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Moment Closure Hierarchies for Kinetic Theories

C. David Levermore[1]

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This paper presents a systematic *nonperturbative* derivation of a hierarchy of closed systems of moment equations corresponding to any classical kinetic theory. The first member of the hierarchy is the Euler system, which is based on Maxwellian velocity distributions, while the second member is based on non-isotropic Gaussian velocity distributions. The closure proceeds in two steps. The first ensures that every member of the hierarchy is hyperbolic, has an entropy, and formally recovers the Euler limit. The second involves modifying the collisional terms so that members of the hierarchy beyond the second also recover the correct Navier–Stokes behavior. This is achieved through the introduction of a generalization of the BGK collision operator. The simplest such system in three spatial dimensions is a "14-moment" closure, which also recovers the behavior of the Grad "13-moment" system when the velocity distributions lie near local Maxwellians. The closure procedure can be applied to a general class of kinetic theories.

KEY WORDS: Kinetic theory; moment closures; hyperbolic systems; entropy, BGK.

1. INTRODUCTION

Fluid dynamical descriptions of gases rest on the assumption that the mean free path of a particle (the average distance travelled between collisions) is much smaller than the macroscopic length scales of interest. In that case the velocity distribution of particles will approach a local equilibrium parametrized by so-called fluid variables (typically the mass density, fluid velocity, and temperature) whose evolution will be governed either by the compressible Euler equations, which approximate the velocity distribution by a local equilibrium, or the compressible Navier–Stokes equations, which account for small deviations of the velocity distribution from a local

[1] Department of Mathematics and Program in Applied Mathematics, University of Arizona, Tucson, Arizona 85721; e-mail: lvrmr@math.arizona.edu.

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equilibrium. Such fluid dynamical equations are routinely solved numerically to effectively model gases in a variety of applications. However, when the basic assumption of fluid dynamics breaks down the deviation of the velocity distribution from a local equilibrium may become large and Navier–Stokes equations can yield momentum and energy fluxes that are inconsistent with nonnegative particle densities and that may even be wrong by orders of magnitude.

Deviations of the velocity distribution from a local equilibrium can be modeled by a kinetic theory of dilute gases like that governed by the Boltzmann equation. The gas is then described by single-particle phase-space densities (one for each species) rather than fluid dynamical variables and the evolution of these phase-space densities is then governed by kinetic equations. In the fluid dynamical regime of small mean free paths the (compressible) Navier–Stokes equations can be systematically recovered as the first-order correction to the Euler equations by using either a Hilbert or Chapman–Enskog expansion. Far outside the fluid dynamical regime one may abandon fluid dynamics in favor of the full kinetic model, which may be effectively solved via molecular dynamics or Monte Carlo methods[4] at low enough densities. However, because of its phase space description and numerical stiffness, the computational cost of doing so in regimes near the fluid dynamical limit becomes too prohibitive in both time and storage requirements to allow for general usage.

This leaves a gap in our ability to efficiently model gases in the regime that lies between free molecular flow and fluid dynamics, the so-called transition regime. The objective of this article is to present models that fail gracefully as one leaves the fluid dynamical regime. More precisely, we seek models that properly capture the fluid dynamical regime when the mean free path is much smaller than the macroscopic length scales, while in the transition regime they give values for the momentum and energy fluxes (and other quantities) that are at least consistent with the nonnegativity of the particle density, and are thereby hopeful of the correct order of magnitude. By doing so, such models may provide a bridge over the transition regime that may be useful in the construction of hybrid fluid/kinetic simulations.

One strategy to describe deviations from fluid dynamics is to close systems of moment equations such as typified by the 13-moment closure of Grad.[18] This strategy introduces dynamical equations for velocity moments of the particle distribution beyond those of the conserved mass, momentum, and energy densities. The additional equations are not local conservation laws, but rather local relaxation laws that include moments of the collision operator. Any closure of this enlarged system must approximate both the higher flux moments and the collision operator

moments. These closures often use relations that are only justified when the particle distribution is near a local equilibrium, such as Grad's moment truncation of the fluxes in terms of generalized Hermite polynomials relative to the local Maxwellian, and his so-called "diagonal approximation" of the collision operator. The resulting systems of equations involve shorter spatial-temporal scales, but retain the assumption of closeness to the local equilibria, thereby taking on a perturbative nature.

Such systems of moment equations present many problems that must be faced if they are to be useful tools for simulation in the transition regime. The most significant of these problems are: (1) complexity due to the large number of equations, (2) stiffness near the fluid dynamical limit, (3) loss of realizability of its predicted moments, and (4) breakdown away from moderate regimes. The first problem is intrinsic to this general strategy and carries a substantial computational cost for any simulation. This problem is being mitigated by advances in supercomputers. The second is also intrinsic but can be resolved by a proper choice of numerical scheme.[24]third problem is more serious because it means that the predicted values of the moments can evolve to the point where they violate inequalities that must be satisfied if they are to be realized by any nonnegative density. This problem can be monitored by checking that the predicted moments satisfy appropriate inequalities during a simulation. The last problem arises because such systems can dynamically become elliptic (develop complex characteristics) and hence become ill posed, after which the meaning of the solution becomes suspect.

This paper presents a systematic *nonperturbative* derivation of a whole hierarchy of closed systems of moment equations corresponding to any classical kinetic theory. The first member of the hierarchy is the Euler system, which is based on Maxwellian velocity distributions, while the second closure is based on nonisotropic Gaussian velocity distributions. The closure procedure has two steps. The first ensures that every member of the hierarchy is hyperbolic, has an entropy, and possesses realizability of its predicted moments, thus ensuring that, unlike the perturbative approach, difficulties such as (3) and (4) above do not arise. Moreover, every member formally recovers the Euler limit. The second step involves a modification of the collisional terms that is a nonlinear generalization of the "diagonal approximation" of Grad and which ensures and those members of the hierarchy beyond the Gaussian closure recover the correct Navier–Stokes behavior. The simplest such system in three spatial dimensions is a "14-moment" closure which also recovers the Grad "13-moment" system when the velocity distributions lie near local Maxwellians.

The remainder of this paper is organized as follows. Section 2 abstracts the salient structures associated with classical kinetic equations,

thereby providing a simple general framework for the subsequent theory. Section 3 reviews classical fluid dynamical descriptions, including the Euler limit and the Navier–Stokes approximation, and discusses their breakdown. Section 4 presents the first step of the moment closure prescription and proves the corresponding claims made in the last paragraph. Section 5 works out the case of the Gaussian closure. Section 6 examines the collisional terms for higher order closures. It then introduces a generalization of the BGK collision operator, thereby completing the second step of the closure prescription. Section 7 indicates the generalization of this theory to more general kinetic equations. Finally, Section 8 gives a concluding discussion.

2. CLASSICAL KINETIC EQUATIONS

This paper will treat as illustrative the case of a gas composed of a single species of identical classical particles contained within a fixed spatial domain $\Omega \subset \mathbb{R}^D$. Kinetic theories describe such a gas through the evolution of a nonnegative density $F = F(t, x, v)$ over the single-particle phase space $\Omega \times \mathbb{R}^D$. This evolution is usually governed by a kinetic equation of the form

$$\partial_t F + v \cdot \nabla_x F = \mathscr{C}(F) \tag{2.1}$$

where the collision operator $F \mapsto \mathscr{C}(F)$ acts only on the v dependence of F locally at each (t, x). The exact nature of the domain Ω as well as any associated boundary conditions play a minor role in what follows, and so will remain unspecified. More general kinetic systems will be discussed in Section 7.

The integral of any scalar or vector-valued measurable function $f = f(v)$ over the D-dimensional Lebesgue measure dv^D will be denoted by $\langle f \rangle$; thus

$$\langle f \rangle = \int f(v)\, dv^D \tag{2.2}$$

All functions in this paper are understood to be Lebesgue measurable in all variables.

The collision operator $\mathscr{C}$ is assumed to be defined over a domain $\mathscr{D}(\mathscr{C})$ that is contained within the cone of nonnegative functions of v. It will be assumed that $\mathscr{C}$ possesses three properties, discussed below, that relate to dynamical conservation, dissipation, and symmetry, and which are shared by a wide variety of classical collision operators.

First, the operator $\mathscr{C}$ is assumed to have 1, v and $|v|^2$ as locally conserved quantities; this means

$$\langle \mathscr{C}(f) \rangle = 0, \qquad \langle v\mathscr{C}(f) \rangle = 0, \qquad \langle |v|^2 \mathscr{C}(f) \rangle = 0$$

$$\text{for every} \quad f \in \mathscr{D}(\mathscr{C}) \tag{2.3}$$

Moreover, it is assumed that every locally conserved quantity is a linear combination of these three, so that for any $g = g(v)$ the following statements are equivalent:

$$\begin{aligned} &\text{(i)} \quad \langle g\mathscr{C}(f) \rangle = 0 \qquad \text{for every} \quad f \in \mathscr{D}(\mathscr{C}) \\ &\text{(ii)} \quad g \in \mathbb{E} \equiv \operatorname{span}\{1, v_1, v_2, \ldots, v_D, |v|^2\} \end{aligned} \tag{2.4}$$

The relations (2.3) represent the physical laws of mass, momentum, and energy conservation during collisions and (2.4) states that there are no other conservation laws. A consequence of (2.3) is that solutions of the kinetic equation (2.1) formally satisfy the local conservation laws

$$\begin{aligned} \partial_t \langle F \rangle + \nabla_x \cdot \langle vF \rangle &= 0 \\ \partial_t \langle vF \rangle + \nabla_x \cdot \langle v \vee vF \rangle &= 0 \\ \partial_t \langle \tfrac{1}{2}|v|^2 F \rangle + \nabla_x \cdot \langle \tfrac{1}{2}|v|^2 vF \rangle &= 0 \end{aligned} \tag{2.5}$$

corresponding to mass, momentum and energy conservation respectively. Here $\vee$ denotes the symmetric tensor outer product that acts on a symmetric k-tensor and a symmetric l-tensor by symmetrizing their usual tensor outer product.

Second, the operator $\mathscr{C}$ is assumed to satisfy the local dissipation relation

$$\langle \log f \mathscr{C}(f) \rangle \leqslant 0 \qquad \text{for every} \quad f \in \mathscr{D}(\mathscr{C}) \tag{2.6}$$

The quantity on the left of (2.6) is the so-called local entropy dissipation rate. The local equilibria of $\mathscr{C}$ are assumed to be characterized by the vanishing of the local entropy dissipation rate and to be given by the class of Maxwellian densities, i.e., those of the form

$$f = \mathscr{E}(\rho, u, \theta) \equiv \frac{\rho}{(2\pi\theta)^{D/2}} \exp\left(-\frac{|v-u|^2}{2\theta} \right) \tag{2.7}$$

for some $(\rho, u, \theta) \in \mathbb{R}_+ \times \mathbb{R}^D \times \mathbb{R}_+$. More precisely, for every $f \in \mathscr{D}(\mathscr{C})$ the following statements are assumed to be equivalent:

$$\text{(i)} \quad \langle \log f \mathscr{C}(f) \rangle = 0$$
$$\text{(ii)} \quad \mathscr{C}(f) = 0 \tag{2.8}$$
$$\text{(iii)} \quad f \text{ is a Maxwellian density given by (2.7)}$$

These assumptions about $\mathscr{C}$ merely abstract some of the consequences of Boltzmann's celebrated H-theorem. Relation (2.6) implies that solutions of the kinetic equation (2.1) formally satisfy the local dissipation law

$$\partial_t \langle F \log F - F \rangle + \nabla_x \cdot \langle v(F \log F - F) \rangle = \langle \log F \mathscr{C}(F) \rangle \leqslant 0 \tag{2.9}$$

corresponding to entropy dissipation. In this paper we adopt the sign convention of diminishing entropy, which, while at variance with much of the physics literature, is both mathematically and physically more natural.

Third, the operator $\mathscr{C}$ is assumed to commute with translational and orthogonal transformations. Specifically, given any $f = f(v)$, then for every vector $w \in \mathbb{R}^D$ and for every orthogonal matrix $O \in \mathbb{R}^{D \times D}$ define transformed functions $\mathscr{T}_u f$ and $\mathscr{T}_o f$ by

$$\mathscr{T}_u f = \mathscr{T}_u f(v) \equiv f(v - u), \qquad \mathscr{T}_o f = \mathscr{T}_o f(v) \equiv f(O^T v) \tag{2.10}$$

It is assumed that if f is in $\mathscr{D}(\mathscr{C})$, then so are $\mathscr{T}_u f$ and $\mathscr{T}_o f$ with

$$\mathscr{T}_u \mathscr{C}(f) = \mathscr{C}(\mathscr{T}_u f), \qquad \mathscr{T}_o \mathscr{C}(f) = \mathscr{C}(\mathscr{T}_o f) \tag{2.11}$$

This relation reflects the Galilean invariance of the microscopic collisional dynamics and implies that when $\Omega = \mathbb{R}^D$, the kinetic equation (2.1) formally retains Galilean invariance. Specifically, whenever $F = F(t, x, v)$ satisfies (2.1), then, for every vector $u \in \mathbb{R}^D$ and orthogonal matrix $O \in \mathbb{R}^{D \times D}$, so do the actions of the Galilean group on F,

$$\begin{aligned} \mathscr{A}_u F &= \mathscr{A}_u F(t, x, v) \equiv F(t, x - ut, v - u) \\ \mathscr{A}_o F &= \mathscr{A}_o F(t, x, v) \equiv F(t, O^T x, O^T v) \end{aligned} \tag{2.12}$$

Of course, the set of solutions of (2.1) is also invariant under space and time translations.

