonparabolic band approximation) For nonparabolic bands according to (2.3), i.e. $\gamma(\varepsilon) = 2\varepsilon(1 + \delta\varepsilon)$, we can specify the above formulas, as in Example 2.15:

$$D_{ij} = \frac{8\sqrt{2}\pi}{3} \tau e^{\lambda_0} \int_0^\infty \varepsilon^{i+j+3/2} \frac{(1+\delta\varepsilon)^{3/2}}{1+2\delta\varepsilon} e^{-\varepsilon/T} d\varepsilon,$$
$$m_i = 4\sqrt{2}\pi e^{\lambda_0} \int_0^\infty \varepsilon^{i+1/2} (1+\delta\varepsilon)^{1/2} (1+2\delta\varepsilon) e^{-\varepsilon/T} d\varepsilon, \quad i = 0, 1.$$

These expressions coincide with those in [15]. $\square$

Example 3.4. (Parabolic band approximation) For $\delta = 0$, the integrals of the previous example can be computed explicitly. Since

$$m_i = 4\sqrt{2}\pi e^{\lambda_0} \int_0^\infty \varepsilon^{i+1/2} e^{-\varepsilon/T} d\varepsilon = 4\sqrt{2}\pi e^{\lambda_0} T^{i+3/2} \Gamma(i + \tfrac{3}{2}), \tag{3.9}$$

we compute the moments

$$m_0 = (2\pi)^{3/2}T^{3/2}e^{\lambda_0}, \quad m_1 = \frac{3}{2}(2\pi)^{3/2}T^{5/2}e^{\lambda_0} = \frac{3}{2}m_0T.$$

Calling $n = m_0$ the particle density, $m_1 = \frac{3}{2}nT$ can be interpreted as the electron energy with the temperature T. The diffusion coefficients become

$$D_{ij} = \frac{8\sqrt{2}\pi}{3}\tau e^{\lambda_0}\int_0^\infty \varepsilon^{i+j+3/2}e^{-\varepsilon/T}d\varepsilon = \frac{8\sqrt{2}\pi}{3}\tau e^{\lambda_0}T^{i+j+5/2}\Gamma(i+j+\tfrac{5}{2}),$$

and computing the Gamma functions, we derive for $D = (D_{ij})$,

$$D = \tau nT\begin{pmatrix} 1 & \frac{5}{2}T \\ \frac{5}{2}T & \frac{35}{4}T^2 \end{pmatrix}.$$

The relaxation time τ may be defined as the inverse of the (averaged) collision rate which generally depends on the energy. For instance, we may take

$$\tau = \tau_0\Big(\frac{\langle M_F\rangle}{\langle \varepsilon M_F\rangle}\Big)^\beta,$$

where $\tau_0 > 0$ and $\beta \in \mathbb{R}$ [47]. Then $\tau = \tau_0(m_0/m_1)^\beta = (\frac{2}{3})^\beta\tau_0T^{-\beta}$, and the diffusion matrix can be written as

$$D = \Big(\frac{2}{3}\Big)^\beta\tau_0m_0T^{1-\beta}\begin{pmatrix} 1 & \frac{5}{2}T \\ \frac{5}{2}T & \frac{35}{4}T^2 \end{pmatrix}.$$

We observe that D is very similar to the matrix derived in [15] for $\beta = 1$ but the coefficients are different. The matrix of [15] can be obtained if the relaxation time depends on the microscopic kinetic energy, $\tau = \tau(\varepsilon) = \varepsilon_0/\varepsilon$ for some $\varepsilon_0 > 0$, such that

$$D_{ij} = \frac{8\sqrt{2}\pi}{3}e^{\lambda_0}\int_0^\infty \tau(\varepsilon)\varepsilon^{i+j+3/2}e^{-\varepsilon/T}d\varepsilon = \frac{8\sqrt{2}\pi\varepsilon_0}{3}e^{\lambda_0}T^{i+j+3/2}\Gamma(i+j+\tfrac{3}{2}),$$

which gives the matrix

$$D = \frac{2}{3}\varepsilon_0 n\begin{pmatrix} 1 & \frac{3}{2}T \\ \frac{3}{2}T & \frac{15}{4}T^2 \end{pmatrix}. \quad \square$$

