THEORETICAL AND APPLIED MECHANICS
Volume 42 (2015) Issue 4, 261–276 DOI: 10.2298/TAM1504261P

MOMENT CLOSURE HIERARCHIES FOR RAREFIED GASES

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Abstract. The paper proposes an approximate closure procedure for hierarchies of macroscopic equations for rarefied gases, derived as moment equations from the Boltzmann equation in kinetic theory of gases. The procedure is based upon application of the maximum entropy principle. If the exact minimizer is exploited, moments of the distribution function may diverge, unless the restriction on the structure of the moments is introduced. In this paper, a perturbative approach is proposed by restricting the set of admissible functions in the variational problem. This leads to an approximate minimizer, but the procedure can be applied to an arbitrary choice of the moments.

1. Introduction

Macroscopic models in continuum thermomecanics consist of the balance laws, which express physical conservation laws, and the constitutive relations, which describe the response of the particular medium. In modern continuum theories, it is mandatory that constitutive relations are compatible with the entropy inequality, i.e. entropy inequality has to be satisfied for any thermodynamic process which occurs in the medium. Typical examples are the constitutive relations for Newtonian viscous fluids and Fourier's law of heat conduction, leading to the so-called Navier-Stokes-Fourier (NSF) theory [1, 2].

Apart from the widespread acceptance of the NSF theory, there appears one important shortcoming: it does not predict unconditionally the finite speeds of propagation of disturbances. This paradox—often called the paradox of infinite pulse speeds—was successfully overcome within the framework of extended thermodynamics (ET), where the list of usual state variables (mass, momentum and energy density) was extended by the fluxes of momentum and energy [3]. Classical conservation laws were adjoined with balance laws—evolution equations—for the new state variables. The closure problem, which consists of determination of the new non-convective fluxes and the source terms, was resolved by the application

2010 *Mathematics Subject Classification:* 76P05; 82C40.
Key words and phrases: rarefied gases, moment equations, maximum entropy principle.

of the entropy principle in which the entropy flux was treated as constitutive quantity, as well.

Later development revealed formal equivalence between ET and the kinetic theory of monatomic gases [4]. Actually, extended models can be regarded as moment equations-evolution equations for the moments of distribution function derived from the Boltzmann equation. The closure, furnished through the application of entropy principle, appeared to be equivalent to Grad's closure procedure, obtained by approximating the distribution function in the form of Hermite polynomials [5].

The parallelism between continuum and kinetic theory can be transferred from the balance laws to the entropy inequality, as well. For a properly defined kinetic entropy, the celebrated H-theorem shows the dissipative character of the entropy functional, thus presenting a kinetic counterpart of the entropy inequality. Moreover, it shows that equilibrium distribution maximizes the entropy functional. This fact was extrapolated by Kogan [6] to non-equilibrium processes. To reach this goal, Kogan relied on the maximum entropy principle (MEP): the actual velocity distribution function is the one that maximizes the kinetic entropy, subject to the constraints that actually correspond to the state variables taken into account. If the state of the gas is described by the standard fields of mass, momentum and energy, the MEP recovers the equilibrium distribution. If, in addition to equilibrium variables (mass, momentum and energy), one takes into account the non-equilibrium ones—the stress tensor and the heat flux—the non-equilibrium velocity distribution function is obtained. In such a way, Grad's 13 moments distribution function was recovered within the framework of MEP.

Further efforts within ET yielded a particular framework, called molecular extended thermodynamics [3], which provided a general framework for the closure by MEP in the context of ET [7]. Furthermore, it was shown [4, 8, 9] that Lagrange multipliers, used to solve the constrained variational problem by MEP, correspond to the main field components used in exploitation of the entropy principle in ET. These findings were later put into a stringent mathematical form by Levermore [10].

Application of MEP in solving the moment closure led to an exact solution which is not always convergent. Physically appropriate solution required an expansion of the maximizer in the neighborhood of the equilibrium velocity distribution function—the Maxwellian—in order to obtain the convergent moments. To develop a non-perturbative procedure, Levermore [10] formalized the findings of [3] and introduced the additional requirement which imposed restriction on the choice of the moments. In such a way, some important cases were ruled out (e.g. the Grad's one). Since this closure appears to be too restrictive, our aim is to formalize (in the spirit of [10]) a perturbative approach to MEP ab initio, which will circumvent Levermore's restriction and facilitate arbitrary choice of moments.

The rest of the paper is organized as follows. First, a brief overview of Boltzmann equation, H-theorem and moment hierarchies will be given. After that, formal closure by the maximum entropy principle will be presented in the case of Euler's and Grad's equations. Levermore's exact closure will then be presented. Finally, the perturbative closure using MEP will be developed, which removes the restrictions present in the exact approach.

2. Boltzmann equation and moment hierarchies

In the kinetic theory of gases [11], the state of the gas is described statistically by the velocity distribution function $f : \mathbb{R} \times \mathbb{R}^3 \times \mathbb{R}^3 \to \mathbb{R}^+$, $f(t, \mathbf{x}, \mathbf{v})$, where $f(t, \mathbf{x}, \mathbf{v})\,\mathrm{d}\mathbf{x}\,\mathrm{d}\mathbf{v}$ presents the number of atoms at time t in the infinitesimal volume $\mathrm{d}\mathbf{x}\,\mathrm{d}\mathbf{v}$ of the phase space. The evolution of the velocity distribution function is described by the Boltzmann equation:

$$\partial_t f + \mathbf{v} \cdot \nabla_{\mathbf{x}} f = Q(f, f). \tag{2.1}$$

where $Q(f, f)$ represents the collision integral describing the mutual interaction between the particles. It acts only on $\mathbf{v}$-dependence of f locally, at each $(t, \mathbf{x})$. In the sequel, we shall use the velocity dependent functions $\phi(\mathbf{v})$ averaged over the velocity space, thus introducing the following notation:

$$\langle \phi \rangle = \int_{\mathbb{R}^3} \phi(\mathbf{v})\,\mathrm{d}\mathbf{v}.$$

It will be assumed that all the functions are measurable in all variables, i.e. that all integrals that appear in the sequel make sense.