In addition to the three properties of $\mathscr{C}$ discussed above, it will be assumed that for a given and absolute equilibrium $\mathscr{E}$ (independent of space and time) the linearization of the kinetic equation (2.1) about $F = \mathscr{E}$ has analogous structural features. Formally setting $F = \mathscr{E}(1 + \delta g)$ into (2.1) and dropping terms of order δ_2 results in the linearization

$$\partial_t g + v \cdot \nabla_x g + \mathscr{L}_{\mathscr{E}} g = 0 \tag{2.13}$$

where $\mathscr{L}_\mathscr{E}$ is defined to act linearly on $g = g(v)$ by

$$\mathscr{L}_\mathscr{E} g \equiv -\frac{1}{\mathscr{E}} D\mathscr{C}(\mathscr{E})\,\mathscr{E} g \equiv -\frac{1}{\mathscr{E}} \partial_\delta \mathscr{C}(\mathscr{E}(1+\delta g))\Big|_{\delta=0} \tag{2.14}$$

The operator $\mathscr{L}_\mathscr{E}$ is assumed to be closed and densely defined with domain $\mathscr{D}(\mathscr{L}_\mathscr{E})$ in $\mathbb{H}_\mathscr{E}$, the Hilbert space with the weighted inner product $(h \mid g)_\mathscr{E} = \langle h\mathscr{E} g\rangle$). Typically, the linearized kinetic equation (2.13) is well-posed over $\mathbb{H}_\mathscr{E}$ and, as for the case of the Boltzmann equation, is related to the initial-value problem for (2.1) through the notion of entropic convergence.[26]

Some properties of $\mathscr{L}_\mathscr{E}$ follow formally from those of $\mathscr{C}$. First, differentiating the relation $\mathscr{C}(\mathscr{E}(\rho, u, \theta)) = 0$ with respect to an arbitrary parametrization of (ρ, u, θ) leads to the relation

$$\mathscr{L}_\mathscr{E} \frac{\dot{\mathscr{E}}}{\mathscr{E}} = -\frac{1}{\mathscr{E}} D\mathscr{C}(\mathscr{E})\,\dot{\mathscr{E}} = 0 \tag{2.15}$$

where by (2.7) the logarithmic derivative of $\mathscr{E} = \mathscr{E}(\rho, u, \theta)$ is

$$\frac{\dot{\mathscr{E}}}{\mathscr{E}} = \frac{\dot{\rho}}{\rho} + \frac{(v-u)\cdot\dot{u}}{\theta} + \left(\frac{|v-u|^2}{2\theta} - \frac{D}{2}\right)\frac{\dot{\theta}}{\theta} \tag{2.16}$$

Considering the variations $\dot{\rho}$, $\dot{u}$, and $\dot{\theta}$ as independent shows that the space of locally conserved quantities $\mathbb{E}$ defined in (2.4) is contained in $\mathscr{N}(\mathscr{L}_\mathscr{E})$, the null space of $\mathscr{L}_\mathscr{E}$. Second, applying the definition (2.14) of $\mathscr{L}_\mathscr{E}$ to the local conservation relations (2.3) shows that

$$\langle \mathscr{E}\mathscr{L}_\mathscr{E} g\rangle = 0 \qquad \langle v\mathscr{E}\mathscr{L}_\mathscr{E} g\rangle = 0, \qquad \langle |v|^2\,\mathscr{E}\mathscr{L}_\mathscr{E} g\rangle = 0$$
$$\text{for every} \quad g \in \mathscr{D}(\mathscr{L}_\mathscr{E}) \tag{2.17}$$

This implies that $\mathbb{E} \subset \mathscr{N}(\mathscr{L}_\mathscr{E}^\dagger)$, where $\mathscr{L}_\mathscr{E}^\dagger$ is the adjoint of $\mathscr{L}_\mathscr{E}$ over $\mathbb{H}_\mathscr{E}$ with domain $\mathscr{D}(\mathscr{L}_\mathscr{E}^\dagger)$. Third, taking the second variation of the dissipation relation (2.6) gives

$$\langle g\mathscr{E}\mathscr{L}_\mathscr{E} g\rangle = -\tfrac{1}{2}\partial_{\delta\delta}\langle \log(\mathscr{E}(1+\delta g))\,\mathscr{C}(\mathscr{E}(1+\delta g))\rangle|_{\delta=0} \geqslant 0 \tag{2.18}$$

whereby it follows that $g \in \mathscr{N}(\mathscr{L}_\mathscr{E} + \mathscr{L}_\mathscr{E}^\dagger$ if and only if $\langle g\mathscr{E}\mathscr{L}_\mathscr{E} g\rangle_\mathscr{E} = 0$, which then implies

$$\mathscr{N}(\mathscr{L}_\mathscr{E}) = \mathscr{N}(\mathscr{L}_\mathscr{E}^\dagger) \subset \mathscr{N}(\mathscr{L}_\mathscr{E} + \mathscr{L}_\mathscr{E}^\dagger) \tag{2.19}$$

By the inferences from (2.16) and (2.17) above, $\mathbb{E}$ is a subset of each of these spaces.

We shall assume that $\mathscr{D}(\mathscr{L}_\varepsilon^\dagger) = \mathscr{D}(\mathscr{L}_\varepsilon)$ and that all the above inclusions are equalities. More precisely, for every $g \in \mathscr{D}(\mathscr{L}_\varepsilon)$ the following statements are assumed to be equivalent:

$$\begin{aligned} &\text{(i)} \quad \langle g \mathscr{E} \mathscr{N}_\varepsilon g \rangle = 0 \\ &\text{(ii)} \quad \mathscr{L}_\varepsilon g = 0 \\ &\text{(iii)} \quad \mathscr{L}_\varepsilon^\dagger g = 0 \\ &\text{(iv)} \quad g \in \mathbb{E} \end{aligned} \tag{2.20}$$

An important special case which includes all classical collision operators is when $\mathscr{L}_\varepsilon$ is self-adjoint ($\mathscr{L}_\varepsilon^\dagger = \mathscr{L}_\varepsilon$). In this case (2.18) implies that (i), (ii), and (iii) in (2.20) are always equivalent, so the only assertion in (2.20) is the equivalence of (iv) to the others.

In addition, it shall be assumed that $\mathscr{L}_\varepsilon$ satisfies the Fredholm alternative $\mathscr{R}(\mathscr{L}_\varepsilon) = \mathbb{E}^\perp$, where $\mathscr{R}(\mathscr{L}_\varepsilon)$ denotes the range of $\mathscr{L}_\varepsilon$. Specifically, this means we are assuming that $\mathscr{R}(\mathscr{L}_\varepsilon)$ is closed, a property that does not hold for all classical collision operators, but does hold for that of Boltzmann in the case of Maxwell molecules or hard potentials with an angular cutoff.[7] One could include the case of the soft potentials if the Fredholm assumption is replaced with the weaker one that $\mathscr{L}_\varepsilon$ satisfies the Fredholm alternative in a space that is appropriately related to $\mathbb{H}_\varepsilon$,[14] but for simplicity we will not do so here.

The Fredholm alternative implies that the equation $\mathscr{L}_\varepsilon g = f$ has a solution if and only if $f \in \mathbb{E}^\perp$, in which case there is a unique solution in $\mathbb{E}^\perp$ denoted by $g = \mathscr{L}_\varepsilon^{-1} f$. Let $\mathscr{P}_\varepsilon$ be the orthogonal projection of $\mathbb{H}_\varepsilon$ onto $\mathbb{E}$, which acts on $g = g(v)$ as

$$\begin{aligned} \mathscr{P}_\varepsilon g = \frac{1}{\rho}\Bigg[\langle \mathscr{E} g \rangle + \frac{(v-u)\langle (v-u)\, \mathscr{E} g \rangle}{\theta} \\ + \left(\frac{|v-u|^2}{2\theta} - \frac{D}{2} \right) \frac{2}{D} \left\langle \left(\frac{|v-u|^2}{2\theta} - \frac{D}{2} \right) \mathscr{E} g \right\rangle \Bigg] \end{aligned} \tag{2.21}$$

The operator $\mathscr{L}_\varepsilon^{-1}$ is the unique bounded pseudoinverse of $\mathscr{L}_\varepsilon$ such that

$$\mathscr{L}_\varepsilon \, \mathscr{L}_\varepsilon^{-1} = \mathscr{I} - \mathscr{P}_\varepsilon, \qquad \mathscr{L}_\varepsilon^{-1} \, \mathscr{L}_\varepsilon \subset \mathscr{I} - \mathscr{P}_\varepsilon \tag{2.22}$$

where $\mathscr{I} - \mathscr{P}_\varepsilon$ is the orthogonal projection of $\mathbb{H}_\varepsilon$ onto $\mathbb{E}^\perp$. The dissipation relation (2.18) ensures that the quadratic forms associated with $\mathscr{L}_\varepsilon$ and $\mathscr{L}_\varepsilon^{-1}$ enjoy the positivity properties:

$$\begin{aligned} \langle g \mathscr{E} \mathscr{L}_\varepsilon g \rangle > 0 \qquad &\text{for every nonzero} \quad g \in \mathbb{E}^\perp \cap \mathscr{D}(\mathscr{L}_\varepsilon) \\ \langle g \mathscr{E} \mathscr{L}_\varepsilon^{-1} g \rangle > 0 \qquad &\text{for every nonzero} \quad g \in \mathbb{E}^\perp \end{aligned} \tag{2.23}$$

In the case that $\mathscr{L}_{\mathscr{E}}$ is self-adjoint this means that $\mathscr{L}_{\mathscr{E}}$ and $\mathscr{L}_{\mathscr{E}}^{-1}$ are positive definite over $\mathbb{E}^{\perp}$.

Finally, fix a local equilibrium $\mathscr{E} = \mathscr{E}(\rho, u, \theta)$. Every orthogonal matrix $O \in \mathbb{R}^{D \times D}$ defines the transformation $\mathscr{O}_O \equiv \mathscr{T}_u \mathscr{T}_O \mathscr{T}_u^{-1}$, where $\mathscr{T}_u$ and $\mathscr{T}_O$ are defined by (2.10). It is easily checked that $\mathscr{O}_O \mathscr{E} = \mathscr{E}$ and that $\mathscr{O}_O$ is an orthogonal transformation over $\mathbb{H}_{\mathscr{E}}$. Linearizing the commutation relations (2.11) about $\mathscr{E}$ shows that for every orthogonal matrix $O \in \mathbb{R}^{D \times D}$, if $g \in \mathscr{D}(\mathscr{L}_{\mathscr{E}})$, then so is $\mathscr{O}_O g$ and

$$\mathscr{O}_O \mathscr{L}_{\mathscr{E}} g = \mathscr{L}_{\mathscr{E}} \mathscr{O}_O g \tag{2.24}$$

In other words, the operator $\mathscr{L}_{\mathscr{E}}$ commutes with the orthogonal transformations $\mathscr{O}_O$. This symmetry is usually applied in one of two ways. First, specializing (2.24) to the case $O = -I$ shows that the space of all functions that are even (odd) in $v - u$ is invariant under $\mathscr{L}_{\mathscr{E}}$; this is the so-called even/odd symmetry of $\mathscr{L}_{\mathscr{E}}$. Second, because the measure $d\overset{D}{v}$ is invariant under action by any $\mathscr{O}_O$ it follows that

$$\begin{aligned} \langle g \mathscr{E} \mathscr{L}_{\mathscr{E}} g \rangle &= \langle \mathscr{O}_O (g \mathscr{E} \mathscr{L}_{\mathscr{E}} g) \rangle = \langle (\mathscr{O}_O g)\, \mathscr{E} \mathscr{L}_{\mathscr{E}} \mathscr{O}_O g \rangle \\ \langle g \mathscr{E} \mathscr{L}_{\mathscr{E}}^{-1} g \rangle &= \langle \mathscr{O}_O (g \mathscr{E} \mathscr{L}_{\mathscr{E}}^{-1} g) \rangle = \langle (\mathscr{O}_O g)\, \mathscr{E} \mathscr{L}_{\mathscr{E}}^{-1} \mathscr{O}_O g \rangle \end{aligned} \tag{2.25}$$

for every orthogonal matrix $O \in \mathbb{R}^{D \times D}$. This so-called orthogonal symmetry simplifies the evaluation of many tensors that appear subsequently.

3. FLUID DYNAMICAL DESCRIPTIONS

Fluid dynamical descriptions of the gas are those with an evolution governed by the local conservation laws (2.5) in which the phase-space density F is approximated in terms of the locally conserved spatial densities. The local densities are determined by the fluid variables ρ, u and θ through the defining relations

$$\langle F \rangle = \rho, \qquad \langle vF \rangle = \rho u, \qquad \left\langle \frac{1}{2} |v|^2 F \right\rangle = \frac{1}{2} \rho |u|^2 + \frac{D}{2} \rho \theta \tag{3.1}$$

These relations are consistent with the previous usage of ρ, u, and θ in the formula for the local Maxwellian density (2.7) in that they reduce to identities when F is given by (2.7). The local fluxes can then be written as

$$\langle v \vee vF \rangle = \rho u \vee u + \rho \theta I + \Sigma \tag{3.2a}$$

$$\left\langle \frac{1}{2} |v|^2 vF \right\rangle = \frac{1}{2} \rho |u|^2 u + \frac{D+2}{2} \rho \theta u + \Sigma u + q \tag{3.2b}$$

where the stress Σ and the heat flux q take on values of a traceless symmetric matrix in $\mathbb{R}^{D \vee D}$ and a vector in $\mathbb{R}^D$, respectively. The local conservation laws (2.5) become

$$\begin{aligned} \partial_t \rho + \nabla_x \cdot (\rho u) &= 0 \\ \partial_t (\rho u) + \nabla_x \cdot (\rho u \vee u) + \nabla_x (\rho\theta) + \nabla_x \cdot \Sigma &= 0 \\ \partial_t \left(\frac{1}{2} \rho |u|^2 + \frac{D}{2} \rho\theta \right) + \nabla_x \cdot \left(\frac{1}{2} \rho |u|^2 u + \frac{D+2}{2} \rho\theta u + \Sigma u + q \right) &= 0 \end{aligned} \tag{3.3}$$

A fluid dynamical closure is then specified by so-called constitutive relations that express the stress Σ and heat flux q in terms of ρ, u, and θ and their derivatives, whereby the evolution of (ρ, u, θ) is then governed by (3.3).

Rather than specifying Σ and q independently, one can first solve (3.2) for Σ and q in terms of F as

$$\Sigma = \theta \langle AF \rangle, \qquad q = \theta^{3/2} \langle BF \rangle \tag{3.4}$$

where the dimensionless traceless symmetric $D \times D$-matrix A and the dimensionless D-vector B are given by

$$A = \frac{(v-u) \vee (v-u)}{\theta} - \frac{1}{D} \frac{|v-u|^2}{\theta} I \tag{3.5a}$$

$$B = \left(\frac{|v-u|^2}{2\theta} - \frac{D+2}{2} \right) \frac{v-u}{\theta^{1/2}} \tag{3.5b}$$

Then a fluid dynamical closure can be specified by choosing an expression for F in terms of ρ, u and θ and their derivatives. Sometimes this approach also yields a local entropy dissipation law from (2.9) that is consistent with (3.3).

The simplest such closure arises upon making the approximation that F has the form of the unique local Maxwellian density given by (2.7). In this case both the stress Σ and the heat flux q vanish identically, thereby reducing (3.3) to the Euler equations

$$\begin{aligned} \partial_t \rho + \nabla_x \cdot (\rho u) &= 0 \\ \partial_t (\rho u) + \nabla_x \cdot (\rho u \vee u) + \nabla_x (\rho\theta) &= 0 \\ \partial_t \left(\frac{1}{2} \rho |u|^2 + \frac{D}{2} \rho\theta \right) + \nabla_x \cdot \left(\frac{1}{2} \rho |u|^2 u + \frac{D+2}{2} \rho\theta u \right) &= 0 \end{aligned} \tag{3.6}$$

The local entropy dissipation law (2.9) becomes

$$\partial_t(\rho\sigma) + \nabla_x \cdot (\rho u\sigma) \leqslant 0 \tag{3.7}$$

where the specific entropy $\sigma = \sigma(\rho, \theta)$ is given by

$$\sigma \equiv \frac{1}{\rho} \langle \mathscr{E} \log \mathscr{E} - \mathscr{E} \rangle = \log\left(\frac{\rho}{(2\pi\theta)^{D/2}}\right) - \frac{D+2}{2} \tag{3.8}$$

Classical solutions of the Euler system (3.6) satisfy (3.7) as an equality, while weak solutions (like shocks) that are obtained through a "viscosity method" will generally satisfy (3.7) as an inequality (in the sense of distributions).[25]

In fact, classical solutions of the Euler system (3.6) satisfy a large family of formal local conservation laws in the form

$$\partial_t(\rho h(\sigma)) + \nabla_x \cdot (\rho u h(\sigma)) = 0 \tag{3.9}$$

where $h = h(\sigma)$ is any differentiable function over $\mathbb{R}$. The density ρh is a strictly convex function of the mass, momentum, and energy densities of (3.6) whenever,[20, 21]

$$h'(\sigma) > 0, \qquad \frac{2}{D+2} h'(\sigma) + h''(\sigma) > 0 \tag{3.10}$$

In that case ρh is called a strictly convex entropy density for (3.6) and weak solutions satisfy the local dissipation laws

$$\partial_t(\rho h(\sigma)) + \nabla_x \cdot (\rho u h(\sigma)) \leqslant 0 \tag{3.11}$$

The choice $h(\sigma) = \sigma$ in (3.11) recovers (3.7).