3.3. Fourth-order moment equations. Finally, we consider the case $N = 2$ and $\kappa = (1, \varepsilon, \varepsilon^2)$. The coefficients are taken from Example 2.15, which uses the hypotheses of Proposition 2.13. The balance equations are given by (2.7) which, taking into account Example 2.6, read as

$$\partial_t m_0 + \mathrm{div} J_0 = 0, \tag{3.10}$$

$$\partial_t m_1 + \mathrm{div} J_1 - \nabla V\cdot J_0 = W_1, \tag{3.11}$$

$$\partial_t m_2 + \mathrm{div} J_2 - 2\nabla V\cdot J_1 = W_2, \tag{3.12}$$

where W_i are the averaged inelastic collision terms (see Proposition 2.4) and the fluxes are given by (2.13),

$$J_i = -D_{i0}(\nabla\lambda_0 + \nabla V\lambda_1) - D_{i1}(\nabla\lambda_1 + 2\nabla V\lambda_2) - D_{i2}\nabla\lambda_2, \quad i = 0, 1, 2.$$

The diffusion coefficients are expressed as in Example 2.15 with $N = 2$. In the limiting case $\delta \to 0$ we obtain the parabolic band approximation which allows for a more explicit formulation of the fourth-order model. Since the parabolic band approximation cannot be taken directly in the case $N = 2$ (the entropy maximization problem may be unsolvable; see Remark 2.2), we derive the model for $\delta = 0$ by taking formally the limit $\delta \to 0$ in the expressions for D_{ij} and m_i in Example 2.15. This leads to

$$m_i = 4\sqrt{2}\pi e^{\lambda_0}\int_0^\infty \varepsilon^{i+1/2}e^{\lambda_1\varepsilon+\lambda_2\varepsilon^2}d\varepsilon, \quad D_{ij} = \frac{8\sqrt{2}\pi}{3}\tau e^{\lambda_0}\int_0^\infty \varepsilon^{i+j+3/2}e^{\lambda_1\varepsilon+\lambda_2\varepsilon^2}d\varepsilon, \tag{3.13}$$

where $i, j = 0, 1, 2$. We must have $\lambda_2 < 0$ in order to guarantee integrability. Notice that we can express the diffusion coefficients in terms of the moments,

$$D_{ij} = \frac{2\tau}{3}m_{i+j+1}. \tag{3.14}$$

The moments m_j for $j \geq 3$ are defined as above. In section 4 we discuss several reformulations of this model and compare it with higher-order models in the literature.

4. Properties of the model equations. We suppose that (H1)-(H5) hold and that the weight functions are given by $\kappa_i = \varepsilon^i$, $i = 0, \ldots, N$. Then, by (2.12), (2.13) and (2.18), the higher-order moment model can be written as

$$\partial_t m_i + \mathrm{div} J_i - iJ_{i-1}\cdot\nabla V = W_i, \quad J_i = -\sum_{j=0}^N \big(D_{ij}\nabla\lambda_j + jD_{i,j-1}\nabla V\lambda_j\big), \tag{4.1}$$

where $i = 0, \ldots, N$, $D_{i,-1} = 0$, and the moments m_i and the Lagrange multipliers λ_j are related by the formula

$$m_i = \int_B \varepsilon(p)^i \exp\Big(\sum_{j=0}^N \varepsilon(p)^j\lambda_j\Big)dp. \tag{4.2}$$

In this section we show that these equations can be written in two different ways, which allows to recover some important properties of the model.

4.1. Drift-diffusion formulation. We can write the fluxes in a drift-diffusion formulation which allows a numerical decoupling of the stationary higher-order moment model.

PROPOSITION 4.1. *Let (H1)-(H5) and the assumptions of Lemma 2.12 hold and let $\kappa_i = \varepsilon^i$ for $i = 0, \ldots, N$. Then we can write*

$$J_i = -\nabla d_i - F_i(d)d_i\nabla V,$$

where $d_i = D_{i0}$, $d = (d_0, \ldots, d_N)^\top$, and

$$F_i(d) = \sum_{j=1}^N j\frac{D_{i,j-1}}{D_{i0}}\lambda_j, \quad i = 0, \ldots, N.$$

The Lagrange multipliers λ_j are implicitly given by the values of d_i,

$$d_i = -\langle \varepsilon^i u \otimes \phi_0 \rangle, \quad L\phi_0 = ue^{\lambda\cdot\kappa}.$$

The operator L is the linearization of the elastic collision operator, see (H4). The mapping $d = d(\lambda)$ can be inverted since $\det d'(\lambda) = \det D > 0$.