An outstanding feature of the collision integral $Q(f, f)$ is the existence of the *collision invariants*:

$$\langle Q(f, f) \rangle = 0, \quad \langle \mathbf{v} Q(f, f) \rangle = \mathbf{0}, \quad \langle |\mathbf{v}|^2 Q(f, f) \rangle = 0. \tag{2.2}$$

They express conservation properties of the macroscopic quantities—the mass density, the momentum density and the energy density, respectively:

$$\langle f \rangle, \quad \langle \mathbf{v} f \rangle, \quad \Big\langle \frac{1}{2} |\mathbf{v}|^2 f \Big\rangle.$$

which are interpreted as moments of the distribution function. This leads to the recovery of macroscopic conservation laws of mass, momentum and energy from the Boltzmann equation (2.1):

$$\begin{aligned} &\partial_t \langle f \rangle + \nabla_{\mathbf{x}} \cdot \langle \mathbf{v} f \rangle = 0, \\ &\partial_t \langle \mathbf{v} f \rangle + \nabla_{\mathbf{x}} \cdot \langle \mathbf{v} \otimes \mathbf{v} f \rangle = \mathbf{0}, \\ &\partial_t \Big\langle \frac{1}{2} |\mathbf{v}|^2 f \Big\rangle + \nabla_{\mathbf{x}} \cdot \Big\langle \frac{1}{2} |\mathbf{v}|^2 \mathbf{v} f \Big\rangle = 0 \end{aligned} \tag{2.3}$$

Along with the reconstruction of macroscopic conservation laws, the Boltzmann equation recovers the entropy inequality, as well. For the entropy production functional $D(f)$:

$$D(f) := \langle \log f\, Q(f, f) \rangle \leqslant 0,$$

celebrated H-theorem claims that $D(f) \leqslant 0$ for any non-negative f, and that the following three statements are equivalent:

(1) for any $\mathbf{v} \in \mathbb{R}^3$, $Q(f, f) = 0$;
(2) entropy production vanishes, $D(f) = 0$;
(3) there exists $n > 0$, $\theta > 0$ and $\mathbf{u} \in \mathbb{R}^3$, such that:

$$f = \frac{n}{(2\pi\theta)^{3/2}} \exp\left\{ -\frac{|\mathbf{v} - \mathbf{u}|^2}{2\theta} \right\} =: f_M, \tag{2.4}$$

where f_M denotes the equilibrium velocity distribution (the so-called Maxwellian).

An immediate consequence of the entropy production inequality is the dissipation inequality:

$$\partial_t\langle f(\log f-1)\rangle+\nabla_{\mathbf{x}}\langle \mathbf{v}f(\log f-1)\rangle=\langle Q(f,f)\log f\rangle\leqslant 0.$$

Taking into account the mass balance law $(4)_1$, and defining the entropy density $H(f)$ and the entropy flux $J(f)$:

$$H(f):=\langle f\ \log f\rangle,\quad \mathbf{J}(f):=\langle \mathbf{v}\,f\ \log f\rangle,$$

the macroscopic entropy inequality can be recovered:

$$\partial_t H+\nabla_{\mathbf{x}}\mathbf{J}=D\leqslant 0.$$

An important distinction between the entropy inequality in continuum theories and the dissipation inequality in kinetic theory has to be stressed: in continuum theories the dissipation inequality is a postulate, while in kinetic theory it is a theorem drawn from the basic principles.

Our main concern will not be the Boltzmann equation itself, but the so-called moment hierarchies [4, 5, 10]. Let $\mathbb{M}$ be the finite-dimensional linear subspace of functions of $\mathbf{v}$, usually assumed to be polynomials, and let $M=\dim\mathbb{M}$ be its dimension. The basis of $\mathbb{M}$ consists of functions $m_i(\mathbf{v})$, $i=1,\dots,M$, which can be recast into the vector $\mathbf{m}(\mathbf{v})=(m_1(\mathbf{v}),\dots,m_M(\mathbf{v}))^T$, and used to define the *moments of the distribution function*:

$$\langle \mathbf{m}f\rangle=(\langle m_1 f\rangle,\dots,\langle m_M f\rangle)^T.$$

Evolution of the moments of the distribution function is determined by the transfer equations for moments—*moment equations*:

$$\partial_t\langle \mathbf{m}f\rangle+\nabla_{\mathbf{x}}\cdot\langle \mathbf{v}\mathbf{m}f\rangle=\langle \mathbf{m}Q(f,f)\rangle, \tag{2.5}$$

obtained by averaging the Boltzmann equation (2.1) over the velocity space, against the vector of basis functions of $\mathbb{M}$. They are often called the moment hierarchies since, in most physically relevant situations, the basis functions are polynomials with an increasing degree of velocities. In such a way, the Boltzmann equation is replaced, and in a certain sense approximated, by a finite set of macroscopic balance equations, i.e., the moment equations (2.5). Evolution of the state of the gas is then tracked by the evolution of the finite number of moments in the physical space, rather than the evolution of the distribution function itself in the phase space. In (2.5), $\langle \mathbf{m}f\rangle$ represent the densities, $\langle \mathbf{v}\mathbf{m}f\rangle=(\langle \mathbf{v}m_1 f\rangle,\dots,\langle \mathbf{v}m_M f\rangle)^T$ are the fluxes, and $\langle \mathbf{m}Q(f,f)\rangle=(\langle m_1 Q(f,f)\rangle,\dots,\langle m_M Q(f,f)\rangle)^T$ are the source terms (productions).

3. Formal closure by the maximum entropy principle

The moment hierarchy (2.5) can be regarded as a system of governing equations for the densities. However, this system is not closed and the moment closure problem arises—one has to express the densities, the fluxes and the productions as functions of M variables, usually chosen to be the densities themselves. This

problem is equivalent to the problem of derivation of constitutive relations in continuum theories.