Deviations from the local equilibrium approximation can be computed systematically using a Chapman–Enskog analysis of the scaled kinetic equation

$$\partial_t F + v \cdot \nabla_x F = \frac{1}{\varepsilon} \mathscr{C}(F) \tag{3.12}$$

where ε is a dimensionless number that gives the order of the mean free path over the macroscopic gradient length scales.[2, 7] The Chapman–Enskog expansion of F in powers of ε has the form

$$F = \mathscr{E}(\rho, u, \theta)(1 + \varepsilon g^{(1)} + \varepsilon^2 g^{(2)} + \cdots) \tag{3.13}$$

where the leading order is the local equilibrium given by

$$\mathscr{E}(\rho, u, \theta) = \frac{\rho}{(2\pi\theta)^{D/2}} \exp\left(-\frac{|v-u|^2}{2\theta}\right) \tag{3.14}$$

for $(\rho(t,x), u(t,x), \theta(t,x)) \in \mathbb{R}_+ \times \mathbb{R}^D \times \mathbb{R}_+$ consistent with (3.1). Placing (3.13) into (3.1), the $g^{(n)}$ must satisfy the consistency constraint

$$\langle \mathscr{E} g^{(n)} \rangle = 0, \qquad \langle v \mathscr{E} g^{(n)} \rangle = 0, \qquad \langle \tfrac{1}{2}|v|^2 \mathscr{E} g^{(n)} \rangle = 0 \tag{3.15}$$

which simply states that each $g^{(n)}$ belongs to $\mathbb{E}^\perp$. Placing (3.13) into (3.12), the $g^{(n)}$ at each (t,x) are then expressed locally in terms of (ρ, u, θ) and their spatial derivatives, where time derivatives of the fluid variables are eliminated at each order using (3.3).

The Navier–Stokes approximation involves keeping just the first-order correction in the Chapman–Enskog expansion (3.13). It is found that $g^{(1)} \in \mathbb{E}^\perp$ satisfies

$$\mathscr{L}_{\mathscr{E}} g^{(1)} = -(\mathscr{I} - \mathscr{P}_{\mathscr{E}}) \frac{v \cdot \nabla_x \mathscr{E}}{\mathscr{E}} \tag{3.16}$$

where $\mathscr{P}_{\mathscr{E}}$ is the orthogonal projection of $\mathbb{H}_{\mathscr{E}}$ onto $\mathbb{E}$ given by (2.21). Using (2.16) and (2.21), we find that the right side of (3.16) takes the form

$$(\mathscr{I} - \mathscr{P}_{\mathscr{E}}) \frac{v \cdot \nabla_x \mathscr{E}}{\mathscr{E}} = \frac{1}{2} A : \left(\nabla_x u + (\nabla_x u)^T - \frac{2}{D} \nabla_x \cdot u I\right) + \frac{1}{\theta^{1/2}} B \cdot \nabla_x \theta \tag{3.17}$$

The right side of (3.16) is clearly in $\mathbb{E}^\perp$, and hence in $\mathscr{R}(\mathscr{L}_{\mathscr{E}})$ by the Fredholm alternative, so its solution can be expressed using the pseudoinverse $\mathscr{L}_{\mathscr{E}}^{-1}$ and the relation (3.17) as

$$\begin{aligned} g^{(1)} &= \mathscr{L}_{\mathscr{E}}^{-1} (\mathscr{I} - \mathscr{P}_{\mathscr{E}}) \frac{v \cdot \nabla_x \mathscr{E}}{\mathscr{E}} \\ &= -\frac{1}{2} \mathscr{L}_{\mathscr{E}}^{-1} A : \left(\nabla_x u + (\nabla_x u)^T - \frac{2}{D} \nabla_x \cdot u I\right) - \frac{1}{\theta^{1/2}} \mathscr{L}_{\mathscr{E}}^{-1} B \cdot \nabla_x \theta \end{aligned} \tag{3.18}$$

The first-order correction to the local equilibrium approximation is thereby linearly proportional to gradients of the fluid variables.

By using (3.18) in the Chapman–Enskog expansion (3.13) and dropping all the higher order terms, we obtain the Navier–Stokes approximation for F and, as it has served its purpose, discard ε. When this approximation is substituted into formula (3.4) and the even/odd symmetry of $\mathscr{L}_{\mathscr{E}}$ is used to infer that the three-tensors $\langle A \mathscr{E} \mathscr{L}_{\mathscr{E}}^{-1} B \rangle$ and

$\langle B\mathscr{E}\mathscr{L}_\mathscr{E}^{-1} A\rangle$ vanish identically, then we are led to the Navier–Stokes closure

$$\Sigma = \theta\langle A\mathscr{E}g^{(1)}\rangle = -\frac{1}{2}\theta\langle A\mathscr{E}\mathscr{L}_\mathscr{E}^{-1} A\rangle : (\nabla_x u + (\nabla_x u)^T - \frac{2}{D}\nabla_x \cdot uI) \quad (3.19a)$$

$$q = \theta^{3/2}\langle B\mathscr{E}g^{(1)}\rangle = -\theta\langle B\mathscr{E}\mathscr{L}_\mathscr{E}^{-1}B\rangle \cdot \nabla_x\theta \quad (3.19b)$$

The symmetry of $\mathscr{L}_\mathscr{E}$ with respect to orthogonal transformations (2.25) and the fact that $\mathrm{tr}(A) = 0$ imply that the components of the four-tensor $\langle A\mathscr{E}\mathscr{L}_\mathscr{E}^{-1} A\rangle$ and the two-tensor $\langle B\mathscr{E}\mathscr{L}_\mathscr{E}^{-1}B\rangle$ satisfy the identities

$$\langle A_{ij}\mathscr{E}\mathscr{L}_\mathscr{E}^{-1} A_{kl}\rangle = \frac{1}{(D-1)(D+2)}\langle A : \mathscr{E}\mathscr{L}_\mathscr{E}^{-1} A\rangle \left(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk} - \frac{2}{D}\delta_{ij}\delta_{kl}\right)$$

$$\langle B_i\mathscr{E}\mathscr{L}_\mathscr{E}^{-1} B_k\rangle = \frac{1}{D}\langle B\cdot\mathscr{E}\mathscr{L}_\mathscr{E}^{-1} B\rangle\,\delta_{ik} \quad (3.20)$$

Moreover, the only appearance of u in the above integrands is through $v-u$, so by the translation invariance of $d\vec{v}^D$ the above tensors depend only on ρ and θ. Therefore, using the identities (3.20), we find that the Navier–Stokes closure (3.19) becomes

$$\Sigma = -\mu\left(\nabla_x u + (\nabla_x u)^T - \frac{1}{D}\nabla_x \cdot uI\right) \quad (3.21a)$$

$$q = -\kappa\nabla_x\theta \quad (3.21b)$$

where the viscosity $\mu = \mu(\rho, \theta)$ and the heat conduction $\kappa = \kappa(\rho, \theta)$ are given by

$$\mu = \theta\frac{1}{(D-1)(D+2)}\langle A : \mathscr{E}\mathscr{L}_\mathscr{E}^{-1} A\rangle \quad (3.22a)$$

$$\kappa = \theta\frac{1}{D}\langle B\cdot\mathscr{E}\mathscr{L}_\mathscr{E}^{-1}B\rangle \quad (3.22b)$$

The positivity of μ and κ is a consequence of (2.23), while the fact they are bounded above follows from the boundedness of $\mathscr{L}_\mathscr{E}^{-1}$. The functional independence of μ and κ on u is a consequence of Galilean invariance. Whenever $\mathscr{C}$ is homogeneous of degree two in F (as for the classical Boltzmann collision operator), then both $\mathscr{L}_\mathscr{E}$ and $\mathscr{E}$ will be homogeneous of degree one in ρ, whereby μ and κ will be independent of ρ as well.

Fluid dynamics breaks down when the macroscopic gradient lengths are comparable to the mean free path of the flow. The viscous stress and

heat conduction terms in the fluxes of the usual Navier–Stokes equations then become large enough to lead to unphysical effects. One such effect is the development of unrealizable values for the moments of the fluid particle distribution. This is clearly seen to arise in (3.2a) for the Navier–Stokes closure (3.21a), recast as

$$\langle (v-u) \vee (v-u)F \rangle = \rho\theta I - \mu \left(\nabla_x u + (\nabla_x u)^T - \frac{2}{D} \nabla_x \cdot uI \right) \quad (3.23)$$

whenever the expression on the right side of (3.23) is no longer a nonnegative-definite matrix (the left side being manifestly so). This means that the approximation has become so bad that there is no distribution of particles that is consistent with the predicted values of the momentum flux computed from the fluid variables. A more refined moment realizability analysis[27] leads to the requirement of the nonnegative definiteness of the dimensionless symmetric $D \times D$-matrix

$$I - \frac{\mu}{\rho\theta} \left(\nabla_x u + (\nabla_x u)^T - \frac{2}{D} \nabla_x \cdot uI \right) - \frac{2}{D} \frac{\kappa^2}{\rho^2\theta^3} \nabla_x \theta \, (\nabla_x \theta)^T \quad (3.24)$$

In practice, any simulation using the Navier–Stokes closure should be suspect whenever the eigenvalues of the matrix (3.24) become significantly different than unity. Such a difference would indicate that higher order terms in the Chapman–Enskog expansion are becoming important. However, the problem of unrealizable moments is *not* remedied by proceeding to the next few higher order terms in the Chapman–Enskog expansion[5, 34] (to the Burnett or super–Burnett equations), because if those terms are important, then all the remaining ones are, too. The fundamental physical difficulty is that the underlying distribution of particles has variations on small scales and is therefore far from any local equilibrium.

One strategy to maintain moment realizability within fluid dynamical closures involves the introduction of so-called flux-limited closures such as was explored in ref. 29 within the context of a discrete-velocity kinetic theory, but that is not the approach we will take here.

4. MOMENT CLOSURES

An alternative strategy for describing deviations from local equilibria was developed by Grad[18] based on moment equations. In general, the development of moment equations begins with the choice of a finite-dimensional linear subspace $\mathbb{M}$ of functions of v (usually chosen to be polynomials). Let M be the dimension of this space and $\{m_i = m_i(v)\}_{i=1}^{M}$ be a

basis. Denote the column M-vector of these basis elements by $\mathbf{m} = \mathbf{m}(v)$, so that every $m \in \mathbb{M}$ has a unique representation in the form $m(v) = \boldsymbol{\alpha}^T \mathbf{m}(v)$ for some $\boldsymbol{\alpha} \in \mathbb{R}^M$, where $\boldsymbol{\alpha}^T$ is the matrix transpose of the column vector $\boldsymbol{\alpha}$. Now taking the moments of the kinetic equation (2.1) over the vector $\mathbf{m}(v)$ leads to the system

$$\partial_t \langle \mathbf{m} F \rangle + \nabla_x \cdot \langle v \mathbf{m} F \rangle = \langle \mathbf{m} \mathscr{C}(F) \rangle \tag{4.1}$$

It must be noted that it is not even known for the Boltzmann equation whether the quantities appearing in this equation are well-defined functions for every solution F. However, recent work has shown this to be the case for the spatially homogeneous case[11] (also see refs. 9 and 35) and for the nearly homogeneous case,[1] thereby giving some hope that it might be more generally true. For present purposed we shall suppose these quantities are well defined and consider system (4.1) formally. The so-called "moment closure problem" is then to express the above densities $\langle \mathbf{m} F \rangle$, fluxes $\langle v \mathbf{m} F \rangle$, and collisional terms $\langle \mathbf{m} \mathscr{C}(F) \rangle$, as a function of M variables (traditionally the densities themselves), thus formally closing the system.

Moment closures must be devised while remaining mindful that the resulting system should be well-posed, respect physical symmetries, yield moments that are realized by some nonnegative velocity density of particles, and recover the proper fluid dynamical approximations. These goals can be achieved in part by requiring that $\mathbb{M}$ satisfy the following conditions:

$$\begin{aligned} &\text{(I)} \quad \mathbb{E} \equiv \operatorname{span}\{1, v, |v|^2\} \subset \mathbb{M} \\ &\text{(II)} \quad \mathbb{M} \text{ is invariant under the actions of } \mathscr{T}_u \text{ and } \mathscr{T}_o \end{aligned} \tag{4.2}$$

The span notation used here in the definition of $\mathbb{E}$ and throughout this paper will be applied to a collection of scalars, vectors, and tensors and will mean all scalar-valued linear combinations of their components. In particular, $\mathbb{E}$ consists of all linear combinations of the scalars 1 and $|v|^2$ and the components of the vector v. Condition (I) above is a minimal requirement if any fluid dynamical approximation is to be recovered, while condition (II) is needed if the theory is to be Galilean invariant. For example, one such choice of $\mathbb{M}$ that was studied extensively by Grad is

$$\mathbb{M} = \operatorname{span}\{1, v, v \vee v, |v|^2 v\} \tag{4.3}$$

which in three dimensions provided the basis for his 13-moment closure. This choice was made to include the momentum and energy fluxes of (2.5)

among the moment densities, which can therefore be expressed in terms of ρ, u, θ, Σ, and q by (3.1) and (3.2).

Given any $\mathbb{M}$ satisfying conditions (I) and (II) of (4.2), Grad proposed the following two-step closure procedure.[18] The first step is to expand F in terms of Hermite polynomials relative to the weight $\mathscr{E}(\rho, u, \theta)$. For $\mathbb{M}$ given by (4.3) this leads to

$$F = \mathscr{E}\left(1 + \frac{1}{2}\frac{1}{\rho\theta}\Sigma : A + \frac{2}{D+2}\frac{1}{\rho\theta^{3/2}} q \cdot B\right) \tag{4.4}$$

The moment flux terms in (4.1) can then generally be evaluated by direct integration. The second step had two motivations: that the collision term in (4.1) could almost never be evaluated explicitly, and that it seldom yields the correct behavior in the fluid regime. To overcome these difficulties Grad introduced the so-called diagonal approximation in which the collision operator $\mathscr{C}(F)$ is modified by linearizing it about $F = \mathscr{E}$ and then "diagonalizing" it with respect to the Hermite polynomials so as to recover the correct transport coefficients. This modification takes the form

$$\mathscr{C}(F) = -\frac{1}{2}\frac{\theta}{\mu}\mathscr{E}A : \langle AF\rangle - \frac{2}{D+2}\frac{\theta}{\kappa}\mathscr{E}B \cdot \langle BF\rangle - \cdots \tag{4.5}$$

where μ and κ are the viscosity and heat conduction given by (3.22). This simplification allows both the collision term in (4.1) to be evaluated and the correct Navier–Stokes behavior to be recovered.

The moment closure prescribed here places an additional requirement on the linear subspace $\mathbb{M}$. Given any $\mathbb{M}$, this requirement is formulated in terms of the associated subset

$$\mathbb{M}_c \equiv \{m \in \mathbb{M} : \langle \exp(m(v))\rangle < \infty\} \tag{4.6}$$

The convexity of the exponential function ensures that $\mathbb{M}_c$ is a convex cone in $\mathbb{M}$. We will construct a self-consistent closure of the kinetic equation (2.1) for each $\mathbb{M}$ satisfying conditions (I), (II), and also

$$\text{(III)} \quad \text{the cone } \mathbb{M}_c \text{ has a nonempty interior in } \mathbb{M} \tag{4.7}$$

We shall call such subspaces *admissible* and all other subspaces *inadmissible*.