Proof. We claim that the first sum in the second equation in (4.1) equals ∇D_{0i}. Indeed, from

$$L(\nabla\phi_{jk}) = u_k\varepsilon^j \sum_{\ell=0}^N \nabla\lambda_\ell \varepsilon^\ell M_F = \sum_{\ell=0}^N \nabla\lambda_\ell u_k \varepsilon^{j+\ell} M_F = L\Big(\sum_{\ell=0}^N \nabla\lambda_\ell \phi_{j+\ell,k}\Big)$$

and the unique solvability in $N(L)^\perp$, we obtain the relation

$$\nabla\phi_j = \sum_{\ell=0}^N \nabla\lambda_\ell\phi_{j+\ell} + cM_F,$$

where c is a constant vector. Hence, by (2.14), setting $j = 0$,

$$\nabla D_{i0} = -\langle \varepsilon^i u \otimes \nabla\phi_0\rangle = -\sum_{\ell=0}^N \nabla\lambda_\ell \langle \varepsilon^i u \otimes \phi_\ell\rangle = -\sum_{\ell=0}^N \nabla\lambda_\ell D_{i\ell}.$$

Then (4.1) becomes

$$J_i = -\nabla D_{i0} - D_{i0}\nabla V \sum_{j=0}^N j\,\frac{D_{i,j-1}}{D_{i0}}\lambda_j,$$

showing the first assertion.

It remains to show that the determinant of the matrix $d'(\lambda)$ is positive. Since

$$L\Big(\frac{\partial\phi_{jk}}{\partial\lambda_\ell}\Big) = u_k\varepsilon^j \frac{\partial M_F}{\partial\lambda_\ell} = u_k\varepsilon^{j+\ell}M_F = L\phi_{j+\ell,k},$$

which gives $\partial\phi_0/\partial\lambda_\ell = \phi_\ell + cM_F$ and thus,

$$\frac{\partial D_{i0}}{\partial\lambda_\ell} = -\Big\langle \varepsilon^i u \otimes \frac{\partial\phi_0}{\partial\lambda_\ell}\Big\rangle = -\langle \varepsilon^i u\otimes\phi_\ell\rangle = D_{i\ell}, \tag{4.3}$$

the Jacobian of $d(\lambda)$ consists of the elements $\partial d_i/\partial\lambda_j = \partial D_{i0}/\partial\lambda j = D_{ij}$. The matrix $D = (D_{ij})$ is positive definite (see Lemma 2.12), and we have $\det d'(\lambda) = \det D > 0$. □

Remark 4.2. The decoupling of the higher-order moment model can be done as follows. Under the assumptions of the above proposition, the stationary model reads as

$$\mathrm{div} J_i = i\nabla V\cdot J_{i-1} + W_i, \quad J_i = -\nabla d_i - F_i(d)d_i\nabla V, \quad i = 0,\ldots,N.$$

We assume that V is given, and $W_i = W_i(d,V)$ may depend on d and V. We also write $J_i = J_i(d,V)$. During the iteration procedure, we may "freeze" the nonlinearities: Let $\widetilde{d}$ be given (e.g., from the previous iteration step) and consider the system

$$\mathrm{div} J_i(d,V) = i\nabla V\cdot J_{i-1}(d,V) + W_i(\widetilde{d},V), \quad J_i(d,V) = -\nabla d_i - F_i(\widetilde{d})d_i\nabla V.$$

This system is decoupled since each equation is a scalar elliptic differential equation for d_i. Furthermore, the linear equations can by "symmetrized" by local Slotboom variables as described, for instance, in [15] in order to treat the convective part $F_i(\widetilde{d})d_i\nabla V$. Finally, the "symmetrized" equations can be numerically discretized by mixed finite elements [15, 28]. We will numerically explore this idea for a higher-order moment model in a future paper. □

EXAMPLE 4.3. (Energy-transport model) In the case of the energy-transport equations ($N = 1$), the functions $F_i(\lambda)$ in Proposition 4.1 simplify. Introducing the particle temperature $T = -1/\lambda_1$ as in Example 3.2, we obtain $F_0(d) = F_1(d) = \lambda_1 = -1/T$ and hence,

$$J_i = -\nabla d_i + \frac{d_i}{T}\nabla V, \quad i = 0, 1.$$

The temperature is implicitly defined through the relation

$$f(T) = \frac{d_1}{d_0} = \frac{D_{10}}{D_{00}} = \frac{\langle \varepsilon u \otimes \phi_0\rangle}{\langle u \otimes \phi_0\rangle},$$

where ϕ_0 solves $L\phi_0 = uM_F$. A similar expression has been given in [15] but only in the case of monotone energy bands. For given d_0 and d_1, this defines T uniquely since $f'(T) = \det D/(Td_0)^2 > 0$. In order to check this derivative, we first compute

$$L\Big(\frac{\partial\phi_0}{\partial T}\Big) = \frac{\partial}{\partial T}(ue^{\lambda_0-\varepsilon/T}) = \frac{1}{T^2}\varepsilon u M_F = \frac{1}{T^2}L\phi_1.$$