It is a well known fact that physical entropy, either in macroscopic or in kinetic sense, attains the maximum in equilibrium. Moreover, it was shown by Boltzmann that the equilibrium distribution is the one which has the highest probability to occur. On the other hand, the velocity distribution function determines the state of the gas in the kinetic theory, but all the information we acquire about the system is the macroscopic one. The maximum entropy principle synthesizes these facts into a unifying procedure, and appears as a tool which resolves the moment closure problem. In the sequel, we shall demonstrate the application of MEP to the moment closure problem in equilibrium case, yielding the Euler's gas dynamics equations, and non-equilibrium 13 moments case, yielding the Grad's moment equations.

3.1. Euler's equations: the local equilibrium closure. Consider the physical entropy:

$$h = -k\langle f \log f\rangle, \tag{3.1}$$

and assume that the state of the gas is determined by the so-called equilibrium variables—the mass density ρ, the momentum density $\rho\mathbf{u}$ and the internal energy density $\rho\varepsilon$, defined as moments of the distribution function:

$$\rho = \langle mf\rangle; \quad \rho\mathbf{u} = \langle m\mathbf{v}f\rangle; \quad \rho\varepsilon = \left\langle \frac{1}{2}m|\mathbf{C}|^2 f\right\rangle. \tag{3.2}$$

In (3.1) and (3.2) k is the Boltzmann constant, m is the atomic mass of the gas, $\mathbf{u}$ is the mass average velocity, ε is the internal energy, and $\mathbf{C} = \mathbf{v} - \mathbf{u}$ is the peculiar velocity. Transfer equations for the moments (3.2) are, actually, the conservation laws of mass, momentum and energy (presented using index notation and summation convention):

$$\begin{aligned}
&\frac{\partial\rho}{\partial t} + \frac{\partial}{\partial x_i}(\rho u_i) = 0\\
&\frac{\partial}{\partial t}(\rho u_j) + \frac{\partial}{\partial x_i}(\rho u_j u_i + p_{ji}) = 0\\
&\frac{\partial}{\partial t}\Big(\frac{1}{2}\rho|\mathbf{u}|^2 + \rho\varepsilon\Big) + \frac{\partial}{\partial x_i}\Big\{\Big(\frac{1}{2}\rho|\mathbf{u}|^2 + \rho\varepsilon\Big)u_i + p_{ji}v_j + q_i\Big\} = 0
\end{aligned} \tag{3.3}$$

In $(3.3)_{2,3}$ the non-convective fluxes appear:

$$p_{ij} = \langle mC_iC_jf\rangle; \quad q_i = \left\langle \frac{1}{2}m|\mathbf{C}|^2C_if\right\rangle,$$

that have the physical meaning of pressure (stress) tensor and heat flux, respectively. They are subject to the closure procedure, which will be achieved through MEP.

The maximum entropy principle emerges from the extremal property of the entropy in equilibrium. It can be expressed as a variational problem with constraints: find the distribution function f which maximizes the physical entropy, $h \to \max$, subject to constraints (3.2). The exact solution $\hat{f}_E$ of the problem is obtained using the method of Lagrange multipliers and reads:

$$\hat{f}_E = \exp\Big\{ -1 - \frac{m}{k}\Big[\lambda_E^{(0)} + \lambda_{iE}^{(1)} C_i + \frac{1}{2}\lambda_E^{(2)} |\mathbf{C}|^2\Big]\Big\},$$

where subscript E indicates that solution corresponds to the equilibrium constraints, while superscripts suggest the order of the moment (degree of velocity) corresponding to the multiplier. The multipliers are determined by the compatibility of $\hat{f}_E$ with the constraints (3.2), and eventually expressed in terms of the moments ρ, $\mathbf{u}$ and the kinetic temperature $T = (3m/2k)\varepsilon$. The final form of the distribution function as solution of the variational problem is:

$$\hat{f}_E = \frac{\rho/m}{(2\pi(k/m)T)^{3/2}} \exp\left\{ -\frac{|\mathbf{C}|^2}{2(k/m)T}\right\}. \tag{3.4}$$

This solution resolves the closure problem such that:

$$p_{ij} = \langle m C_i C_j \hat{f}_E\rangle = p \quad \delta_{ij},\ p = \rho\frac{k}{m}T; \quad q_i = \Big\langle \frac{1}{2} m |\mathbf{C}|^2 C_i \hat{f}_E \Big\rangle = 0,$$

where p is the pressure and δ_{ij} the Kronecker delta.

Two important remarks are in order. First, taking into account the definition of the peculiar velocity $\mathbf{C}$ and the relations $n = \rho/m$ and $\theta = (k/m)T$, by comparison of (3.4) and (2.4) it becomes evident that formally $\hat{f}_E = f_M$. In other words, the equilibrium distribution function is recovered by MEP. However, ρ, $\mathbf{u}$ and T need not be constants—they may be the functions of $(t, \mathbf{x})$. In such a way, the distribution function (3.4) is not an exact equilibrium distribution, but rather the local one (the local Maxwellian). This means that the state of the gas is locally, at every $(t, \mathbf{x})$, described by the Maxwellian distribution with ρ, $\mathbf{u}$ and T changing with t and $\mathbf{x}$. Consequently, $\hat{f}_E$ does not satisfy the Boltzmann equation (2.1) identically, and moments of the distribution function (3.2) can not be arbitrary. They have to satisfy Euler's equations (3.3).

3.2. Grad's equations: the non-equilibrium closure. Grad [5] developed the moment method and constructed the hierarchy of governing equations of balance type. One of the aims was to derive the set of equations which will capture the non-equilibrium processes (for other features, like hyperbolicity, one may consult [4]). The central role was played by the non-equilibrium approximation of the distribution function which comprised the finite number of moments.