It is clear from (4.6) that only polynomials $m(v)$ such that $m(v) \to -\infty$ as $|v| \to \infty$ comprise $\mathbb{M}_c$. Hence, condition (III) of (4.7) can only be met by linear spaces of polynomials over v with even maximal degree. In particular, the $\mathbb{M}$ of the Grad 13-moment closure (4.3) is inadmissible. In

general, a linear space of even maximal degree that is invariant under translational and orthogonal transformations and contains $\mathbb{E}$ can be admissible, but might not be. Examples of such admissible spaces with maximal degree two and four are

$$\begin{aligned}
&\text{maximal degree} = 2: && \mathbb{M} = \operatorname{span}\{1, v, |v|^2\} \equiv \mathbb{E} \\
& && \mathbb{M} = \operatorname{span}\{1, v, v \vee v\} \\
&\text{maximal degree} = 4: && \mathbb{M} = \operatorname{span}\{1, v, v \vee v, |v|^2 v, |v|^4\} \\
& && \mathbb{M} = \operatorname{span}\{1, v, v \vee v, v \vee v \vee v, |v|^4\} \\
& && \mathbb{M} = \operatorname{span}\{1, v, v \vee v, v \vee v \vee v, |v|^2 v \vee v\} \\
& && \mathbb{M} = \operatorname{span}\{1, v, v \vee v, v \vee v \vee v, v \vee v \vee v \vee v\}
\end{aligned} \tag{4.8}$$

while an example of an inadmissible space of maximal degree four that satisfies conditions (I) and (II) but not (III) is

$$\mathbb{M} = \operatorname{span}\left\{1, v, v \vee v, v \vee v \vee v, |v|^2 \left(v \vee v - \frac{1}{D} |v|^2 I\right)\right\} \tag{4.9}$$

In three spatial dimensions the admissible spaces listed in (4.8) have dimension 5, 10, 14, 21, 26, and 35, respectively. Each of these spaces except the fourth is generated by its highest degree basis elements ($|v|^2$, $v \vee v$, $|v|^4$, $|v|^2 v \vee v$, and $v \vee v \vee v \vee v$ in the examples) through the action of the translations $\mathscr{T}_u$ in condition (II) of (4.2). For each even degree $2n$ there are $n+1$ such spaces, one for each possible trace of the $2n$-fold tensor product of v. Spaces such as the fourth one above become prevalent as n increases. Of course, there is no need to consider only spaces of polynomials, but they will be used here to illustrate the closure procedure.

The closure procedure may now be stated simply. Let F in the moment system (4.1) have the form

$$F = \mathscr{M}(\boldsymbol{\alpha}) \equiv \exp(\boldsymbol{\alpha}^T \mathbf{m}(v)) \tag{4.10}$$

where $\boldsymbol{\alpha}^T$ is the transpose of some $\boldsymbol{\alpha} = \boldsymbol{\alpha}(t, x)$ with values in $\mathbb{R}^M$ such that $\boldsymbol{\alpha}^T \mathbf{m}(v)$ lies in the cone $\mathbb{M}_c$. This results in the system of M equations (4.1) for the M unknowns $\boldsymbol{\alpha}$ given by

$$\partial_t \langle \mathbf{m} \mathscr{M}(\boldsymbol{\alpha}) \rangle + \nabla_x \cdot \langle v \mathbf{m} \mathscr{M}(\boldsymbol{\alpha}) \rangle = \langle \mathbf{m} \mathscr{C}(\mathscr{M}(\boldsymbol{\alpha})) \rangle \tag{4.11}$$

where the moment densities, moment fluxes, and collisional terms are expressed in terms of α as the integrals

$$\langle \mathbf{m} \mathscr{M}(\boldsymbol{\alpha}) \rangle, \quad \langle v \mathbf{m} \mathscr{M}(\boldsymbol{\alpha}) \rangle, \quad \langle \mathbf{m} \mathscr{C}(\mathscr{M}(\boldsymbol{\alpha})) \rangle \tag{4.12}$$

Each admissible space $\mathbb{M}$ generates such a closure, and the hierarchy of such closures is partially ordered by the relation $\subset$ acting on the admissible spaces.

For admissible spaces of maximal degree two the first two integrals in (4.12) may be evaluated explicitly, allowing direct study of the moment system (4.11). For example, when $\mathbb{M} = \text{span}\{1, v, |v|^2\}$ one can see from (4.10) that $\mathcal{M} = \mathcal{E}$, so that the collisional term vanishes and (4.11) becomes the Euler system (3.6). Less trivial is the case when $\mathbb{M} = \text{span}\{1, v, v \vee v\}$. In that case the moment densities and fluxes can always be evaluated as Gaussian integrals and even the collisional term can be evaluated for many classical collision operators $\mathcal{C}$. While this so-called Gaussian closure improves upon the Euler system by having a nontrivial stress, it still has a heat flux that is identically zero. Regardless of this deficiency, this closure will be examined in considerable detail in the next section.

For admissible spaces of maximal degree four or more the integrals in (4.12) are impossible to evaluate explicitly as functions of $\boldsymbol{\alpha}$. Indeed, the efficient evaluation of these integrals would seem a formidable obstruction to any practical implementation of these closures. However, the moment system (4.11) has remarkable structural features that make it highly attractive theoretically and that facilitate its practical implementation. This structure can be brought out by recasting the moment system (4.11) in terms of the density potential h^* and the flux potential j^* defined over the cone $\mathbb{M}_c$ by

$$h^*(\boldsymbol{\alpha}) \equiv \langle \mathcal{M}(\boldsymbol{\alpha}) \rangle, \qquad j^*(\boldsymbol{\alpha}) \equiv \langle v\mathcal{M}(\boldsymbol{\alpha}) \rangle \tag{4.13}$$

and the vector of collisional relaxation terms $\mathbf{r}^*$ defined by

$$\mathbf{r}^*(\boldsymbol{\alpha}) \equiv \langle \mathbf{m}\mathcal{C}(\mathcal{M}(\boldsymbol{\alpha})) \rangle \tag{4.14}$$

Differentiating (4.13) with respect to $\boldsymbol{\alpha}$ using (4.10) yields the relations

$$h^*_{\boldsymbol{\alpha}}(\boldsymbol{\alpha}) = \langle \mathbf{m}\mathcal{M}(\boldsymbol{\alpha}) \rangle, \qquad j^*_{\boldsymbol{\alpha}}(\boldsymbol{\alpha}) = \langle v\mathbf{m}\mathcal{M}(\boldsymbol{\alpha}) \rangle \tag{4.15}$$

where the right sides are just the moment densities and fluxes given in (4.12). The closed moment system (4.11) can therefore be put into the so-called potential form of Godunov[13]

$$\partial_t h^*_{\boldsymbol{\alpha}}(\boldsymbol{\alpha}) + \nabla_x \cdot j^*_{\boldsymbol{\alpha}}(\boldsymbol{\alpha}) = \mathbf{r}^*(\boldsymbol{\alpha}) \tag{4.16}$$

Moreover, because each component of v is in $\mathbb{M}$, each component of the flux potential j^* is itself a moment density and hence expressible in terms of first derivatives of the density potential h^*. Therefore, evaluating the left side of (4.16) requires only a twice differentiable evaluation of the scalar

function h^* in terms of $\boldsymbol{\alpha}$. Of course, such an evaluation of h^* is generally going to be quite complicated, but this is the price to be paid for the structural simplicity that emerges below.

The moment system (4.11) has many desirable properties that can be read off from its potential form (4.16), many of which are lacking in traditional closures. The most important of these is its hyperbolicity, which ensures that the system is at least linearly well-posed. This property follows from the fact that the density potential $h^* = h^*(\boldsymbol{\alpha})$ is a strictly convex function with a positive-definite Hessian matrix

$$h^*_{\boldsymbol{\alpha}\boldsymbol{\alpha}}(\boldsymbol{\alpha}) = \langle \mathbf{m}\mathbf{m}^T \mathscr{M}(\boldsymbol{\alpha}) \rangle \tag{4.17}$$

Indeed, a direct calculation using (4.10) shows that for every $\boldsymbol{\gamma} \in \mathbb{R}^M$ one has

$$\boldsymbol{\gamma}^T h^*_{\boldsymbol{\alpha}\boldsymbol{\alpha}}(\boldsymbol{\alpha})\, \boldsymbol{\gamma} = \langle (\boldsymbol{\gamma}^T \mathbf{m})^2\, \mathscr{M}(\boldsymbol{\alpha}) \rangle \geqslant 0 \tag{4.18}$$

with equality if and only if $\boldsymbol{\gamma} = 0$. The hyperbolicity of (4.16) then becomes evident upon rewriting it in the form

$$h^*_{\boldsymbol{\alpha}\boldsymbol{\alpha}}(\boldsymbol{\alpha})\, \partial_t \boldsymbol{\alpha} + j^*_{\boldsymbol{\alpha}\boldsymbol{\alpha}}(\boldsymbol{\alpha}) \cdot \nabla_x \boldsymbol{\alpha} = \mathbf{r}^*(\boldsymbol{\alpha}) \tag{4.19}$$

By the positive definiteness of $h^*_{\boldsymbol{\alpha}\boldsymbol{\alpha}}$ and the symmetry of $j^*_{\boldsymbol{\alpha}\boldsymbol{\alpha}}$, this has the Godunov form of a symmetric hyperbolic system for $\boldsymbol{\alpha}$.[13] The characteristic velocities associated with any wave vector $k \in \mathbb{R}^D$ are determined by the critical values of the Rayleigh quotient

$$\boldsymbol{\gamma} \mapsto \frac{\boldsymbol{\gamma}^T k \cdot j^*_{\boldsymbol{\alpha}\boldsymbol{\alpha}}(\boldsymbol{\alpha})\, \boldsymbol{\gamma}}{\boldsymbol{\gamma}^T h^*_{\boldsymbol{\alpha}\boldsymbol{\alpha}}(\boldsymbol{\alpha})\, \boldsymbol{\gamma}} \tag{4.20}$$

considered as a function over nonzero $\boldsymbol{\gamma} \in \mathbb{R}^M$.

Another important property of the moment system (4.11) that is exposed by the its potential form (4.16) is the existence of an entropy that is locally dissipated. Indeed, multiplying (4.19) on the left by $\boldsymbol{\alpha}^T$ yields

$$\partial_t (\boldsymbol{\alpha}^T h^*_{\boldsymbol{\alpha}}(\boldsymbol{\alpha}) - h^*(\boldsymbol{\alpha})) + \nabla_x \cdot (\boldsymbol{\alpha}^T j^*_{\boldsymbol{\alpha}}(\boldsymbol{\alpha}) - j^*(\boldsymbol{\alpha})) = \boldsymbol{\alpha}^T \mathbf{r}^*(\boldsymbol{\alpha}) \tag{4.21}$$

where

$$\boldsymbol{\alpha}^T \mathbf{r}^*(\boldsymbol{\alpha}) = \langle \boldsymbol{\alpha}^T \mathbf{m} \mathscr{C}(\mathscr{M}(\boldsymbol{\alpha})) \rangle = \langle \log \mathscr{M}(\boldsymbol{\alpha})\, \mathscr{C}(\mathscr{M}(\boldsymbol{\alpha})) \rangle \tag{4.22}$$

The local dissipation relation (2.6) for the collision operator $\mathscr{C}$ then implies that

$$\boldsymbol{\alpha}^T \mathbf{r}^*(\boldsymbol{\alpha}) \leqslant 0 \tag{4.23}$$

while the characterization (2.8) of the equilibria of $\mathscr{G}$ shows that equilibria of $\mathbf{r}^*$ are characterized by the equivalence of the following statements:

$$\begin{aligned} &\text{(i)} \quad \boldsymbol{\alpha}^T \mathbf{r}^*(\boldsymbol{\alpha}) = 0 \\ &\text{(ii)} \quad \mathbf{r}^*(\boldsymbol{\alpha}) = 0 \\ &\text{(iii)} \quad \boldsymbol{\alpha}^T \mathbf{m} \in \mathbb{E} \end{aligned} \tag{4.24}$$

Moreover, the density in (4.21) may be put in the form

$$\begin{aligned} \boldsymbol{\alpha}^T h_{\boldsymbol{\alpha}}^*(\boldsymbol{\alpha}) - h^*(\boldsymbol{\alpha}) &= \langle \boldsymbol{\alpha}^T \mathbf{m} \mathscr{M}(\boldsymbol{\alpha}) \rangle - \langle \mathscr{M}(\boldsymbol{\alpha}) \rangle \\ &= \langle \mathscr{M}(\boldsymbol{\alpha}) \log (\mathscr{M}(\boldsymbol{\alpha})) - \mathscr{M}(\boldsymbol{\alpha}) \rangle \end{aligned} \tag{4.25}$$

from which it is seen to be exactly equal to the entropy density in (2.9) associated with the distribution $\mathscr{M}(\boldsymbol{\alpha})$.

Traditionally moment closures have been expressed in terms of the moment densities, denoted as $\boldsymbol{\alpha}$, which by (4.15) are given as a function of $\boldsymbol{\alpha}$ by

$$\boldsymbol{\rho} \equiv \langle \mathbf{m} \mathscr{M}(\boldsymbol{\alpha}) \rangle = h_{\boldsymbol{\alpha}}^*(\boldsymbol{\alpha}) \tag{4.26}$$

This relation can be inverted in terms of the function $h = h(\boldsymbol{\rho})$, which is the Legendre transform of the strictly convex function h^*. Specifically, h is defined by

$$h(\boldsymbol{\rho}) + h^*(\boldsymbol{\alpha}) = \boldsymbol{\alpha}^T \boldsymbol{\rho} \tag{4.27}$$

where $\boldsymbol{\rho}$ and $\boldsymbol{\alpha}$ are related by (4.26). Then $\boldsymbol{\alpha}$ can be expressed as a function of $\boldsymbol{\rho}$ by

$$\boldsymbol{\alpha} = h_{\boldsymbol{\rho}}(\boldsymbol{\rho}) \tag{4.28}$$

By comparing (4.27) with (4.25), it is seen that $h(\boldsymbol{\rho})$ is the entropy density; this relation thereby gives physical meaning to both $\boldsymbol{\alpha}$ and h^*, which heretofore might have seemed artificial.

The moment system (4.16) can now be formulated in terms of the moment densities as

$$\partial_t \boldsymbol{\rho} + \nabla_x \cdot j_{\boldsymbol{\alpha}}^*(h_{\boldsymbol{\rho}}(\boldsymbol{\rho})) = \mathbf{r}^*(h_{\boldsymbol{\rho}}(\boldsymbol{\rho})) \tag{4.29}$$

An explicit expression of the moment fluxes in terms of the moment densities is no less complicated or impossible than it was for the $\boldsymbol{\alpha}$ formulation

(4.16). The hyperbolicity of this formulation (4.29) becomes evident upon rewriting it as

$$\partial_t \boldsymbol{\rho} + j^*_{\alpha\alpha}(h_{\boldsymbol{\rho}}(\boldsymbol{\rho}))h_{\boldsymbol{\rho}\boldsymbol{\rho}}(\boldsymbol{\rho}) \cdot \nabla_x \boldsymbol{\rho} = \mathbf{r}^*(h_{\boldsymbol{\rho}}(\boldsymbol{\rho})) \tag{4.30}$$

and observing that the Hessian matrix $h_{\boldsymbol{\rho}\boldsymbol{\rho}}(\boldsymbol{\rho})$ is a Friedrichs–Lax symmetrizer[12] of this equation. The equivalence of the Godunov and the Friedrichs–Lax forms for general hyperbolic systems was proved in.[32] Moreover, it is seen easily from (4.27) that the local entropy dissipation law (4.21) can be formulated in terms of the moment densities as

$$\partial_t h(\boldsymbol{\rho}) + \nabla_x \cdot j(\boldsymbol{\rho}) = h_{\boldsymbol{\rho}}(\boldsymbol{\rho})^T \mathbf{r}^*(h_{\boldsymbol{\rho}}(\boldsymbol{\rho})) \tag{4.31}$$

where the entropy flux $j = j(\boldsymbol{\rho})$ is given by

$$j(\boldsymbol{\rho}) + j^*(\boldsymbol{\alpha}) = \boldsymbol{\alpha}^T j^*_{\boldsymbol{\alpha}}(\boldsymbol{\alpha}) \tag{4.32}$$

with $\boldsymbol{\alpha}$ related to $\boldsymbol{\rho}$ by (4.28). Hence, by (4.23) and (4.24), $h = h(\boldsymbol{\rho})$ is a strictly convex entropy for the system (4.29) both in the sense of "extended thermodynamics"[33] and in the more general sense of relaxation systems.[8]

The implicit definition of the entropy density h through (4.27) provides a practical algorithm for computing both h and $\boldsymbol{\alpha}$ as functions of $\boldsymbol{\rho}$. This is particularly useful because there is no explicit expression for h, not even on the level of a quadrature formula such as (4.13) prescribes the density potential h^*, and hence no explicit expression for $\boldsymbol{\alpha}$ as a function of $\boldsymbol{\rho}$. Suppose that the integral in (4.11) that defines the density potential h^* and two of its derivatives can be effectively evaluated through a combination of asymptotics and numerics. Then, given a value of $\boldsymbol{\rho}$, it follows from (4.26) and (4.27) that the values of $\boldsymbol{\alpha}$ and $h(\boldsymbol{\rho})$ can be obtained numerically by solving the minimization problem

$$h(\boldsymbol{\rho}) = -\min_{\boldsymbol{\alpha}} \{h^*(\boldsymbol{\alpha}) - \boldsymbol{\alpha}^T \boldsymbol{\rho}\} \tag{4.33}$$

Of course, the resulting $\boldsymbol{\alpha}$ can then be used to evaluate the moment fluxes $j^*_{\boldsymbol{\alpha}}$ and the collisional vector $\mathbf{r}^*$, which can then be used to update $\boldsymbol{\rho}$ through a difference approximation to (4.16). In particular, as was remarked following (4.16), the moment fluxes can be evaluated as second derivatives of the density potential h^*. More details on numerical algorithms that exploit this approach will be given in Section 8.