Hence, $\partial\phi_0/\partial T = \phi_1/T^2 + cM_F$, where c is a constant. Thus, since $\langle \varepsilon u\otimes\phi_0\rangle = D_{10} = D_{01} = \langle u\otimes\phi_1\rangle$ and $D_{11} = \langle \varepsilon u\otimes\phi_1\rangle$,

$$\begin{aligned} f'(T) &= \frac{1}{T^2d_0^2}\big(\langle\varepsilon u\otimes\phi_1\rangle\langle u\otimes\phi_0\rangle - \langle\varepsilon u\otimes\phi_0\rangle\langle u\otimes\phi_1\rangle\big) \\ &= \frac{1}{T^2d_0^2}(D_{11}D_{00} - D_{10}D_{01}) = \frac{\det D}{T^2d_0^2} > 0. \quad \square \end{aligned}$$

EXAMPLE 4.4. (Fourth-order model) We take $N = 2$ and assume the parabolic band approximation. The functions $F_i(d)$ read as follows:

$$F_i(d) = \lambda_1 + 2\frac{d_{i+1}}{d_i}\lambda_2, \quad i = 0, 1, 2.$$

Notice that, by (3.14), $d_i = (2\tau/3)m_{i+1}$. Moreover, integration by parts gives, using (3.13),

$$\begin{aligned} m_i &= -4\sqrt{2}\pi e^{\lambda_0}\int_0^\infty \frac{2}{2i+3}\varepsilon^{i+3/2}(\lambda_1 + 2\lambda_2\varepsilon)e^{\lambda_1\varepsilon+\lambda_2\varepsilon^2}d\varepsilon \\ &= -\frac{2}{2i+3}(\lambda_1 m_{i+1} + 2\lambda_2 m_{i+2}) = -\frac{3}{(2i+3)\tau}(\lambda_1 d_i + 2\lambda_2 d_{i+1}). \end{aligned} \tag{4.4}$$

Hence,

$$F_i(d) = \frac{1}{d_i}(\lambda_1 d_i + 2\lambda_2 d_{i+1}) = -\frac{(2i+3)\tau}{3}\,\frac{m_i}{d_i},$$

and the fluxes become, for constant relaxation time,

$$J_i = -\nabla d_i - F_i(d) d_i \nabla V = -\frac{2}{3}\tau\Big(\nabla m_{i+1} - \frac{2i+3}{2} m_i \nabla V\Big), \quad i = 0, 1, 2. \tag{4.5}$$

Together with the balance equations (2.12), we obtain a system of three equations for the unknowns m_0, m_1, and m_2. If τ depends on x or t, the variables are τm_0, τm_1, and τm_2. In the expression for J_2, the moment m_3 is needed. However, it can be computed from m_0, m_1, and m_2 using the relation

$$m_3 = -\frac{1}{2\lambda_2}\Big(\frac{5}{2} m_1 + \lambda_1 m_2\Big), \tag{4.6}$$

which comes from (4.4), where λ_1, λ_2 are functions of $m = (m_0, m_1, m_2)$. The fourth-order model with the above current relations can be also seen as a system of parabolic equations in the variables m_1, m_2, and m_3; the particle density m_0 is then a function of m_1, m_2, and m_3.

It remains to show that the function $m(\lambda)$ with $\lambda = (\lambda_0, \lambda_1, \lambda_2)$ can be inverted. This comes from the fact that the matrix $m'(\lambda) = (m_{i+j})_{i,j} \in \mathbb{R}^{3\times 3}$ is positive definite (and hence, its determinant is positive) since it is equal to the Hessian of the strictly convex funtion

$$\lambda \mapsto m_0 = 4\sqrt{2}\pi\tau \int_0^\infty \varepsilon^{1/2} e^{\lambda_0 + \lambda_1\varepsilon + \lambda_2\varepsilon^2} d\varepsilon.$$

The final fourth-order model consists of the balance equations (3.10)-(3.12) and the current relations (4.5) in the variables m_1, m_2, and m_3. □

Remark 4.5. Grasser et al. have derived a related fourth-order model, called the six-moments transport equations (see (124)-(129) in [25]). The model equations are given by (3.10)-(3.12) and (4.5) where

$$m_0 = n, \quad m_1 = \frac{3}{2} nT, \quad m_2 = \frac{5\cdot 3}{4} nT^2 \beta_n. \tag{4.7}$$