Kogan [6] showed that the same distribution function can be obtained using MEP. The main difference with respect to the approximation at the Euler's level is concerned with the state variables—it is assumed that this set is extended with the pressure tensor p_{ij} and the heat flux q_i. In such a way, the complete set of constraints is consisted of 13 moments (the number of moments is reduced by 1 due to relation $p_{ii} = 2\rho\varepsilon$ valid for monatomic gases):

$$\rho = \langle m f\rangle; \quad \rho\mathbf{u} = \langle m\mathbf{v} f\rangle; \quad \rho\varepsilon = \Big\langle \frac{1}{2} m |\mathbf{C}|^2 f\Big\rangle; \tag{3.5}$$

$$p_{ij} = \langle m C_i C_j f\rangle; \quad q_i = \Big\langle \frac{1}{2} m |\mathbf{C}|^2 C_i f\Big\rangle.$$

Transfer equations for the moments (3.5) consist of mass, momentum and energy conservation laws (3.3) and the balance laws for pressure tensor and heat flux:

$$\frac{\partial}{\partial t}(\rho v_i v_j + p_{ij}) + \frac{\partial}{\partial x_k}\{\rho v_i v_j v_k + v_i p_{jk} + v_j p_{ki} + v_k p_{ij} + p_{ijk}\} = P_{ij};$$
$$\frac{\partial}{\partial t}\Big\{\Big(\frac{1}{2}\rho|\mathbf{v}|^2 + \rho\varepsilon\Big)v_i + p_{ij}v_j + q_i\Big\} + \frac{\partial}{\partial x_j}\Big\{\Big(\frac{1}{2}\rho|\mathbf{v}|^2 + \rho\varepsilon\Big)v_i v_j$$
$$+ v_i v_k p_{jk} + v_j v_k p_{ik} + \frac{1}{2}\rho|\mathbf{v}|^2 p_{ij} + q_i v_j + q_j v_i + p_{ijk}v_k + q_{ij}\Big\} = Q_i. \tag{3.6}$$

Note that in (3.6) the new non-convective fluxesappear , as well as the source terms:

$$p_{ijk} = \langle mC_iC_jC_kf\rangle; \qquad q_{ij} = \Big\langle\frac{1}{2}m|\mathbf{C}|^2C_iC_jf\Big\rangle;$$
$$P_{ij} = \langle mC_iC_jQ(f,f)\rangle; \qquad Q_i = \Big\langle\frac{1}{2}m|\mathbf{C}|^2C_iQ(f,f)\Big\rangle,$$

which are the subject of the closure procedure. The MEP now postulates that the actual non-equilibrium distribution function is the one which maximizes the physical entropy (3.1), $h \to \max$, subject to constraints (3.5).

The exact solution of the variational problem expressed by the MEP reads:

$$\hat{f}_{13} = \exp\Big\{-1 - \frac{m}{k}\Big[\lambda^{(0)} + \lambda_i^{(1)}C_i + \frac{1}{2}\lambda^{(2)}|\mathbf{C}|^2 + \lambda_{ij}^{(2)}C_iC_j + \frac{1}{2}\lambda_i^{(3)}|\mathbf{C}|^2C_i\Big]\Big\}. \tag{3.7}$$

The most important shortcoming of the exact solution (3.7) comes from the fact that the highest degree of velocity in the exponent is odd, thus the integrals over the velocity space diverge. The problem is resolved by the formal expansion of $\hat{f}_{13}$ in the neighborhood of local Maxwellian (3.4), leading to the following approximation:

$$\hat{f}_{13} \approx \hat{f}_E\Big\{1 - \frac{m}{k}\Big[\tilde{\lambda}^{(0)} + \tilde{\lambda}_i^{(1)}C_i + \frac{1}{2}\tilde{\lambda}^{(2)}|\mathbf{C}|^2 + \tilde{\lambda}_{ij}^{(2)}C_iC_j + \frac{1}{2}\tilde{\lambda}_i^{(3)}|\mathbf{C}|^2C_i\Big]\Big\},$$

where tilde denotes the difference between actual and equilibrium multiplier, e.g. $\tilde{\lambda}_i^{(1)} = \lambda_i^{(1)} - \lambda_{iE}^{(1)}$, and likewise for the others. It can be shown that 13 moments approximation of the distribution function then reads:

$$\hat{f}_{13} \approx \hat{f}_E\Big\{1 + \frac{2}{\rho}\Big(\frac{m}{2kT}\Big)^2\Big[p_{\langle ij\rangle}C_iC_j + \frac{4}{5}q_iC_i\Big(\frac{m}{2kT}|\mathbf{C}|^2 - \frac{5}{2}\Big)\Big]\Big\}, \tag{3.8}$$

where $p_{\langle ij\rangle} = p_{ij} - (1/3)p_{kk}\delta_{ij}$ is the deviatoric part of the pressure tensor. In such a way, approximate solution (3.8) of the variational problem becomes a perturbation of the equilibrium solution (3.4). Therefore, its validity is, in a certain sense, restricted to a neighborhood of local equilibrium state.

Taking the approximate non-equilibrium distribution (3.8), non-convective fluxes can be computed:

$$p_{ijk} = \langle mC_iC_jC_k\hat{f}_{13}\rangle = \frac{2}{5}(q_i\delta_{jk} + q_j\delta_{ki} + q_k\delta_{ij});$$
$$q_{ij} = \Big\langle\frac{1}{2}m|\mathbf{C}|^2C_iC_j\hat{f}_{13}\Big\rangle = \frac{7}{2}\frac{p}{\rho}p_{ij} - \frac{p^2}{\rho}\delta_{ij}.$$

The source terms can also be computed:

$$P_{ij} = \langle mC_iC_jQ(\hat{f}_{13},\hat{f}_{13})\rangle \approx -\frac{1}{\tau}p_{\langle ij\rangle}; \quad Q_i = \Big\langle\frac{1}{2}m|\mathbf{C}|^2C_iQ(\hat{f}_{13},\hat{f}_{13})\Big\rangle \approx \frac{2}{3\tau}q_i,$$

which completes the solution of the closure problem. Note that the source terms

are given above in the linearized form and that the structure of the term τ depends upon the model of interaction between the atoms (see [12] for the details, as well as for the nonlinear form of source terms).

Final remark about the formal application of MEP is concerned with the nature of the closure procedure. Although the objective is closure of the moment equations, i.e. the closure at macroscopic level, it is actually achieved at the kinetic level through approximation of the non-equilibrium distribution function. The approximate velocity distribution function has to contain finite number of parameters, equal to M—the dimension of the linear subspace $\mathbb{M}$. The finite-dimensional approximation of f can be obtained in different ways, MEP being one of the possibilities.