The choice of the exponential form of the density (4.10) was not made merely to maintain nonnegativity; many other choices would have achieved that objective. Nor was it made merely to ensure hyperbolicity; many other choices would have achieved that objective, too. Rather, its significance lies

in the fact that the exponential function is the Legendre transform of the entropy density $F \mapsto F \log F - F$. It is this relation that leads to the local dissipation properties (4.23) and (4.24), hence capturing the structures identified in ref. 8 as leading to formally well-posed fluid dynamical approximations. This Legendre relation also implies that (4.10) is the unique density F that minimizes the entropy subject to the constraint that its moments $\langle \mathbf{m}F \rangle$ are fixed. More specifically, given a density vector $\boldsymbol{\rho}$, one has

$$h(\boldsymbol{\rho}) = \min_F \{ \langle F \log F - F \rangle : \langle \mathbf{m}F \rangle = \boldsymbol{\rho} \} \tag{4.34}$$

with $\boldsymbol{\alpha}$ related to $\boldsymbol{\rho}$ by (4.28). This kind of so-called *entropy minimization principle* has long played a role in statistical physics to provide various closures,[10, 16] whereas here it is viewed as a logical consequence of the closure capturing the proper structures.

It was shown in ref. 8 how the existence of such an entropy leads formally to both the correct Euler approximation and a consistent Navier–Stokes approximation. In general the Navier–Stokes approximation of the moment system (4.11) will have the same form as that for the kinetic equation (2.1), possibly differing only in the numerical value of the viscosity and heat conductivity coefficients. The question of the correctness of the Navier–Stokes approximation will he addressed in Section 6.

Some recent works have employed exponentially based closures of the form (4.10). Dreyer[10] did so within the context of extended thermodynamics.[33] However, he treated the exponential formally, never imposing a condition like (III), and proceeded to retain only the quadratic terms in the exponent while expanding the rest as a polynomial. Both the entropy and hyperbolic structure are generally lost in the resulting moment equations. Apparently independently, Gorbin and Karlin[16, 17] put forth a general procedure for deriving dynamical equations (not necessarily for moments) for nonequilibrium systems based on an *entropy minimization principle*. When the form of the density is given by (4.10), their closure procedure replaces one of the moment densities with the entropy density as a fundamental variable, superficially leading to a system that is formally equivalent to (4.11). So long as the solutions of this system are classical, then the solutions will likewise be equivalent. However, when the solutions become weak due to the development of singularities, then the profound differences in the underlying viewpoints lead to quantitative differences in the solutions. This can be best understood by applying their procedure to the family of Maxwellians, formally obtaining the Euler equations (3.6). However, their fundamental equations are the mass and momentum local

conservation laws of (3.6) and the entropy equation (3.7) taken as an equality, which is inconsistent with energy conservation for weak solutions. Indeed, they do not address how to handle the eventual development of singularities at all. Moreover, they address neither the hyperbolicity of the resulting systems nor the recovery of the Euler and Navier–Stokes approximations.

5. THE GAUSSIAN CLOSURE

The linear space $\mathbb{M} = \mathbb{G} \equiv \text{span}\{1, v, v \vee v\}$ is the smallest admissible space that properly contains $\mathbb{E}$, and thus generates the simplest closure of the type developed in the last section which extends beyond the Euler system. The dimension of $\mathbb{G}$ is $(D+1)(D+2)/2$ in general, ten when $D=3$. The entropy-minimizing densities (4.10) for this space can be parametrized by $\rho \in \mathbb{R}_+$, $u \in \mathbb{R}^D$, and $\Theta \in \mathbb{R}_+^{D \vee D}$, where $\mathbb{R}_+^{D \vee D}$ denotes the set of symmetric, positive-definite $D \times D$ matrices; they take the form of Gaussian densities, given by

$$\mathcal{G}(\rho, u, \Theta) \equiv \frac{\rho}{[\det(2\pi\Theta)]^{1/2}} \exp\left(-\frac{1}{2}(v-u)\cdot\Theta^{-1}(v-u)\right) \tag{5.1}$$

This translates into the notation of the last section by identifying $\mathbf{m}(v) = (1, v, v \vee v)^T$ and

$$\boldsymbol{\alpha} = \left(\log\left(\frac{\rho}{[\det(2\pi\Theta)]^{1/2}}\right) - \frac{1}{2}u\cdot\Theta^{-1}u,\ \Theta^{-1}u,\ -\frac{1}{2}\Theta^{-1}\right)^T \tag{5.2}$$

so that $\mathcal{G}(\rho, u, \Theta) = \mathcal{M}(\boldsymbol{\alpha})$. The positive definiteness of Θ is required for condition (III) of (4.7) to be satisfied. Relation (5.2) may be easily inverted to express (ρ, u, Θ) directly in terms of $\boldsymbol{\alpha}$. However, the simplicity of this closure stems from the fact that all moments can be computed for Gaussian densities and these moments can be expressed better in the (ρ, u, Θ) than in the $\boldsymbol{\alpha}$ notation. For example, integration of the basic moments $1, v, v \vee v$, and $v \vee v \vee v$ over the Gaussian density $\mathcal{G}(\rho, u, \Theta)$ yields

$$\begin{aligned}
\langle \mathcal{G}(\rho, u, \Theta)\rangle &= \rho \\
\langle v\mathcal{G}(\rho, u, \Theta)\rangle &= \rho u \\
\langle v \vee v\mathcal{G}(\rho, u, \Theta)\rangle &= \rho u \vee u + \rho\Theta \\
\langle v \vee v \vee v\mathcal{G}(\rho, u, \Theta)\rangle &= \rho u \vee u \vee u + 3\rho\Theta \vee u
\end{aligned} \tag{5.3}$$

Taking the trace of the $v \vee v$ moment and comparing with (3.1) shows that $\theta = (1/D)\,\mathrm{tr}(\Theta)$. Comparing (5.3) with (3.2), we find that the stress Σ and heat flux q are given by

$$\Sigma = \rho(\Theta - \theta I), \qquad q = 0 \tag{5.4}$$

Notice that when $\Theta = \theta I$ the Gaussian density $\mathscr{G}$ reduces to the equilibrium density $\mathscr{E}$ and formulas (5.3) and (5.4) reduce to their values for the Euler closure. Because Gaussian densities admit no heat flux, the Gaussian closure is of limited practical interest; however, it provides an approximation that in some respects lies between the Euler and the Navier–Stokes approximations.

The moment equations governing $\rho = \rho(t,x)$, $u = u(t,x)$, and $\Theta = \Theta(t,x)$ are

$$\partial_t \rho + \nabla_x \cdot (\rho u) = 0 \tag{5.5a}$$

$$\partial_t (\rho u) + \nabla_x \cdot (\rho u \vee u + \rho\Theta) = 0 \tag{5.5b}$$

$$\partial_t (\rho u \vee u + \rho\Theta) + \nabla_x \cdot (\rho u \vee u \vee u + 3\rho\Theta \vee u) = \Xi(\rho, \Theta) \tag{5.5c}$$

where, following (4.14), the collisional term Ξ is shown to be independent of u by first using the translation invariance (2.11) and then using local conservation (2.3) to obtain

$$\begin{aligned} \Xi(\rho, \Theta) &\equiv \langle v \vee v \mathscr{C}(\mathscr{G}(\rho, 0, \Theta)) \rangle \\ &= \langle (v-u) \vee (v-u)\, \mathscr{C}(\mathscr{G}(\rho, u, \Theta)) \rangle \\ &= \langle v \vee v \mathscr{C}(\mathscr{G}(\rho, u, \Theta)) \rangle \end{aligned} \tag{5.6}$$

The local energy conservation law is recovered by taking the trace of (5.5c),

$$\partial_t \left(\frac{1}{2}\rho |u|^2 + \frac{D}{2}\rho\theta \right) + \nabla_x \cdot \left(\frac{1}{2}\rho |u|^2 u + \frac{D}{2}\rho\theta u + \rho\Theta u \right) = 0 \tag{5.7}$$

Notice that when $\Theta = \theta I$ the momentum equation (5.5b) and the energy equation (5.7) reduce to those given by the Euler closure (3.6).

The Gaussian closure has a long history in kinetic theory—remarkably, longer than the Boltzmann equation itself. Indeed, six years before Boltzmann[6] showed that Maxwell's general "equation of continuity" could be reformulated as an evolution equation for F, Maxwell himself raised the possibility of applying this closure to a gas of what are now known as the Maxwell molecules.[31] Maxwell did not pursue the matter because his theory of gas dynamics, in which the molecules were assumed to be near

local equilibrium, did not require it. In the 1950s and 1960s, however, the closure was rediscovered and advocated by many (for example, see refs. 22 and 23) as a way to derive closed systems of moment equations to describe gases that are not near local equilibrium. None of these works, however, treated it within the context of a larger hierarchy such as the one studied here.

The physical content of the moment equations (5.5) is brought out more clearly when they are expressed in terms of the convective, or Lagrangian, derivative $\partial_t + u \cdot \nabla_x$. Using (5.5a) to eliminate time derivatives of ρ from (5.5b) and (5.5c) gives

$$(\partial_t + u \cdot \nabla_x)\, \rho + \rho \nabla_x \cdot u = 0 \tag{5.8a}$$

$$\rho(\partial_t + u \cdot \nabla_x)\, u + \nabla_x \cdot (\rho \Theta) = 0 \tag{5.8b}$$

$$\rho(\partial_t + u \cdot \nabla_x)(u \vee u + \Theta) + 2u \vee \nabla_x \cdot (\rho \Theta) + \rho(\Theta \cdot \nabla_x u + (\nabla_x u)^T \cdot \Theta) = \Xi(\rho, \Theta) \tag{5.8c}$$

It is seen from (5.8b) that

$$\rho(\partial_t + u \cdot \nabla_x)(u \vee u) + 2u \vee \nabla_x \cdot (\rho \Theta) = 0 \tag{5.9}$$

Subtracting (5.9) from (5.8c) and dividing by ρ leads to

$$(\partial_t + u \cdot \nabla_x)\, \Theta + (\Theta \cdot \nabla_x u + (\nabla_x u)^T \cdot \Theta) = \frac{1}{\rho} \Xi(\rho, \Theta) \tag{5.10}$$

This equation clearly shows both the distortion of Θ by the velocity flow field u and the fact that its evolution is consistent with it remaining a symmetric matrix.

In order to see that Θ also remains positive definite, multiply (5.10) on the left by Θ^{-1} and then take the trace to obtain

$$\operatorname{tr}(\Theta^{-1}(\partial_t + u \cdot \nabla_x)\, \Theta) + 2\nabla_x \cdot u = \frac{1}{\rho} \operatorname{tr}(\Theta^{-1} \Xi(\rho, \Theta)) \tag{5.11}$$

Upon using the general identity $\partial_s \log(\det \Theta) = \operatorname{tr}(\Theta^{-1} \partial_s \Theta)$ and (5.8a), one finds

$$(\partial_t + u \cdot \nabla_x) \log\left(\frac{\det \Theta}{\rho^2}\right) = (\partial_t + u \cdot \nabla_x) \log(\det \Theta) - 2(\partial_t + u \cdot \nabla_x) \log(\rho)$$

$$= \frac{1}{\rho} \operatorname{tr}(\Theta^{-1} \Xi(\rho, \Theta)) \tag{5.12}$$

Now recalling the definition (5.6) of $\Xi(\rho, \Theta)$, the form (5.1) of $\mathscr{G}(\rho, u, \Theta)$, and the local entropy dissipation (2.6), one has

$$\begin{aligned}\tfrac{1}{2}\operatorname{tr}(\Theta^{-1}\Xi(\rho,\Theta)) &= \tfrac{1}{2}\langle (v-u)\cdot\Theta^{-1}(v-u)\,\mathscr{C}(\mathscr{G}(\rho,u,\Theta))\rangle \\ &= -\langle \log(\mathscr{G}(\rho,u,\Theta))\,\mathscr{C}(\mathscr{G}(\rho,u,\Theta))\rangle \geqslant 0 \end{aligned} \tag{5.13}$$

It follows from (5.12) that $\det\Theta$ never passes through zero so long as ρ remains positive. Hence, its eigenvalues remain bounded away from zero and Θ remains positive definite.

After multiplying (5.12) by $-\frac{1}{2}$ and using the density equation (5.8a) yet again, we can bring it into the divergence form

$$\partial_t(\rho\sigma) + \nabla_x\cdot(\rho u\sigma) = -\tfrac{1}{2}\operatorname{tr}(\Theta^{-1}\Xi(\rho,\Theta)) \tag{5.14}$$

where σ is the specific entropy, which is given by

$$\sigma \equiv \frac{1}{\rho}\langle \mathscr{G}\log\mathscr{G} - \mathscr{G}\rangle = \log\left(\frac{\rho}{[\det(2\pi\Theta)]^{1/2}}\right) - \frac{D+2}{2} \tag{5.15}$$

Moreover, for any $(\rho, u, \Theta)\in\mathbb{R}_+\times\mathbb{R}^D\times\mathbb{R}_+^{D\times D}$ the following statements are equivalent:

$$\begin{aligned} &\text{(i)} \quad \operatorname{tr}(\Theta^{-1}\Xi(\rho,\Theta)) = 0 \\ &\text{(ii)} \quad \Xi(\rho,\Theta) = 0 \\ &\text{(iii)} \quad \Theta = \theta I \qquad \text{for some} \quad \theta\in\mathbb{R}_+ \end{aligned} \tag{5.16}$$

Just as for the Euler equations, the Gaussian moment equations (5.8) admit a large family of formal dissipation laws in the form

$$\partial_t(\rho h(\sigma)) + \nabla_x\cdot(\rho u h(\sigma)) = -\tfrac{1}{2}h'(\sigma)\operatorname{tr}(\Theta^{-1}\Xi(\rho,\Theta)) \tag{5.17}$$

where $h = h(\sigma)$ is any differentiable function over $\mathbb{R}$. Moreover, ρh will be an entropy density for (5.8) in the sense of ref. 8 whenever $h'(\sigma) > 0$, and strictly convex whenever h satisfies (3.10). The choice $h(\sigma) = \sigma$ in (5.17) recovers (5.14).