Here, the variables are the particle density n, the electron temperature T, and the kurtosis β_n. This notation is inspired from the energy-transport model in the parabolic band approximation (see Example 3.4), where $m_2 = \frac{15}{4} nT^2$ (see (3.9)). In this sense, β_n measures the deviation from the heated Maxwellian $M_F = e^{\lambda_0 - \varepsilon/T}$. More generally, the kurtosis is defined by

$$\beta_n = \frac{3}{5}\frac{m_0 m_2}{m_1^2}.$$

By the Cauchy-Schwarz inequality,

$$\begin{aligned} m_1^2 &= 32\pi^2 e^{2\lambda_0}\Big(\int_0^\infty \varepsilon^{1/4}\varepsilon^{5/4} e^{\lambda_1\varepsilon+\lambda_2\varepsilon^2} d\varepsilon\Big)^2 \\ &\le 32\pi^2 e^{2\lambda_0}\int_0^\infty \varepsilon^{1/2} e^{\lambda_1\varepsilon+\lambda_2\varepsilon^2} d\varepsilon \int_0^\infty \varepsilon^{5/2} e^{\lambda_1\varepsilon+\lambda_2\varepsilon^2} d\varepsilon = m_0 m_2, \end{aligned}$$

we obtain the restriction $\beta_n \ge 3/5$.

Grasser et al. [25] define heuristically m_3 in terms of the lower-order moments by setting

$$m_3 = \frac{7\cdot 5\cdot 3}{8} nT^2 \beta_n^c, \tag{4.8}$$

where the constant exponent c is fitted from Monte-Carlo simulations of the Boltzmann equation, computing the numerical moment m_3^{MC}. It has been found that the choice $c=3$ gives the smallest deviation of the ratio m_3^{MC}/m_3 from the desired value one [25].

In the model derived in Example 4.4, m_3 is implicitly defined in terms of the lower-order moments, see (4.6). Using notation (4.7) and setting $\lambda_1=-1/T$ as in the energy-transport equations, we obtain from (4.6)

$$m_3=-\frac{15}{8}\frac{(1-\beta_n)nT}{\lambda_2}.$$

The expression (4.8) is obtained by setting $\lambda_2=-(1-\beta_n)/7T^2\beta_n^c$. Since it should hold $\lambda_2<0$, we conclude the restriction $\beta_n\le 1$. Together with the above condition, the kurtosis has to satisfy the inequality $3/5\le\beta_n\le 1$ [22]. Clearly, $\beta_n=1$ corresponds to the energy-transport case for which $\lambda_2=0$.

Thus, the model of Grasser et al. is contained in our model hierarchy with the heuristic choice $\lambda_2=-(1-\beta_n)/7T^2\beta_n^c$. $\square$

4.2. Dual entropy variable formulation. It is well known from non-equilibrium thermodynamics that the electric force terms in (4.1) can be removed by employing so-called dual entropy variables [17, 36]. Here, we extend this methodology to higher-order moment models by defining the (generalized) dual entropy variables $\nu=(\nu_0,\ldots,\nu_N)^\top$ by $\lambda=P\nu$, where $\lambda=(\lambda_0,\ldots,\lambda_N)^\top$ are the Lagrange multipliers (or the primal entropy variables), and the transformation matrix $P=(P_{ij})\in\mathbb{R}^{(N+1)\times(N+1)}$ is defined by

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

where $i,\ j=0,\ldots,N$. The dual-entropy formulation "symmetrizes" the system of equations [13]. It is well known that the existence of such variables is equivalent to the existence of an entropy functional [14, 35]. We need the following properties of the transformation matrix P.

LEMMA 4.6.

(i) The matrix $Q=(Q_{ij})$ given by $Q_{ij}=\binom{j}{i}a_{ij}V^{j-i}$ is the inverse of P.

(ii) For all $i,\ j=0,\ldots,N$,

$$\sum_{k=0}^N(j-k)P_{ik}Q_{kj}=-\sum_{k=0}^N(j-k)Q_{ik}P_{kj}=j\delta_{i,j-1}V,$$

where $j\delta_{i,j-1}=0$ for $j=0$.