4. Maximum entropy principle and the exact moment closure

It was the intention of molecular extended thermodynamics to develop a systematic moment closure procedure, based upon the maximum entropy principle, that goes beyond Grad's 13 moments approximation. Basis of this approach was laid by Dreyer [7], while systematic exposition was given in [3]. Later development of the subject was rounded up mathematically by Levermore [10] with an emphasis on *exact closure*. In this section we shall recall the core ideas of the exact moment closure by MEP using Levermore's notation.

Formal closure procedure based upon MEP, although illustrated by particular examples, reveals certain general features of the approach, and of the method of moments itself as well. First, the basis of the linear subspace $\mathbb{M}$ in the case of Euler's equations is consisted of collision invariants (2.2), which corresponds to the equilibrium solution of the Boltzmann equation. Further inspection shows that linear space of Grad's equations contains the linear space of Euler's equations as a subspace—so-called *equilibrium subspace*. Second, it can be shown that moment equations in both cases are invariant with respect to Galilean transformations, just as Boltzmann equation is. Therefore, it is required that crucial properties of the Boltzmann equation—the existence of equilibrium solution and invariance with respect to Galilean transformations—have to be preserved and transferred to the moment equations (2.5) in general case. These requirements can be expressed as restrictions on the structure of $\mathbb{M}$:

(1) $\mathbb{M}$ contains the equilibrium subspace $\mathbb{E}$: $\mathbb{E} = \operatorname{span}\{1, \mathbf{v}, |\mathbf{v}|^2\} \subset \mathbb{M}$;
(2) $\mathbb{M}$ is invariant under $\mathcal{T}_u$ and $\mathcal{T}_o$,

where $\mathcal{T}_u$ and $\mathcal{T}_o$ denote the groups of translations and orthogonal transformations. Note that equilibrium subspace $\mathbb{E}$ produces the equilibrium macroscopic moments—mass, momentum and energy density (2.3)—which are contained in the local equilibrium velocity distribution (3.4). In the special case of Grad's 13 moments approximation, the linear subspace can be expressed as:

$$\mathbb{M}_{13} = \operatorname{span}\{1, \mathbf{v}, \mathbf{v} \otimes \mathbf{v}, |\mathbf{v}|^2, |\mathbf{v}|^2\mathbf{v}\}, \tag{4.1}$$

and obviously $\mathbb{E} \subset \mathbb{M}_{13}$.

As presented in previous Section, the core idea of MEP is to put the extremal properties of the kinetic entropy into a variational setting, taking into account

macroscopic information about the system. To put it in a general form, consider the linear subspace $\mathbb{M}$ of functions of $\mathbf{v}$ and let $\mathbf{m}(\mathbf{v}) \in \mathbb{R}^M$ be the vector of its basis functions. Therefore, MEP can be formulated as follows:

The actual approximate velocity distribution function for any process is the one which brings the entropy functional minimal value:

$$\langle f \log f - f \rangle \to \min, \tag{4.2}$$

and which is compatible with macroscopic information, taken as constraints, available through the moments of the distribution function:

$$\langle \mathbf{m} f \rangle = \boldsymbol{\rho}(t, \mathbf{x}) \in \mathbb{R}^M. \tag{4.3}$$

The variational problem (4.2)-(4.3) has an exact solution:

$$\hat{f} = \exp(m(\mathbf{v})); \quad m(\mathbf{v}) = \boldsymbol{\alpha} \cdot \mathbf{m}, \quad \boldsymbol{\alpha}(t, \mathbf{x}) \in \mathbb{R}^M \tag{4.4}$$

where $\boldsymbol{\alpha}(t, \mathbf{x})$ are the Lagrange multipliers, determined by the constraints (4.3):

$$\langle \mathbf{m} \hat{f} \rangle = \langle \mathbf{m} \exp(m(\mathbf{v})) \rangle = \boldsymbol{\rho}, \tag{4.5}$$

i.e. by the compatibility with macroscopic variables. However, the moments of the exact solution (4.4) may not be finite at all—the fact well-known from the earliest applications of the MEP. To avoid this problem, Levermore [10] introduced an additional requirement:

$$\langle \exp(m(\mathbf{v})) \rangle < \infty, \tag{4.6}$$

which restricts the structure of the linear subspace $\mathbb{M}$. Levermore's condition (4.6) has the following important consequences:

- $m(\mathbf{v}) = \boldsymbol{\alpha}(t, \mathbf{x}) \cdot \mathbf{m} \to -\infty$ as $|\mathbf{v}| \to \infty$
- linear spaces of polynomials must have even maximal degree; some examples of the admissible linear spaces are the following (more examples are given in [10]):

$$\mathbb{M} = \operatorname{span}\{1, \mathbf{v}, |\mathbf{v}|^2\} \equiv \mathbb{E}; \quad \mathbb{M} = \operatorname{span}\{1, \mathbf{v}, \mathbf{v} \otimes \mathbf{v}\};$$
$$\mathbb{M} = \operatorname{span}\{1, \mathbf{v}, \mathbf{v} \otimes \mathbf{v}, |\mathbf{v}|^2 \mathbf{v}, |\mathbf{v}|^4\}.$$

These consequences imply that the moment closure, restricted by (4.6), has non-perturbative character. However, weak point of this restriction is that it rules out some important linear subspaces, like Grad's one (4.1), since they have odd maximal degree.