Now we turn to the second step of our closure procedure, namely, the treatment of the collisional term $\Xi(\rho, \Theta)$. In doing so, we will illustrate some key difficulties faced for higher order closures within the context of the simpler Gaussian closure. The effect of the collision term on deviations

from the local equilibrium approximation can be computed systematically using a "Chapman–Enskog" analysis of the scaled moment equation

$$\partial_t(\rho u \vee u + \rho\Theta) + \nabla_x \cdot (\rho u \vee u \vee u + 3\rho\Theta \vee u) = \frac{1}{\varepsilon}\Xi(\rho, \Theta) \quad (5.18)$$

where ε is a dimensionless number that gives the order of the collisional length scales over the macroscopic gradient length scales. The traceless part of (5.10) is then simply

$$(\partial_t + u \cdot \nabla_x)(\Theta - \theta I) + \left(\Theta \cdot \nabla_x u + (\nabla_x u)^T \cdot \Theta - \frac{2}{D}\operatorname{tr}(\Theta \cdot \nabla_x u) I\right) = \frac{1}{\varepsilon\rho}\Xi(\rho, \Theta) \quad (5.19)$$

The Chapman–Enskog procedure then expands Θ in ε as

$$\Theta = \theta I + \varepsilon\,\Theta^{(1)} + \varepsilon^2\Theta^{(2)} + \cdots \quad (5.20)$$

where, upon setting (5.20) into (5.19), each $\Theta^{(k)}$ is to be expressed in terms of the fluid variables (ρ, u, θ) and their spatial derivatives subject to the constraint $\operatorname{tr}(\Theta^{(k)}) = 0$.

The "Navier–Stokes" approximation is obtained from the leading balance, which occurs at order ε^0, where $\Theta^{(1)}$ is found to satisfy

$$\rho\theta\left(\nabla_x u + (\nabla_x u)^T - \frac{2}{D}\nabla_x \cdot u I\right) = \Theta^{(1)} : \partial_\Theta \Xi(\rho, \theta I) \quad (5.21)$$

Here the right side is computed directly from (5.6) to be

$$\Theta^{(1)} : \partial_\Theta \Xi(\rho, \theta I) = -\langle v \vee v D\mathscr{C}(\mathscr{E}(\rho, 0, \theta))\,\Theta^{(1)} : \partial_\Theta \mathscr{G}(\rho, 0, \theta I)\rangle \quad (5.22)$$

where $D\mathscr{C}(\mathscr{E})$ is defined in (2.14). The derivative of $\mathscr{G}$ above is computed from (5.1) as

$$\begin{aligned}\Theta^{(1)} : \partial_\Theta \mathscr{G}(\rho, 0, \theta I) &= \mathscr{E}(\rho, 0, \theta)\left(\frac{1}{2} v \cdot \Theta^{-1}\Theta^{(1)}\Theta^{-1} v - \frac{1}{2}\operatorname{tr}(\Theta^{-1}\Theta^{(1)})\right)\Big|_{\Theta = \theta I} \\ &= \frac{1}{2}\mathscr{E}(\rho, 0, \theta)\frac{1}{\theta}\left(\frac{v \vee v}{\theta} - I\right) : \Theta^{(1)} \end{aligned} \quad (5.23)$$

Combining (5.22) and (5.23) while using definitions (2.14) of $\mathscr{L}_\mathscr{E}$ and (3.5a) of A gives

$$\Theta^{(1)} : \partial_\Theta \Xi(\rho, \theta I) = -\tfrac{1}{2}\langle A\mathscr{E}\mathscr{L}_\mathscr{E} A\rangle : \Theta^{(1)} \quad (5.24)$$

By the orthogonal symmetry of $\mathscr{L}_{\mathscr{E}}$ and the fact that $\mathrm{tr}(A)=0$, the components of $\langle A\mathscr{E}\mathscr{L}_{\mathscr{E}}A\rangle$ satisfy the identity

$$\langle A_{ij}\mathscr{E}\mathscr{L}_{\mathscr{E}}A_{kl}\rangle=\eta_G\left(\delta_{ik}\delta_{jl}+\delta_{il}\delta_{jk}-\frac{2}{D}\delta_{ij}\delta_{kl}\right) \tag{5.25}$$

where $\eta_G=\eta_G(\rho,\theta)$ is defined by

$$\eta_G=\frac{1}{(D-1)(D+2)}\langle A:\mathscr{E}\mathscr{L}_{\mathscr{E}}A\rangle \tag{5.26}$$

The right side of (5.21) can be evaluated by using (5.24) and (5.25) and recalling that $\mathrm{tr}(\Theta^{(1)})=0$ to obtain

$$\rho\theta\left(\nabla_x u+(\nabla_x u)^T-\frac{2}{D}\nabla_x\cdot uI\right)=-\eta_G\Theta^{(1)} \tag{5.27}$$

Hence, the stress $\rho\Theta^{(1)}$ takes the form

$$\rho\Theta^{(1)}=-\mu_G(\rho,\theta)\left(\nabla_x u+(\nabla_x u)^T-\frac{2}{D}\nabla_x\cdot uI\right) \tag{5.28}$$

where μ_G is the viscosity for the Gaussian closure, which is given by

$$\mu_G(\rho,\theta)=\frac{\rho^2\theta}{\eta_G(\rho,\theta)} \tag{5.29}$$

The positivity of both η_G and μ_G is a consequence of (2.23).

When $\mathscr{L}_{\mathscr{E}}$ is self-adjoint ($\mathscr{L}_{\mathscr{E}}^{\dagger}=\mathscr{L}_{\mathscr{E}}$) then a direct comparison can be made between the Navier–Stokes viscosity μ, given by (3.22a), and the Gaussian viscosity μ_G, given by (5.26) and (5.29). The Cauchy–Schwarz inequality can be used to obtain

$$\begin{aligned}\frac{\mu}{\mu_G}&=\left(\frac{1}{(D-1)(D+2)}\frac{1}{\rho}\right)^2\langle A:\mathscr{E}\mathscr{L}_{\mathscr{E}}A\rangle\langle A:\mathscr{E}\mathscr{L}_{\mathscr{E}}^{-1}A\rangle\\&\geqslant\left(\frac{1}{(D-1)(D+2)}\frac{1}{\rho}\langle A:\mathscr{E}A\rangle\right)^2=1\end{aligned} \tag{5.30}$$

Hence, we find that

$$0<\mu_G(\rho,\theta)\leqslant\mu(\rho,\theta) \tag{5.31}$$

with equality if and only if $\mathscr{L}_{\mathscr{E}}A=\lambda A$ for some positive eigenvalue λ, in which case $\eta_G=\rho\lambda$ and $\mu=\mu_G=\rho\theta/\lambda$. This is the case for the Boltzmann

equation when applied to the Maxwell gas,[7] but not when applied to more general gases. For most classical collision operators $\mathscr{L}_{\mathscr{C}}$ is indeed self-adjoint and inequality (5.31) is strict.

The Gaussian moment equations (5.5) are very explicit, with the exception of the collision term $\Xi(\rho, \Theta)$ defined by (5.6). For some collision operators $\mathscr{C}$ the integrals in (5.6) can be performed and a simple expression for $\Xi(\rho, \Theta)$ obtained;[28] however, that is the exception rather than the rule. In any event, as the remarks after (5.31) indicate, the associated viscosity μ_G will generally be smaller than the Navier–Stokes viscosity μ. If the solution to the moment equations is to properly extend into fluid dynamical regimes, it is important to modify the collision operator so as to match the moment viscosity and the Navier–Stokes viscosity.

In cases when $\Xi(\rho, \Theta)$ is effectively computable, this may be achieved by replacing $\mathscr{C}$ with the rescaled collision operator

$$\tilde{\mathscr{C}}(F) = \frac{\mu_G(\rho, \theta)}{\mu(\rho, \theta)} \mathscr{C}(F) \tag{5.32}$$

where ρ and θ are recovered from the moments of F by using (3.1). This modified collision operator satisfies all the conservation, dissipation, and symmetry requirements laid down in Section 2, so the foregoing theory applies directly. The associated collision term is then

$$\tilde{\Xi}(\rho, \Theta) = \frac{\mu_G(\rho, \theta)}{\mu(\rho, \theta)} \Xi(\rho, \Theta) \tag{5.33}$$

The resulting modified moment equations (5.5) will recover the correct Navier–Stokes momentum equation.

In cases when the evaluation of $\Xi(\rho, \Theta)$ is difficult or impossible, a more drastic modification of the collision operator is in.order. About the simplest thing to do is to replace $\mathscr{C}$ with the BGK collision operator[3]

$$\tilde{\mathscr{C}}(F) = \frac{\rho\theta}{\mu(\rho, \theta)} (\mathscr{E}(\rho, u, \theta) - F) \tag{5.34}$$

As before, this modified collision operator satisfies all the requirements laid down in Section 2, and the foregoing theory applies directly. By inserting (5.34) into (5.6), we easily find the associated collision term in the moment equation (5.5c) to be

$$\tilde{\Xi}(\rho, \Theta) = \frac{\rho^2\theta}{\mu(\rho, \theta)} (\theta I - \Theta) \tag{5.35}$$

As before, the resulting modified moment equations (5.5) will recover the correct Navier–Stokes momentum equation. However, this expression for the collision term has the virtue of being very easy to compute, requiring only knowledge of the Navier–Stokes viscosity μ. For this reason, the BGK modification (5.35) is the most practical to implement. The resulting equations are exactly those obtained by neglecting third-order moments in $v-u$ when evaluating the flux of the equation for the second-order moments while modeling the collisional terms with a simple relaxation tuned to recover the Navier–Stokes viscosity.

6. COLLISIONAL TERMS FOR HIGHER ORDER CLOSURES

Although simple, the Gaussian closure presented in the last section does not recover the correct Navier–Stokes approximation because the Gaussian densities (5.1) have no heat flux (5.4), and therefore no heat conduction term can arise in the energy equation (5.7). However, all admissible subspaces of degree four, (4.8), and higher have a nontrivial heat flux and hence hold out the possibility that the correct Navier–Stokes approximation can be recovered as the first correction to the Euler equations. In this section it is shown that all such higher order closures lead to the correct form (3.21) of the Navier–Stokes stress and heat flux. When $\mathscr{L}_g$ is self-adjoint the values of the viscosity and heat conduction derived from such closures will generally be less than the correct physical values. However, similar to what was done to recover the physical viscosity for the Gaussian closure, it will be shown that the collision operator can be modified so as to recover the correct physical viscosity and heat conduction.

Deviations of solutions of the moment system (4.14) from the local equilibrium approximation can be computed systematically using a "Chapman–Enskog" analysis of the scaled moment system

$$\partial_t \langle \mathbf{m}\mathscr{M}(\boldsymbol{\alpha})\rangle + \nabla_x \cdot \langle v\mathbf{m}\mathscr{M}(\boldsymbol{\alpha})\rangle = \frac{1}{\varepsilon}\langle \mathbf{m}\mathscr{C}(\mathscr{M}(\boldsymbol{\alpha}))\rangle \tag{6.1}$$

where $\mathscr{M}(\boldsymbol{\alpha})$ is defined in (4.8). The fluid dynamical variables (ρ, u, θ) are related to $\boldsymbol{\alpha}$ by

$$\langle \mathscr{M}(\boldsymbol{\alpha})\rangle = \rho, \qquad \langle v\mathscr{M}(\boldsymbol{\alpha})\rangle = \rho u, \qquad \left\langle \frac{1}{2}|v|^2 \mathscr{M}(\boldsymbol{\alpha})\right\rangle = \frac{1}{2}\rho|u|^2 + \frac{D}{2}\rho\theta \tag{6.2}$$

and satisfy the conservation laws (3.3) with the stress and the heat flux given by

$$\Sigma = \theta\langle A\mathscr{M}(\boldsymbol{\alpha})\rangle, \qquad q = \theta^{3/2}\langle B\mathscr{M}(\boldsymbol{\alpha})\rangle \tag{6.3}$$

The Chapman–Enskog procedure then expands $\boldsymbol{\alpha}$ in ε as

$$\boldsymbol{\alpha} = \boldsymbol{\alpha}^{(0)} + \varepsilon\, \boldsymbol{\alpha}^{(1)} + \varepsilon^2 \boldsymbol{\alpha}^{(2)} + \cdots \tag{6.4}$$

where $\boldsymbol{\alpha}^{(0)}$ is determined by the fluid variables through the relation

$$\mathscr{M}(\boldsymbol{\alpha}^{(0)}) = \mathscr{E}(\rho, u, \theta) \tag{6.5}$$

and where, upon setting (6.4) into (6.1), each $\boldsymbol{\alpha}^{(k)}$ is to be expressed in terms of the fluid variables (ρ, u, θ) and their spatial derivatives subject to the constraint (6.2).

By substituting (6.4) into the exponential form (4.8), we obtain the expansion

$$\mathscr{M}(\boldsymbol{\alpha}) = \mathscr{E}(1 + \varepsilon\, \mathbf{m}^T \boldsymbol{\alpha}^{(1)} + \varepsilon^2 [\mathbf{m}^T \boldsymbol{\alpha}^{(2)} + \tfrac{1}{2}(\mathbf{m}^T \boldsymbol{\alpha}^{(1)})^2] + \cdots) \tag{6.6}$$

Upon setting this expansion into relation (6.2) while recalling (6.5), one finds at order ε the constraint

$$\langle \mathscr{E} \mathbf{m}^T \rangle\, \boldsymbol{\alpha}^{(1)} = 0, \qquad \langle v \mathscr{E} \mathbf{m}^T \rangle\, \boldsymbol{\alpha}^{(1)} = 0, \qquad \langle |v|^2 \mathscr{E} \mathbf{m}^T \rangle\, \boldsymbol{\alpha}^{(1)} = 0 \tag{6.7}$$

Next, setting expansion (6.6) into the moment equations (6.1), we find that the leading order balance yields

$$\partial_t \langle \mathbf{m} \mathscr{E} \rangle + \nabla_x \cdot \langle v \mathbf{m} \mathscr{E} \rangle = -\langle \mathbf{m} \mathscr{E} \mathscr{L}_\mathscr{E} \mathbf{m}^T \rangle\, \boldsymbol{\alpha}^{(1)} \tag{6.8}$$

The nonconservative part of these equations can be isolated by multiplying on the left by an arbitrary $\boldsymbol{\gamma}^T$ where

$$\boldsymbol{\gamma} \in \mathbb{F}^\perp \equiv \{\boldsymbol{\gamma} \in \mathbb{R}^M : \boldsymbol{\gamma}^T \mathbf{m} \in \mathbb{E}^\perp\} \tag{6.9}$$

By so doing, we obtain

$$\begin{aligned} \boldsymbol{\gamma}^T \langle \mathbf{m} \mathscr{E} \mathscr{L}_\mathscr{E} \mathbf{m}^T \rangle\, \boldsymbol{\alpha}^{(1)} &= -\boldsymbol{\gamma}^T \left\langle \mathbf{m} \mathscr{E} \frac{\partial_t \mathscr{E} + v \cdot \nabla_x \mathscr{E}}{\mathscr{E}} \right\rangle \\ &= -\boldsymbol{\gamma}^T \left\langle \mathbf{m} \mathscr{E} (I - \mathscr{P}_\mathscr{E}) \frac{v \cdot \nabla_x \mathscr{E}}{\mathscr{E}} \right\rangle \end{aligned} \tag{6.10}$$

Because the vectors multiplying $\boldsymbol{\gamma}^T$ in the left-most and right-most expressions of (6.10) are both in $\mathbb{F}^\perp$, the $\boldsymbol{\gamma}^T$ may now be removed and (3.17) used to find that $\boldsymbol{\alpha}^{(1)}$ satisfies

$$\langle \mathbf{m}\mathscr{E}\mathscr{L}_{\mathscr{E}}\mathbf{m}^T\rangle\,\boldsymbol{\alpha}^{(1)} = -\frac{1}{2}\langle \mathbf{m}\mathscr{E}A\rangle : \left(\nabla_x u + (\nabla_x u)^T - \frac{2}{D}\nabla_x\cdot uI\right)$$
$$-\frac{1}{\theta^{1/2}}\langle \mathbf{m}\mathscr{E}B\rangle\cdot\nabla_x\theta \tag{6.11}$$