(iii) For all $i=0,\ldots,N-1,\ j=1,\ldots,N$,

$$-jP_{i,j-1}+(i+1)P_{i+1,j}=0.$$

Proof. (i) By the definition of the coefficients a_{ij}, we have $\sum_k P_{ik}Q_{kj}=0$ for all $i>j$. Let $i<j$. Then

$$\begin{aligned}\sum_{k=0}^N P_{ik}Q_{kj}&=\sum_{k=i}^j(-1)^{i+k}\binom{k}{i}\binom{j}{k}V^{j-i}=V^{j-i}\sum_{k=i}^j(-1)^{i+k}\binom{j}{i}\binom{j-i}{k-i}\\&=V^{j-i}\binom{j}{i}\sum_{\ell=0}^{j-i}(-1)^\ell\binom{j-i}{\ell}=0.\end{aligned}$$

Furthermore, for $i=j$, we obtain

$$\sum_{k=0}^N P_{ik}Q_{ki} = \sum_{k=i}^i (-1)^{i+k}\binom{k}{i}\binom{i}{k} = 1.$$

(ii) The definition of a_{ij} yields $\sum_k (j-k)P_{ik}Q_{kj}=0$ for $i\geq j$. Next, let $i<j-1$. Then

$$\begin{aligned}\sum_{k=0}^N (j-k)P_{ik}Q_{kj} &= V^{j-i}\sum_{k=i}^{j-1}(j-k)(-1)^{i+k}\binom{k}{i}\binom{j}{k}\\ &= V^{j-i}\sum_{k=i}^{j-1}(-1)^{i+k}j\binom{j-1}{i}\binom{j-1-i}{k-i}\\ &= jV^{j-i}\binom{j-1}{i}\sum_{\ell=0}^{j-1-i}(-1)^\ell\binom{j-1-i}{\ell}=0.\end{aligned}$$

If $i=j-1$ then

$$\sum_{k=0}^N (j-k)P_{ik}Q_{kj} = V\sum_{k=j-1}^{j-1}(j-k)(-1)^{j-1+k}\binom{k}{j-1}\binom{j}{k} = V\binom{j-1}{j-1}\binom{j}{j-1} = jV.$$

The second equality is shown in a similar way.

(iii) For $i\geq j$ we have $P_{i,j-1}=0$ and $P_{i+1,j}=0$. If $i<j$ then

$$-jP_{i,j-1}+(i+1)P_{i+1,j} = (-1)^{i+j+1}V^{j-1-i}\Big(-j\binom{j-1}{i}+(i+1)\binom{j}{i+1}\Big)=0.$$

This shows the lemma. □

PROPOSITION 4.7. *Define the dual entropy variables $\nu=(\nu_0,\dots,\nu_N)^\top$, the transformed moments $\rho=(\rho_0,\dots,\rho_N)^\top$, and the thermodynamic fluxes $F=(F_0,\dots,F_N)^\top$ by*

$$\lambda = P\nu, \quad \rho = P^\top m \quad \textit{and} \quad F = P^\top J.$$

Then the model equations (4.1) *can be equivalently written as*

$$\partial_t\rho_i + \mathrm{div}F_i = (P^\top W + V^{-1}\partial_t VRm)_i, \quad F_i = -\sum_{j=0}^N C_{ij}\nabla\nu_i,$$

where $W=(0,W_1,\dots,W_N)^\top$, $R=(R_{ij})$ is given by $R_{ij}=(i-j)P_{ji}$, and the new diffusion matrix $C=(C_{ij})$ is defined by $C=P^\top DP$.

Notice that the new diffusion matrix C is symmetric and positive definite if and only if D is symmetric and positive definite (see Lemma 2.12).

Proof. First we prove the relation for the new fluxes. Employing the definitions $C=P^\top DP$ and $\nu=Q\lambda$ and the property $QP=I$ (I being the identity matrix), we

obtain

$$\begin{aligned}\sum_{j=0}^N C_{ij}\nabla\nu_j &= \sum_{j,k,\ell,n=0}^N P_{ki}D_{k\ell}P_{\ell j}\nabla(Q_{jn}\lambda_n)\\ &= \sum_{j,k,\ell,n=0}^N P_{ki}D_{k\ell}(P_{\ell j}Q_{jn}\nabla\lambda_n + P_{\ell j}\nabla Q_{jn}\lambda_n)\\ &= \sum_{k,\ell=0}^N P_{ki}D_{k\ell}\nabla\lambda_\ell + \sum_{k,\ell,n=0}^N P_{ki}D_{k\ell}\Big(\sum_{j=0}^N (n-j)P_{\ell j}Q_{jn}\Big)V^{-1}\nabla V\lambda_n,\end{aligned}$$

since $\nabla Q_{jn} = (n-j)V^{-1}\nabla V Q_{jn}$. Now, using Lemma 4.6 (ii),

$$\begin{aligned}\sum_{j=0}^N C_{ij}\nabla\nu_j &= \sum_{k,\ell=0}^N P_{ki}D_{k\ell}\nabla\lambda_\ell + \sum_{k,\ell,n=0}^N P_{ki}D_{k\ell}n\delta_{\ell,n-1}\nabla V\lambda_n\\ &= \sum_{k,n=0}^N P_{ki}(D_{kn}\nabla\lambda_n + nD_{k,n-1}\nabla V\lambda_n) = -\sum_{k=0}^N P_{ki}J_k = -F_i.\end{aligned}$$