Odd maximal degree of the linear subspace $\mathbb{M}$ leads to divergent moments of the distribution function (4.5). This physically inadmissible result can be avoided by expansion of the exact solution (4.4) in the neighborhood of local equilibrium velocity distribution (3.4). Strictly speaking, this kind of solution assumes decomposition of the linear subspace $\mathbb{M} = \mathbb{E} \oplus \mathbb{P}$, where $\mathbb{E}$ is the equilibrium subspace and $\mathbb{P}$ is the non-equilibrium, perturbative part of $\mathbb{M}$. The vector of basis functions can then be split in two parts:

$$\mathbf{m}(\mathbf{v}) = (\mathbf{m}_E(\mathbf{v}), \mathbf{m}_P(\mathbf{v}))^T; \quad \mathbf{m}_E(\mathbf{v}) = (1, \mathbf{v}, |\mathbf{v}|^2)^T,$$

which also leads to splitting of the exact solution (4.4):

$$\hat{f} = \exp(m_E(\mathbf{v}))\exp(m_P(\mathbf{v}));$$
$$m_E(\mathbf{v}) = \boldsymbol{\alpha}_E \cdot \mathbf{m}_E, \quad m_P(\mathbf{v}) = \boldsymbol{\alpha}_P \cdot \mathbf{m}_P.$$

The first element in the product, $\exp(m_E(\mathbf{v}))$, recovers the equilibrium distribution (3.4). Thus, convergence of the moments (4.5) is achieved by expansion of the second element in power series. Usually, the second element is linearized over $\mathbb{P}$ [6, 7]. This corresponds to Grad's solution of the moment closure problem. One may also go beyond the linear terms in power series and obtain the higher order macroscopic models [13]. In any case, power series expansion over $\mathbb{P}$ gives perturbative character to the solution obtained by MEP, and restricts it to the neighborhood of equilibrium one. On the other hand, it does not rule out the solutions obtained with constraints over the linear subspaces with odd maximal degree.

5. Perturbative moment closure

Non-perturbative moment closure does not impose restrictions on the set of admissible functions in the variational problem (4.2)-(4.3), but restricts the structure of the linear subspace $\mathbb{M}$. Since it is too restrictive, due to condition (4.6), the idea is to establish a framework for a perturbative solution of the variational problem which will avoid this restriction. Namely, instead of expanding the non-equilibrium part of the solution *a posteriori*, one may restrict the set of admissible functions over which the solution of the variational problem is sought and obtain convergent moments (4.3). This procedure is akin to the Ritz direct method of the calculus of variations [14]. It will be shown that restriction on the set of admissible functions, along with suitable smallness assumption, removes the necessity for the condition (4.6), and removes the restrictions on the linear subspace $\mathbb{M}$, as well.

The framework for the perturbative moment closure will be developed in three steps. The first step establishes the equilibrium solution. The second one constructs the perturbative non-equilibrium solution over suitably chosen set of admissible functions. To obtain the explicit form of the velocity distribution function, one has to determine the Lagrange multipliers as a part of the variational problem with constraints. This is made possible in the third step, by introducing the appropriate smallness assumption on the entropy functional.

5.1. Equilibrium solution. To determine the equilibrium solution, we shall formulate the variational problem in the equilibrium linear subspace $\mathbb{E}$. Find the velocity distribution function f, that minimizes the entropy functional:

$$\langle f \log f - f \rangle \to \min, \tag{5.1}$$

such that it is compatible with the macroscopic variables:

$$\langle \mathbf{m}_E f \rangle = \boldsymbol{\rho}_E(t, \mathbf{x}) \in \mathbb{R}^5, \quad \mathbf{m}_E = (1, \mathbf{v}, |\mathbf{v}|^2)^T. \tag{5.2}$$

The vector of equilibrium macroscopic (state) variables $\boldsymbol{\rho}_E$ comprises the mass density, the momentum density and the energy density:

$$\boldsymbol{\rho}_E = (\rho, \rho\mathbf{u}, \rho|\mathbf{u}|^2 + 2\rho\varepsilon)^T.$$

The variational problem with constraints (5.1)-(5.2) is solved using the method of Lagrange multipliers, and introducing the extended functional:

$$\langle f \log f - f - \boldsymbol{\lambda}_E \cdot \mathbf{m}_E f \rangle \to \min, \tag{5.3}$$

where $\boldsymbol{\lambda}_E$ is the vector of Lagrange multipliers. Exact solution of the variational problem (5.3) is:

$$\langle \log f_E - \boldsymbol{\lambda}_E \cdot \mathbf{m}_E \rangle = 0 \quad \Rightarrow \quad f_E = \exp(\boldsymbol{\lambda}_E \cdot \mathbf{m}_E), \tag{5.4}$$

while the multipliers are determined from the constraints (5.2):

$$\langle \mathbf{m}_E \exp(\boldsymbol{\lambda}_E \cdot \mathbf{m}_E) \rangle = \boldsymbol{\rho}_E. \tag{5.5}$$

The equilibrium solution (5.4), with Lagrange multipliers which satisfy (5.5), can be expressed in traditional form (3.4) [3, 6].

Note that (5.4)-(5.5) recovers the local Maxwellian distribution which does not satisfy the Boltzmann equation (2.1). However, f_E (or, actually, $\boldsymbol{\rho}_E$) satisfies the moment equations (2.5) that are reduced to:

$$\partial_t \langle \mathbf{m}_E f_E \rangle + \nabla_{\mathbf{x}} \cdot \langle \mathbf{v} \mathbf{m}_E f_E \rangle = \mathbf{0}.$$

5.2. Perturbative non-equilibrium solution. The non-equilibrium velocity distribution function is determined as solution of the variational problem:

$$\langle f \log f - f \rangle \to \min, \tag{5.6}$$

subject to:

$$\langle \mathbf{m} f \rangle = \boldsymbol{\rho}(t, \mathbf{x}) \in \mathbb{R}^M = \mathbb{R}^5 \times \mathbb{R}^{M-5}. \tag{5.7}$$

As indicated in the constraints (5.7), the basis of $\mathbb{M}$ and the vector of state variables are split into equilibrium and non-equilibrium part:

$$\mathbf{m} = (\mathbf{m}_E, \tilde{\mathbf{m}}), \quad \boldsymbol{\rho} = (\boldsymbol{\rho}_E, \tilde{\boldsymbol{\rho}}),$$

where $\tilde{\mathbf{m}}$ is the basis of the non-equilibrium part of $\mathbb{M}$, while $\tilde{\boldsymbol{\rho}}$ denotes the non-equilibrium state variables. The extended functional then reads:

$$\langle f \ \log f - f - \boldsymbol{\lambda} \cdot \mathbf{m} f \rangle \to \min, \tag{5.8}$$

where the vector of Lagrange multipliers $\boldsymbol{\lambda} = (\boldsymbol{\lambda}_E, \tilde{\boldsymbol{\lambda}})$ is also split into equilibrium and non-equilibrium part.