The matrix $\langle \mathbf{m}\mathscr{E}\mathscr{L}_{\mathscr{E}}\mathbf{m}^T\rangle$ is positive definite over $\mathbb{F}^{\perp}$ by (2.23) and therefore has a unique pseudoinverse $\langle \mathbf{m}\mathscr{E}\mathscr{L}_{\mathscr{E}}\mathbf{m}^T\rangle^{-1}$. The unique solution of (6.7) and (6.11) is

$$\boldsymbol{\alpha}^{(1)} = -\frac{1}{2}\langle \mathbf{m}\mathscr{E}\mathscr{L}_{\mathscr{E}}\mathbf{m}^T\rangle^{-1}\langle \mathbf{m}\mathscr{E}A\rangle : \left(\nabla_x u + (\nabla_x u)^T - \frac{2}{D}\nabla_x\cdot uI\right)$$
$$-\frac{1}{\theta^{1/2}}\langle \mathbf{m}\mathscr{E}\mathscr{L}_{\mathscr{E}}\mathbf{m}^T\rangle^{-1}\langle \mathbf{m}\mathscr{E}B\rangle\cdot\nabla_x\theta \tag{6.12}$$

Using the even/odd symmetry of $\mathscr{L}_{\mathscr{E}}$ to infer that

$$\begin{aligned}\langle A\mathscr{E}\mathbf{m}^T\rangle\langle \mathbf{m}\mathscr{E}\mathscr{L}_{\mathscr{E}}\mathbf{m}^T\rangle^{-1}\langle \mathbf{m}\mathscr{E}B\rangle &= 0\\ \langle B\mathscr{E}\mathbf{m}^T\rangle\langle \mathbf{m}\mathscr{E}\mathscr{L}_{\mathscr{E}}\mathbf{m}^T\rangle^{-1}\langle \mathbf{m}\mathscr{E}A\rangle &= 0\end{aligned} \tag{6.13}$$

and substituting (6.12) into (3.4) leads to the "Navier–Stokes" approximation

$$\begin{aligned}\Sigma &= \theta\langle A\mathscr{E}\mathbf{m}^T\rangle\,\boldsymbol{\alpha}^{(1)}\\ &= -\frac{1}{2}\theta\langle A\mathscr{E}\mathbf{m}^T\rangle\langle \mathbf{m}\mathscr{E}\mathscr{L}_{\mathscr{E}}\mathbf{m}^T\rangle^{-1}\langle \mathbf{m}\mathscr{E}A\rangle : \left(\nabla_x u + (\nabla_x u)^T - \frac{2}{D}\nabla_x\cdot uI\right)\\ q &= \theta^{3/2}\langle B\mathscr{E}\mathbf{m}^T\rangle\,\boldsymbol{\alpha}^{(1)}\\ &= -\theta\langle B\mathscr{E}\mathbf{m}^T\rangle\langle \mathbf{m}\mathscr{E}\mathscr{L}_{\mathscr{E}}\mathbf{m}^T\rangle^{-1}\langle \mathbf{m}\mathscr{E}B\rangle\cdot\nabla_x\theta\end{aligned} \tag{6.14}$$

By the symmetry of $\mathscr{L}_{\mathscr{E}}$ with respect to orthogonal transformations (2.25) and the fact that $\operatorname{tr}(A)=0$, the components of the above tensors can be evaluated in the spirit of (3.20), so the "Navier–Stokes" approximation (6.14) becomes

$$\begin{aligned}\Sigma &= -\mu_M\left(\nabla_x u + (\nabla_x u)^T - \frac{2}{D}\nabla_x\cdot uI\right)\\ q &= -\kappa_M\nabla_x\theta\end{aligned} \tag{6.15}$$

where the viscosity $\mu_M = \mu_M(\rho, \theta)$ and the heat conduction $\kappa_M = \kappa_M(\rho, \theta)$ are given by

$$\mu_M = \theta \frac{1}{(D-1)(D+2)} \operatorname{tr}(\langle \mathbf{m}\mathscr{E}A\rangle : A\mathscr{E}\mathbf{m}^T\rangle \langle \mathbf{m}\mathscr{E}\mathscr{L}_\mathscr{E}\mathbf{m}^T\rangle^{-1}) \quad (6.16a)$$

$$\kappa_M = \theta \frac{1}{D} \operatorname{tr}(\langle \mathbf{m}\mathscr{E}B\rangle \cdot \langle B\mathscr{E}\mathbf{m}^T\rangle \langle \mathbf{m}\mathscr{E}\mathscr{L}_\mathscr{E}\mathbf{m}^T\rangle^{-1}) \quad (6.16b)$$

The positivity of μ_M and κ_M is a consequence of (2.23) and the fact that the vectors $\langle \mathbf{m}\mathscr{E}A\rangle$ and $\langle \mathbf{m}\mathscr{E}B\rangle$ are nonzero for closures of higher order than the Gaussian closure. Indeed, for the Gaussian closure the vector $\langle \mathbf{m}\mathscr{E}B\rangle$ is zero, leading to zero heat conduction in that case. The functional independence of μ_M and κ_M on u is a consequence of Galilean invariance.

When $\mathscr{L}_\mathscr{E}$ is self-adjoint ($\mathscr{L}_\mathscr{E}^\dagger = \mathscr{L}_\mathscr{E}$), then a direct comparison can be made between the Navier–Stokes viscosity μ and heat conduction κ given by (3.21) and μ_M and κ_M given by (6.16). For each $g \in \mathbb{E}^\perp$ define the quadratic form $\mathscr{Q}$ acting on $\gamma \in \mathbb{F}^\perp$ as

$$\begin{aligned}\mathscr{Q}(\gamma) &\equiv \gamma^T \langle \mathbf{m}\mathscr{E}\mathscr{L}_\mathscr{E}\mathbf{m}^T\rangle\, \gamma - 2\gamma^T\langle \mathbf{m}\mathscr{E}g\rangle + \langle g\mathscr{E}\mathscr{L}_\mathscr{E}^{-1}g\rangle \\ &= \langle (\gamma^T\mathbf{m} - \mathscr{L}_\mathscr{E}^{-1}g)\,\mathscr{E}\mathscr{L}_\mathscr{E}(\gamma^T\mathbf{m} - \mathscr{L}_\mathscr{E}^{-1}g)\rangle \geqslant 0 \end{aligned} \quad (6.17)$$

This quantity is minimized when

$$\gamma = \gamma(g) \equiv \langle \mathbf{m}\mathscr{E}\mathscr{L}_\mathscr{E}\mathbf{m}^T\rangle^{-1}\langle \mathbf{m}\mathscr{E}g\rangle \quad (6.18)$$

at which value (6.17) becomes

$$\mathscr{Q}(\gamma(g)) = \langle g\mathscr{E}\mathscr{L}_\mathscr{E}^{-1}g\rangle - \langle g\mathscr{E}\mathbf{m}^T\rangle\langle \mathbf{m}\mathscr{E}\mathscr{L}_\mathscr{E}\mathbf{m}^T\rangle^{-1}\langle \mathbf{m}\mathscr{E}g\rangle \geqslant 0 \quad (6.19)$$

with equality if and only if $\mathscr{L}_\mathscr{E}^{-1}g \in \mathbb{M}$.

By letting g in (6.19) be an arbitrary linear combination of the components of first A and then B, one deduces the quadratic form inequalities

$$\begin{aligned}\langle A\mathscr{E}\mathscr{L}_\mathscr{E}^{-1}A\rangle &\geqslant \langle A\mathscr{E}\mathbf{m}^T\rangle\langle \mathbf{m}\mathscr{E}\mathscr{L}_\mathscr{E}\mathbf{m}^T\rangle^{-1}\langle \mathbf{m}\mathscr{E}A\rangle \\ \langle B\mathscr{E}\mathscr{L}_\mathscr{E}^{-1}B\rangle &\geqslant \langle B\mathscr{E}\mathbf{m}^T\rangle\langle \mathbf{m}\mathscr{E}\mathscr{L}_\mathscr{E}\mathbf{m}^T\rangle^{-1}\langle \mathbf{m}\mathscr{E}B\rangle \end{aligned} \quad (6.20)$$

with equality respectively if and only if each component of $\mathscr{L}_\mathscr{E}^{-1}A$ or $\mathscr{L}_\mathscr{E}^{-1}B$ is in $\mathbb{M}$. In particular, by using these inequalities to compare the formulas (6.16) for μ_M and κ_M with formulas (3.22) for μ and κ, we find that

$$0 < \mu_M \leqslant \mu, \qquad 0 < \kappa_M \leqslant \kappa \quad (6.21)$$

An important special case for which equality holds in both (6.20) and (6.21) is when the components of A and B are eigenfunctions of $\mathscr{L}_{\mathscr{E}}$. For the Boltzmann equation this is the case for a gas of Maxwell molecules,[7] but not for more general gases. For most classical collision operators $\mathscr{L}_{\mathscr{E}}$ is indeed self-adjoint and inequalities (6.21) are strict.

In order for the closure to have the proper behavior in the fluid dynamical regime the collision term $\mathbf{r}^*(\boldsymbol{\alpha})$ *must* be modified. This should be done in a way that does not destroy the entropy structure of the moment system. As was done for the Gaussian closure, the idea will be to modify the collision operator $\mathscr{C}(F)$ so as to recover the correct transport coefficients μ and κ while at the same time facilitating the calculation of the collision term $\mathbf{r}^*(\boldsymbol{\alpha})$. In particular, it is desirable from a practical viewpoint that the evaluation of the collision term in (4.14) should be no harder than the evaluation of the fluxes.

The simplest modification to consider is the BGK collision operator

$$\mathscr{C}(F) = \frac{\rho\theta}{\mu(\rho, \theta)} \left(\mathscr{E}(\rho, u, \theta) - F\right) \tag{6.22}$$

where the relaxation rate is normalized as in (5.34) so as to obtain the correct Navier–Stokes viscosity. However, the associated heat conduction will be $\kappa = [(D+2)/2]\,\mu$, which corresponds to a gas with Prandl number $\mathrm{Pr} = 1$, where

$$\mathrm{Pr} \equiv \frac{2}{D+2} \frac{\kappa(\rho, \theta)}{\mu(\rho, \theta)} \tag{6.23}$$

This will generally not give the correct heat flux because for most gases one has $\mathrm{Pr} < 1$. However, provided $\mathrm{Pr} \leqslant 1$, the correct Navier–Stokes heat conduction is recovered by a collision operator of the form

$$\begin{aligned} \mathscr{C}(F) = {} & \frac{\rho\theta}{\mu(\rho, \theta)} \left(\mathscr{E}(\rho, u, \theta) - F\right) \\ & + \left(\frac{D+2}{2} \frac{\rho\theta}{\kappa(\rho, \theta)} - \frac{\rho\theta}{\mu(\rho, \theta)}\right) \left(\mathscr{G}(\rho, u, \Theta) - F\right) \end{aligned} \tag{6.24}$$

where ρ, u, and Θ are determined from F by

$$\langle F \rangle = \rho, \qquad \langle vF \rangle = \rho u, \qquad \langle v \vee vF \rangle = \rho u \vee u + \rho\Theta \tag{6.25}$$

and θ is then determined by $\theta = (1/D)\,\mathrm{tr}(\Theta)$. This collision operator has two relaxation time scales. The first is related to the heat conduction and gives the rate at which the density F relaxes to the Gaussian $\mathscr{G}(\rho, u, \Theta)$.

The second is related to the viscosity and gives the slower rate at which the Gaussian relaxes to the local equilibrium $\mathscr{E}(\rho, u, \theta)$. As we will see below, this two-scale generalization of the BGK collision operator satisfies all the requirements put forth in Section 2.

The collision operator (6.24) is the first in a whole family of multiscale generalizations of the BGK operator. The construction of a K-scale member of this family proceeds as follows. Consider any sequence of K admissible subspaces $\{\mathbb{M}_k\}_{k=1}^K$ ordered by *strict* inclusion and strictly contained within $\mathbb{M}$ as

$$\mathbb{E} = \mathbb{M}_1 \subset \mathbb{M}_2 \subset \cdots \subset \mathbb{M}_K \subset \mathbb{M} \tag{6.26}$$

Denote a column vector of basis elements of $\mathbb{M}_k$ by $\mathbf{m}_k = \mathbf{m}_k(v)$. Define the density

$$\mathscr{M}_k \equiv \exp(\boldsymbol{\alpha}_k^T \mathbf{m}) \tag{6.27a}$$

where $\boldsymbol{\alpha}_k \in \mathbb{R}^M$ is uniquely determined by the relations

$$\boldsymbol{\alpha}_k^T \mathbf{m} \in \mathbb{M}_k, \qquad \langle \mathbf{m}_k \mathscr{M}_k \rangle = \langle \mathbf{m}_k F \rangle \tag{6.27b}$$

Next, associate with these subspaces and densities a corresponding sequence of relaxation rates $\nu_k = \nu_k(\rho, \theta)$ that are strictly ordered so that

$$0 < \frac{\rho\theta}{\mu} = \nu_1 < \nu_2 < \cdots < \nu_K \tag{6.28}$$

If the Prandl number (6.23) is strictly less than one then one must take

$$\mathbb{M}_2 = \mathbb{G} \qquad \text{and} \qquad \nu_2 = \frac{D+2}{2}\frac{\rho\theta}{\kappa} \tag{6.29}$$

Now define-the collision operator

$$\begin{aligned} C(F) &\equiv \nu_1(\mathscr{M}_1 - F) + \sum_{k=2}^{K} (\nu_k - \nu_{k-1})(\mathscr{M}_k - F) \\ &= \sum_{k=1}^{K-1} \nu_k(\mathscr{M}_k - \mathscr{M}_{k+1}) + \nu_K(\mathscr{M}_K - F) \end{aligned} \tag{6.30}$$

As we shall see, this is the nonlinear analog of the diagonal approximation of Grad.

This modified collision operator satisfies all the requirements laid down in Section 2. This is seen most directly when it is expressed as

$$\mathscr{C}(F) = \sum_{k=1}^{K} \eta_k (\mathscr{M}_k - F) \tag{6.31}$$

where $\eta_1 = \nu_1$ and $\eta_k = \nu_k - \nu_{k-1} > 0$ for $k = 2,..., K$. That 1, v, and $|v|^2$ are locally conserved (2.3) by each term in the sum (6.31) is evident from (6.27). That this operator satisfies the local dissipation (2.6) can be seen from

$$\begin{aligned} \langle \log F \mathscr{C}(F) \rangle &= \sum_{k=1}^{K} \eta_k \langle \log F(\mathscr{M}_k - F) \rangle \\ &= \sum_{k=1}^{K} \eta_k \left\langle \log\left(\frac{F}{\mathscr{M}_k}\right)(\mathscr{M}_k - F) \right\rangle \leqslant 0 \end{aligned} \tag{6.32}$$

As each term of this last sum is nonpositive, the only way the sum can vanish is if each term vanishes. This will happen if and only if the $k = 1$ term vanishes because in that case one must have $F = \mathscr{E}$, which would imply all the other terms would also vanish. Hence, the H-theorem (2.8) is satisfied. From this one can argue that the only locally conserved quantities are those in $\mathbb{E}$, thereby establishing (2.4). Finally, the translational and rotational symmetries (2.115 follow for each term in the sum (6.31) from the fact that, being admissible, each $\mathbb{M}_k$ satisfies condition (II) of (4.2).