Next we compute the transformed balance equations. By the definition of F_i,

$$\begin{aligned}\mathrm{div}F_i &= \sum_{j=0}^N \mathrm{div}(P_{ji}J_j) = \sum_{j=0}^N (P_{ji}\mathrm{div}J_j + \nabla P_{ji}\cdot J_j)\\ &= \sum_{j=0}^N P_{ji}(\mathrm{div}J_j - jJ_{j-1}\cdot\nabla V) + \sum_{j=0}^N(\nabla P_{ji}\cdot J_j + jP_{ji}J_{j-1}\cdot\nabla V). \qquad (4.9)\end{aligned}$$

We show that the second sum vanishes. Observing that $\nabla P_{ji} = (i-j)V^{-1}\nabla V P_{ji}$, we find

$$A := \sum_{j=0}^N(\nabla P_{ji}\cdot J_j + jP_{ji}J_{j-1}\cdot\nabla V) = \sum_{j=0}^N\big((i-j)P_{ji}V^{-1}\nabla V\cdot J_j + jP_{ji}J_{j-1}\cdot\nabla V\big).$$

Since the first sum can be rewritten, by Lemma 4.6 (ii), as

$$\begin{aligned}\sum_{j=0}^N (i-j)P_{ji}V^{-1}\nabla V\cdot J_j &= \sum_{j,k=0}^N (i-k)\delta_{jk}P_{ki}V^{-1}J_j\cdot\nabla V\\ &= \sum_{j,k,\ell=0}^N (i-k)P_{j\ell}Q_{\ell k}P_{ki}V^{-1}J_j\cdot\nabla V = \sum_{j,\ell=0}^N\Big(\sum_{k=0}^N(i-k)Q_{\ell k}P_{ki}\Big)P_{j\ell}V^{-1}J_j\cdot\nabla V\\ &= -\sum_{j,\ell=0}^N i\delta_{\ell,i-1}P_{j\ell}J_j\cdot\nabla V = -\sum_{j=0}^N iP_{j+1,i}J_j\cdot\nabla V,\end{aligned}$$

we obtain

$$A = \sum_{j=0}^{N-1}(-iP_{j,i-1} + (j+1)P_{j+1,i})J_j\cdot\nabla V = 0,$$

using Lemma 4.6 (iii). Hence, with the balance equations (4.1), (4.9) becomes

$$\mathrm{div}F_i = \sum_{j=0}^N P_{ji}(-\partial_t m_j + W_j). \tag{4.10}$$

We employ the definition $\rho = P^\top m$ to rewrite the first sum,

$$\begin{aligned}\sum_{j=0}^N P_{ji}\partial_t m_j &= \sum_{j=0}^N \big(\partial_t(P_{ji}m_j) - \partial_t P_{ji} m_j\big) \\ &= \partial_t\rho_i - V^{-1}\partial_t V\sum_{j=0}^N (i-j)P_{ji}m_j = \partial_t\rho_i - V^{-1}\partial_t V\sum_{j=0}^N R_{ij}m_j.\end{aligned}$$

This finishes the proof. □

Example 4.8. (Energy-transport model) The transformation matrix P and its inverse read in the case $N = 1$ as

$$P = \begin{pmatrix} 1 & -V \\ 0 & 1 \end{pmatrix}, \quad Q = \begin{pmatrix} 1 & V \\ 0 & 1 \end{pmatrix}$$

Defining the chemical potential μ by $\lambda_0 = \mu/T$, where $T = -1/\lambda_1 > 0$ is the particle temperature, the dual entropy variables $\nu = Q\lambda$ become (see, e.g. [13, 36])

$$\nu_0 = \lambda_0 + V\lambda_1 = \frac{\mu - V}{T}, \quad \nu_1 = \lambda_1 = -\frac{1}{T}.$$

The quantity $\mu - V$ is known as the *electro-chemical potential*. □

Example 4.9. (Fourth-order model) For $N = 2$, the transformation matrix is given by

$$P = \begin{pmatrix} 1 & -V & V^2 \\ 0 & 1 & -2V \\ 0 & 0 & 1 \end{pmatrix}.$$

Introducing the chemical potential and the temperature as in the previous example and the *second-order temperature* θ as in [23] by $\lambda_2 = -1/\theta T$, the dual entropy variables are

$$\nu_0 = \frac{\mu - V}{T} - \frac{V^2}{\theta T}, \quad \nu_1 = -\frac{1}{T} - \frac{2V}{\theta T}, \quad \nu_2 = -\frac{1}{\theta T}. \quad \square$$