The principal novelty of our study consists of the introduction of the set of admissible functions $\mathcal{D}$. Namely, solution of the variational problem is usually sought in the whole space of measurable non-negative functions. Here, we restrict the solution space to the set of admissible functions of the form:

$$\mathcal{D} = \{ f = f_E(1 + \boldsymbol{\alpha} \cdot \mathbf{m}) : \langle f_E(1 + \boldsymbol{\alpha} \cdot \mathbf{m}) \rangle < \infty, \ \boldsymbol{\alpha} \in \mathbb{R}^M \}, \tag{5.9}$$

where f_E is the equilibrium function (5.4), and the vector $\boldsymbol{\alpha}$ is determined such that (5.8) is satisfied. First, it is obvious that $f_E \boldsymbol{\alpha} \cdot \mathbf{m}$ can be regarded as a perturbation of the equilibrium solution (5.4). Second, since $\mathbb{M}$ is usually the space of polynomials, the restriction $\langle f_E(1 + \boldsymbol{\alpha} \cdot \mathbf{m}) \rangle < \infty$, which replaces the condition (4.6), is practically always satisfied.

The variational problem (5.8) over the set of admissible functions (5.9) can be written as follows:

$$\phi(\boldsymbol{\alpha}) = \langle f_E(1+\boldsymbol{\alpha}\cdot\mathbf{m})\log[f_E(1+\boldsymbol{\alpha}\cdot\mathbf{m})] \\ - f_E(1+\boldsymbol{\alpha}\cdot\mathbf{m}) - \boldsymbol{\lambda}\cdot\mathbf{m} f_E(1+\boldsymbol{\alpha}\cdot\mathbf{m})\rangle \to \min.$$

It may be noticed that the variational problem (5.6)-(5.7) over the infinite-dimensional space of measurable functions is replaced by the finite-dimensional extremal problem over $\mathbb{R}^M$. In other words, one has to determine $\boldsymbol{\alpha}^*(t,\mathbf{x}) \in \mathbb{R}^M$ such that $\phi(\boldsymbol{\alpha}^*) = \phi_{\min}$. Since $\phi(\boldsymbol{\alpha})$ is smooth, the necessary condition for extremum reads:

$$\frac{\partial\phi}{\partial\boldsymbol{\alpha}} = \langle f_E\{\log[f_E(1+\boldsymbol{\alpha}\cdot\mathbf{m})] - \boldsymbol{\lambda}\cdot\mathbf{m}\}\mathbf{m}\rangle = \mathbf{0}. \tag{5.10}$$

The critical value of $\boldsymbol{\alpha}$ is determined by (5.10) only implicitly. Therefore, explicit form of the non-equilibrium velocity distribution can be obtained only if some additional assumptions are introduced.

5.3. The smallness assumption. The additional assumption, which will facilitate the construction of the explicit solution of the variational problem, is the smallness assumption. It was mentioned that $f_E\boldsymbol{\alpha}\cdot\mathbf{m}$ can be regarded as a perturbation of the equilibrium solution. It will be assumed now that this perturbation is small:

$$\langle f_E\log[f_E(1+\boldsymbol{\alpha}\cdot\mathbf{m})]\rangle = \langle f_E\log f_E\rangle + O(\epsilon), \quad \epsilon \ll 1$$

or, equivalently:

$$\langle f_E\log(1+\boldsymbol{\alpha}\cdot\mathbf{m})\rangle = O(\epsilon). \tag{5.11}$$

Taking (5.11) into account, we may approximate the log function:

$$\langle f_E\log(1+\boldsymbol{\alpha}\cdot\mathbf{m})\rangle = \langle f_E\,\boldsymbol{\alpha}\cdot\mathbf{m}\rangle + o(\epsilon),$$

and rewrite the necessary condition (5.10) in the approximate form:

$$\frac{\partial\phi}{\partial\boldsymbol{\alpha}} = \langle f_E\{\log f_E + \boldsymbol{\alpha}\cdot\mathbf{m} - \boldsymbol{\lambda}\cdot\mathbf{m}\}\mathbf{m}\rangle + o(\epsilon) = \mathbf{0}. \tag{5.12}$$

To exploit the equilibrium velocity distribution (5.4), we must embed the equilibrium Lagrange multipliers into the whole space $\mathbb{R}^M$:

$$f_E = \exp(\boldsymbol{\lambda}_E\cdot\mathbf{m}_E) \equiv \exp(\tilde{\boldsymbol{\lambda}}_E\cdot\mathbf{m}), \quad \tilde{\boldsymbol{\lambda}}_E = (\boldsymbol{\lambda}_E, \mathbf{0}),$$

so that (5.12) now reads:

$$\langle f_E\{[\boldsymbol{\alpha} - (\boldsymbol{\lambda} - \tilde{\boldsymbol{\lambda}}_E)]\cdot\mathbf{m}\}\mathbf{m}\rangle + o(\epsilon) = \mathbf{0}. \tag{5.13}$$

From (5.13) one obtains the explicit form of the approximate critical value of $\boldsymbol{\alpha}$:

$$\boldsymbol{\alpha} = \boldsymbol{\lambda} - \tilde{\boldsymbol{\lambda}}_E + o(\epsilon),$$

which leads to the approximate velocity distribution function in $\mathcal{D}$ as solution of the variational problem (5.7), (5.8):

$$\tilde{f} = f_E[1 + (\boldsymbol{\lambda} - \tilde{\boldsymbol{\lambda}}_E)\cdot\mathbf{m}] \in \mathcal{D}. \tag{5.14}$$

The non-equilibrium part of the minimizer (5.14) is expressed in terms of Lagrange multipliers, i.e. their non-equilibrium part. The non-equilibrium Lagrange multipliers have to be compatible with constraints (5.7), which can be rewritten in terms of non-equilibrium macroscopic variables:

$$\langle \tilde{\mathbf{m}} \tilde{f} \rangle = \langle \tilde{\mathbf{m}} f_E [1 + (\boldsymbol{\lambda} - \tilde{\boldsymbol{\lambda}}_E) \cdot \mathbf{m}] \rangle = \tilde{\boldsymbol{\rho}}(t, \mathbf{x}). \tag{5.15}$$

Thus, perturbative solution (5.14)-(5.15) replaces the exact solution (4.4)-(4.5). For polynomial basis functions of $\mathbb{M}$ it always produces convergent moments—macroscopic variables. The restrictions on the linear subspace are removed at the expense of constructing the approximate non-equilibrium solution.