The dual entropy formulation allows to prove entropy dissipation. We define the relative entropy H_0 by

$$H_0(t) = -\int_{\mathbb{R}^3} (m\cdot(\lambda - \bar\lambda) - m_0 + \bar m_0)dx \le 0,$$

where $\lambda = (\lambda_0, \ldots, \lambda_N)^\top$, $m = (m_0, \ldots, m_N)^\top$, and $\bar\lambda = (V, -1, 0, \ldots, 0)^\top$, $\bar m_0 = m_0(\bar\lambda)$ are the equilibrium values (since $e^{\bar\lambda\cdot\kappa} = e^{V-\varepsilon}$ is the equilibrium distribution function in the presence of an electric field). Notice that in the situation of Example 3.4 (i.e. $N = 1$), the relative entropy becomes

$$H = -\int_{\mathbb{R}^3}\Big(n\Big(\ln n - \frac{3}{2}\ln T - \frac{5}{2} - V\Big) + \frac{3}{2}nT + e^V\Big)dx.$$

PROPOSITION 4.10. *Assume that*

$$\int_{\mathbb{R}^3} W\cdot(\lambda-\bar\lambda)dx\le 0. \tag{4.11}$$

Then any (smooth) solution λ to the higher-order moment equations (4.1) *satisfies the entropy inequality*

$$-\frac{dH}{dt}+\int_{\mathbb{R}^3}\sum_{i,j=0}^N C_{ij}\nabla\nu_i\cdot\nabla\nu_j dx\le 0.$$

The second integral on the left-hand side is called *entropy dissipation*. Clearly, it is nonnegative if the diffusion matrix D is positive (semi-) definite. Thus, the entropy is nondecreasing in time.

Proof. We introduce the relative entropy density $h(\lambda)=-m\cdot(\lambda-\bar\lambda)+m_0-\bar m_0$. The moments are given by (4.2) such that $\partial m_0/\partial\lambda_i=m_i$ from which we obtain

$$\frac{\partial h}{\partial\lambda_i}=-\frac{\partial m}{\partial\lambda_i}\cdot(\lambda-\bar\lambda)-m_i+\frac{\partial m_0}{\partial\lambda_i}=-\frac{\partial m}{\partial\lambda_i}\cdot(\lambda-\bar\lambda)$$

and

$$\partial_t m\cdot(\lambda-\bar\lambda)=\sum_{i=0}^N\frac{\partial m}{\partial\lambda_i}\cdot(\lambda-\bar\lambda)\partial_t\lambda_i=-\sum_{i=0}^N\frac{\partial h}{\partial\lambda_i}\partial_t\lambda_i=-\partial_t h(\lambda). \tag{4.12}$$

The balance equations (4.1) are formally equivalent to (4.10); multiplying the latter equations by $\nu_i-\bar\nu_i$, where $\bar\nu=Q\bar\lambda$ and summing over $i=0,\ldots,N$, it follows

$$(P^\top\partial_t m)^\top(\nu-\bar\nu)+(\mathrm{div}F)^\top(\nu-\bar\nu)=(P^\top W)^\top(\nu-\bar\nu).$$

Integrating over x and employing the definition $\nu=Q\lambda$ gives

$$\int_{\mathbb{R}^3}\partial_t m^\top PQ(\lambda-\bar\lambda)dx+\int_{\mathbb{R}^3}\sum_{i,j=0}^N\mathrm{div}(C_{ij}\nabla\nu_j)(\nu_i-\bar\nu_i)dx=\int_{\mathbb{R}^3}W^\top PQ(\lambda-\bar\lambda)dx.$$

Finally, integrating by parts in the second integral, taking into account that $\nabla\bar\nu=0$, and using (4.12) yields

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

which proves the lemma. □

In [7, Lemma 4.11], it has been shown that assumption (4.11) on W holds for an inelastic phonon collision operator, in the case of the energy-transport model. This hypothesis also holds if

$$W_i=-\frac{1}{\tau_1}(m_i-\bar m_i),\quad\text{where }\bar m_i=m_i(\bar\lambda),$$

since

$$W\cdot(\lambda-\bar\lambda)=-\frac{1}{\tau_1}\sum_{i=0}^N\int_B(e^{\kappa\cdot\lambda}-e^{\kappa\cdot\bar\lambda})(\kappa\cdot\lambda-\kappa\cdot\bar\lambda)dp\le 0.$$

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