Like in the case of equilibrium solution (5.4)-(5.5), the non-equilibrium perturbative solution (5.14)-(5.15) does not satisfy the Boltzmann equation (2.1). However, $\tilde{f}$ (actually, the corresponding moments $\boldsymbol{\rho}$ determined by (5.7)) satisfies the moment equations (2.5), which read:

$$\partial_t \langle \mathbf{m} \tilde{f} \rangle + \nabla_{\mathbf{x}} \cdot \langle \mathbf{v} \mathbf{m} \tilde{f} \rangle = \langle \mathbf{m} Q(\tilde{f}, \tilde{f}) \rangle.$$

5.4. A note on linearization. The perturbative moment closure is obtained over the space $\mathcal{D}$ of functions (5.9), that can be regarded as perturbations of the local Maxwellian. Further restriction, i.e. the smallness assumption (5.11), turns the perturbation $f_E \boldsymbol{\alpha} \cdot \mathbf{m}$ into a "small perturbation", leading to a certain kind of *linearization* in the neighborhood of local Maxwellian.

Linearization around equilibrium distribution has certain drawbacks of both mathematical and physical nature. They become especially important when one faces the problem of convergence to equilibrium (nice account on this problem was given by Villani [15, 16]; for the results of quantitative character consult Desvillettes and Villani [17]). How do we cope with this problem?

Our aim was to construct an explicit perturbative moment closure, without restriction on the maximal degree of polynomials in linear spaces $\mathbb{M}$. Linearization is the price we pay for that. However, the solution obtained using MEP, either in equilibrium or in non-equilibrium, is the one which does not satisfy the Boltzmann equation. However, its *moments* satisfy the Euler equations (in equilibrium case), as well as *extended* hierarchy of moment equations in non-equilibrium case. The goal of linearization around local Maxwellian obtained in MEP, is not directed towards the Boltzmann equation and convergence to local equilibrium. It rather comprises the information about non-equilibrium (of small magnitude) through higher order moments in the distribution function, and brings the explicit fluid dynamic limit through the closed set of moment equations. Valuable information about formal derivation of fluid dynamic limits at Euler and Navier-Stokes level can be found in [18].

Finally, the role of MEP must not be overlooked. The principle is exact as long as we deal with global equilibrium. When considered as constrained variational problem in which the moments are assumed to be variable in space and time, like in constraints (5.2) or (5.7), it only mimics the behaviour of f at global equilibrium by applying entropy maximization to the chosen set of moments.

6. Conclusions

In this study we analyzed the moment closure hierarchies—hierarchies of the macroscopic equations—derived from the Boltzmann equation. The moment closure problem can be regarded as a kinetic counterpart for determination of the constitutive relations in classical continuum mechanics. Our main concern was the application of the maximum entropy principle to derivation of the approximate non-equilibrium velocity distribution function, which resolves the closure problem.

Our motif was to remove the restriction on the linear subspace $\mathbb{M}$, over which the solution is sought, which emerged from the Levermore's condition (4.6). This condition imposes severe restrictions on $\mathbb{M}$, and rules out some physically important subspaces at the expense of retaining the exact entropy minimizer. In this study, a perturbative moment closure was proposed. It imposed restriction on the form of admissible functions, rather than the linear subspace itself. The main benefit is the boundedness of the moments of any order for the minimizer which belongs to the set of admissible functions. Moreover, this permitted us to incorporate the classical solutions of the moment closure problem (e.g. Grad's one) into this perturbative moment closure scheme.

There are still interesting open problems for the perturbative moment closure. First, it is well-known that exact closure permits symmetric Godunov form of moment hierarchy [**3**, **9**] and that Lagrange multipliers in MEP correspond to the main field in symmetric hyperbolic systems of balance laws. This property yet remains to be proven for the perturbative moment closure. Moreover, it is of interest to perform a formal extension of this scheme to polyatomic gases, which comprises more microscopic variables. Some recent studies reveal persisting interest in this field [**19**, **20**, **21**], but mathematical framework yet remains to be delineated.

Acknowledgments. This work was partially supported by the Ministry of Education, Science and Technological Development, Republic of Serbia, through the project "Mechanics of nonlinear and dissipative systems–contemporary models, analysis and applications", Project No. ON174016, and by the bilateral project (France-Serbia) CNRS/MSTD No. 25794 "Fluid and kinetic models for gaseous mixtures". The authors are grateful to the unknown referee who stimulated the analysis of linearization, which was added in the revised version.

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ХИЈЕРАРХИЈЕ ЗАТВОРЕНИХ СИСТЕМА ЈЕДНАЧИНА МОМЕНАТА ЗА РАЗРЕЂЕНЕ ГАСОВЕ

Резиме. У раду је изложена апроксимативна процедура формирања затвореног система макроскопских једначина које поседују хијерархијску структуру. Ове једначине имају примену у динамици разређених гасова и изводе се, полазећи од Болцманове једначине кинетичке теорије гасова, као једначине за моменте функције расподеле. Процедура се заснива на примени принципа максимума ентропије. Занимљиво је да моменти функције расподеле, одређени на основу тачног решења варијационог проблема, могу бити дивергентни, што се може избећи ограничењима у погледу структуре момената који се користе приликом максимизације ентропије. У овом раду је предложен пертурбациони метод у ком се уводе рестрикције на скуп допустивих функција варијационог задатка. Овај приступ нас доводи до приближног решења, али зато омогућује произвољан избор момената као ограничења у варијационом задатку.

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(Received 10.11.2015)
(Revised 27.11.2015)