The linear operator $\mathscr{L}_{\mathscr{E}}$ defined by (2.14) can be computed from (6.30) as

$$\begin{aligned} \mathscr{L}_{\mathscr{E}} &= \nu_1(\mathscr{I} - \mathscr{P}_1) + \sum_{k=2}^{K} (\nu_k - \nu_{k-1})(\mathscr{I} - \mathscr{P}_k) \\ &= \sum_{k=1}^{K-1} \nu_k(\mathscr{P}_{k+1} - \mathscr{P}_k) + \nu_K(\mathscr{I} - \mathscr{P}_K) \end{aligned} \tag{6.33}$$

where $\mathscr{P}_k$ is the orthogonal projection onto $\mathbb{M}_k$ in $\mathbb{H}_{\mathscr{E}}$, which is given by

$$\mathscr{P}_k g = \mathbf{m}_k^T \langle \mathbf{m}_k \mathscr{E} \mathbf{m}_k^T \rangle^{-1} \langle \mathbf{m}_k \mathscr{E} g \rangle \tag{6.34}$$

It is evident from (6.33) that $\mathscr{L}_{\mathscr{E}}$ is a bounded self-adjoint operator and over $\mathbb{H}_{\mathscr{E}}$ that its spectral decomposition is given by the last sum in (6.33). The nonzero eigenvalues of $\mathscr{L}_{\mathscr{E}}$ are the ν_k and their corresponding eigenspaces are $\mathbb{E}_k \equiv \mathbb{M}_{k+1} \ominus \mathbb{M}_k$, the orthogonal complement of $\mathbb{M}_k$ in $\mathbb{M}_{k+1}$, where we understand $\mathbb{M}_{K+1} = \mathbb{M}$. The orthogonal projection onto

$\mathbb{E}_k$ in $\mathbb{H}_g$ is then $\mathscr{P}_{k+1} - \mathscr{P}_k$. From these observations it is clear that the pseudoinverse of $\mathscr{L}_g$ is

$$\mathscr{L}_g^{-1} = \sum_{k=1}^{K-1} \frac{1}{\nu_k} (\mathscr{P}_{k+1} - \mathscr{P}_k) + \frac{1}{\nu_K} (\mathscr{I} - \mathscr{P}_K) \tag{6.35}$$

Moreover, the components of the matrix A and vector B are eigenfunctions of $\mathscr{L}_g$. The inequalities in (6.21) are therefore equalities, and the correct Navier–Stokes behavior will be recovered.

The linear space $\mathbb{M} = \text{span}\{1, v, v \vee v, |v|^2 v, |v|^4\}$ generates the simplest such closure that recovers the correct Navier–Stokes approximation. The dimension of this space is $(D+1)(D+4)/2$ in general, and is 14 for $D=3$. One takes as the collision operator (6.24), for which one obtains

$$\mathscr{L}_g = \frac{\rho\theta}{\mu} (\mathscr{P}_g - \mathscr{P}_g) + \frac{D+2}{2} \frac{\rho\theta}{\kappa} (\mathscr{I} - \mathscr{P}_g) \tag{6.36}$$

where $\mathscr{P}_g$ is the orthogonal projection onto $\mathbb{G} = \text{span}\{1, v, v \vee v\}$ in $\mathbb{H}_g$ of the form (6.34). It can be shown that this agrees with the diagonal approximation of Grad for the 13 moment closure (4.5). More generally, $\mathscr{L}_g$ given by (6.33) has the form of a Grad diagonal approximation for a higher order moment closure. The problem of generally determining the relaxation rates ν_k in (6.33) is exactly the same one that Grad faced. One possibility is to choose them so as to match the Chapman–Enskog expansion to higher order than the Navier–Stokes correction. This remains to be done.

Given some choice of the ν_k (hence, of the η_k), the moment closure collisional relaxation term (4.14) can be evaluated as

$$\mathbf{r}^*(\boldsymbol{\alpha}) \equiv \langle \mathbf{m} \mathscr{C}(\mathscr{M}(\boldsymbol{\alpha})) \rangle = \sum_{k=1}^{K} \eta_k (h_{\boldsymbol{\alpha}}^*(\boldsymbol{\alpha}_k) - h_{\boldsymbol{\alpha}}^*(\boldsymbol{\alpha})) \tag{6.37}$$

Similar to the problem we faced in the evaluation of the moment fluxes $j_{\boldsymbol{\alpha}}^*(\boldsymbol{\alpha})$ in the moment system (4.16), the practical implementation of this expression requires only a differentiable evaluation of the scalar function h^* in terms of $\boldsymbol{\alpha}$. Suppose that this can be done through a combination of asymptotics and numerics. Then, given a value of $\boldsymbol{\rho}$, it follows from (6.27) that the values of the $\boldsymbol{\alpha}_k$ can be obtained numerically by solving the restricted minimization problem

$$\min_{\boldsymbol{\alpha}} \{h^*(\boldsymbol{\alpha}) - \boldsymbol{\alpha}^T \boldsymbol{\rho} : \boldsymbol{\alpha}^T \mathbf{m} \in \mathbb{M}_k\} \tag{6.38}$$

This can be done by the same procedure used to solve the minimization problem (4.33) for $\boldsymbol{\alpha}$. The resulting $\boldsymbol{\alpha}_k$ can then be used in (6.37) to evaluate the collisional vector $\boldsymbol{r}^*$. Hence, the practical implementation of the collisional terms in (4.16) is no more difficult than that of the fluxes and is usually a good deal simpler, a fact illustrated by the explicit formulas that arise when using the collision operator (6.24).

Finally, the dissipation properties of this $\mathbf{r}^*$ may be seen directly from formula (6.37). Upon using (6.27b), one obtains

$$\begin{aligned}\boldsymbol{\alpha}^T\mathbf{r}^*(\boldsymbol{\alpha}) &= \sum_{k=1}^{K} \eta_k \boldsymbol{\alpha}^T(h_{\boldsymbol{\alpha}}^*(\boldsymbol{\alpha}_k) - h_{\boldsymbol{\alpha}}^*(\boldsymbol{\alpha})) \\ &= \sum_{k=1}^{K} \eta_k(\boldsymbol{\alpha}-\boldsymbol{\alpha}_k)^T(h_{\boldsymbol{\alpha}}^*(\boldsymbol{\alpha}_k) - h_{\boldsymbol{\alpha}}^*(\boldsymbol{\alpha})) \leqslant 0 \end{aligned} \tag{6.39}$$

which verifies the local dissipation relation (4.23) because the convexity of h^* implies that each term of the last sum in (6.38) is nonpositive. Similarly, the H-theorem like equivalences (4.24) can be seen directly. Indeed, the only way the last sum can vanish is if each term vanishes. This will happen if and only if the $k=1$ term vanishes because in that case one must have $\boldsymbol{\alpha}=\boldsymbol{\alpha}_1$, whereby $\boldsymbol{\alpha}^T\mathbf{m} \in \mathbb{E}$ and all the other terms would also vanish. Hence, the characterization of equilibria (4.24) is satisfied.

7. GENERALIZATIONS

The prescription of Sections 4 and 6 may be generalized to a wide class of kinetic equations. Consider a gas of particles such that the possible state p of a particle at a given location x takes on values in a set $\mathbb{P}$. Associated with each state $p \in \mathbb{P}$ is a velocity $v = v(p) \in \mathbb{R}^D$, which is the velocity of a free particle in state p. At the kinetic level a gas is described by a nonnegative function $F(t, x, p)$ that represents the density of particles with position x and state p in the single-particle phase space at time t. The evolution of $F(t, x, p)$ is assumed to be governed by a kinetic equation of the form

$$\partial_t F + v \cdot \nabla_x F = \mathscr{C}(F) \tag{7.1}$$

Here the interaction of particles through collisions is modeled by the operator $\mathscr{C}$ that acts locally (only on the p variable) and is generally nonlinear. Indeed, it is a nonlinear operator acting on its domain $\mathscr{D}(\mathscr{C})$, a subset of functions over $\mathbb{P}$ that take values in $\mathbb{R}_+$.

A map $e = e(p)$ in $\mathbb{R}^P$ is said to be a locally conserved quantity for the collision operator $\mathscr{C}$ whenever

$$\langle e\mathscr{C}(f)\rangle = 0 \qquad \text{for every} \quad f \in \mathscr{D}(\mathscr{C}) \tag{7.2}$$

The set of all conserved quantities of $\mathscr{C}$ is a linear subspace of $\mathbb{R}^P$ which is assumed to be nontrivial. Let E be the dimension of this space and $\{e_i(p): 1 \leqslant i \leqslant E\}$ a basis. Denote the vector-valued map from $\mathbb{P}$ to $\mathbb{R}^E$ whose components are these basis vectors by $\vec{e} = \vec{e}(p)$. Vectors in $\mathbb{R}^E$ will be denoted with arrows. Thus, $e = e(p)$ is a locally conserved quantity for $\mathscr{C}$ if and only if

$$e = \vec{\beta}^T \vec{e} \qquad \text{for some} \quad \vec{\beta} \in \mathbb{R}^E \tag{7.3}$$

The vector of locally conserved quantities $\vec{e}$ leads to a set of local conservation laws, satisfied by every solution $F = F(t, x, p)$ of the kinetic equation (7.1), that take the form

$$\partial_t \langle \vec{e} F \rangle + \nabla_x \cdot \langle v \vec{e} F \rangle = 0 \tag{7.4}$$

Here $\langle \vec{e} F \rangle$ and $\langle v \vec{e} F \rangle$ are called, respectively, the conserved densities and fluxes corresponding to $\vec{e}$.

The concepts of equilibria, conservation, and dissipation are then tied together by that of entropy. A map $\eta = \eta(f)$ over $\mathbb{R}_+$ is called an entropy density for the collision operator $\mathscr{C}$ whenever

$$\langle \partial_f \eta(f) \mathscr{C}(f) \rangle \leqslant 0 \qquad \text{for every} \quad f \in \mathscr{D}(\mathscr{C}) \tag{7.5}$$

and for every $f \in \mathscr{D}(\mathscr{C})$ the following are equivalent:

$$\begin{aligned} &\text{(i)} \quad \langle \partial_f \eta(f)\, \mathscr{C}(f) \rangle = 0 \\ &\text{(ii)} \quad \mathscr{C}(f) = 0 \\ &\text{(iii)} \quad \partial_f \eta(f) = \vec{\beta}^T \vec{e} \qquad \text{for some} \quad \vec{\beta} \in \mathbb{R}^E \end{aligned} \tag{7.6}$$

An entropy density is called convex if the map $f \mapsto \eta(f)$ is strictly convex with $\partial_{ff} \eta(f) > 0$. Requirement (7.6) merely abstracts some of the consequences of Boltzmann's celebrated H-theorem.[7] It states that the local equilibria of $\mathscr{C}$ are characterized by the vanishing of the entropy dissipation rate and are given by the class of densities determined by solving equation (iii) for f. Indeed, as will be shown below, the form of the local equilibria depends only on η and $\mathbb{E}$, and is completely independent of all other details of the collision operator.

For the classical kinetic theories of Section 2, the quantity $\eta(f) = f \log f - f$ was an entropy density. Other examples of such entropy densities are

$$\begin{aligned} \eta(f) &= f \log f + (1 - f) \log(1 - f) \\ \eta(f) &= f \log f - (1 + f) \log(1 + f) \end{aligned} \tag{7.7}$$

which arise for gases that satisfy Fermi–Dirac or Bose–Einstien statistics, respectively.

An entropy density η leads to a local dissipation law for solutions $F = F(t, x, p)$ of the kinetic equation (7.1)

$$\partial_t \langle \eta(F) \rangle + \nabla_x \cdot \langle v\eta(F) \rangle = \langle \partial_F \eta(F)\, \mathscr{C}(F) \rangle \leqslant 0 \tag{7.8}$$

Here $\langle \eta(F) \rangle$ and $\langle v\eta(F) \rangle$ are called, respectively, the entropy density and entropy flux, while $\langle \partial_F \eta(F)\, \mathscr{C}(F) \rangle$ is called the entropy dissipation rate.

Equation (iii) of (7.6) can be solved for the local equilibria in terms of the Legendre transform of η, which is denoted by $\eta^* = \eta^*(y)$ and is defined implicitly through the relations

$$\eta^*(y) + \eta(z) = yz, \qquad y = \partial_z \eta(z) \tag{7.9}$$

The strict convexity of η ensures that the second equation above can be solved for z in terms of y, thus allowing the elimination of z from the first equation. It is easy to verify the dual nature of this transformation by using implicit differentiation to check that $z = \partial_y \eta^*(y)$; it is then clear from (7.9) that the Legendre transform of η^* is again η. Hence, relation (iii) is equivalent to

$$\text{(iv)} \quad f = \partial_y \eta^*(\vec{\beta}^T \vec{e}) \qquad \text{for some} \quad \vec{\beta} \in \mathbb{R}^E \tag{7.10}$$

The generalization of (4.8) is then

$$\mathscr{M}(\boldsymbol{\alpha}) = \partial_y \eta^*(\boldsymbol{\alpha}^T \mathbf{m}) \qquad \text{for some} \quad \boldsymbol{\alpha} \in \mathbb{R}^M \tag{7.11}$$

The corresponding density and flux potentials are given by

$$h^*(\boldsymbol{\alpha}) = \langle \eta^*(\boldsymbol{\alpha}^T \mathbf{m}) \rangle, \qquad j^*(\boldsymbol{\alpha}) = \langle v\eta^*(\boldsymbol{\alpha}^T \mathbf{m}) \rangle \tag{7.12}$$

Given this, the generalization of the moment closure prescription is straightforward.

Remark. Many kinetic equations admit more than one convex entropy density. Indeed, for linear kinetic equations it is often the case that any strictly convex function of f satisfies (7.6). In such cases the closures one obtains from different entropy densities can be quite different.

8. DISCUSSION

The preceding theory should be considered as a starting point for further study. Three general avenues of investigation are evident: its practical implementation, the nature of its approximations, and its mathematical

foundations. Without trying to be exhaustive, a number of questions related to these avenues are raised below.

The biggest obstacle to a practical implementation of the above theory is the need for algorithms to efficiently evaluate the density potential h^*, defined in (4.13), and two of its derivatives as functions of $\boldsymbol{\alpha}$. The large number of independent variables would seem to make tabular approaches too storage-intensive to be practical. However, one approach might be to approximate the integrals in (4.13) with discrete-velocity quadratures that are designed so as to recover exact expressions when $\mathcal{M}(\boldsymbol{\alpha})$ reduces to a Gaussian. Given a realizable value of $\boldsymbol{\rho}$, the corresponding values of $\boldsymbol{\alpha}$ and $h(\boldsymbol{\rho})$ can then be obtained numerically by iteratively solving the minimization problem (4.33) using a nonlinear conjugate gradient method. Care must be taken to ensure that each iterate remains within the cone $\mathbb{M}_c$ over which h^* takes on finite values. This is a particularly important point because the Maxwellians themselves are realized on the boundary of $\mathbb{M}_c$ for closures of higher order than Gaussian. Because $h^*(\boldsymbol{\alpha})$ approaches $+\infty$ as $\boldsymbol{\alpha}$ approaches any point on the boundary of $\mathbb{M}_c$ that is not in $\mathbb{M}_c$, it is easily seen that h^* is not continuous at a Maxwellian. However, it is also true that at a Maxwellian h^* possesses one-sided derivatives of all orders in directions interior to $\mathbb{M}_c$, the first two of which are given by formulas (4.15) and (4.17). The conjugate gradient method should use the quadrature approximation to these formulas. Convergence should be rather fast, given a good initial guess for $\boldsymbol{\alpha}$ provided by, for example, its value at the previous timestep. If no minimum is found, then the given value of $\boldsymbol{\rho}$ was not realizable and a new one should be computed with a smaller timestep. Such a method has yet to be fully implemented.

The symmetric hyperbolic structure of the moment equations evident in (4.16) lends itself to the practical implementation of generalized Godunov numerical schemes. Such schemes require the development of good approximate Riemann solvers. This might be achieved rather cheaply given a quadrature approximation such as those described in the last paragraph. One simply computes the flux at a given interface as the difference of the appropriate one-way fluxes of the-states on either side, where the one-way fluxes are computed by quadrature over those velocities flowing toward the interface. This approach would be most natural for a Lagrangian implementation where the underlying quadrature set would be naturally centered on the interface. Such an approximate Riemann solver is much more dissipative than an exact one. Its usefulness needs to be tested.

A detailed analysis of the hyperbolic structure of the 35-moment closure (all moments up to fourth order in three dimensions) has recently been carried out by Gombosi *et al.*[15] They found a remarkable factorization of the characteristic polynomial of the system with slab symmetry in

the near-Gaussian approximation and proceeded to classify all the characteristic velocities as either genuinely nonlinear or linearly degenerate. Such knowledge is needed to build more sophisticated approximate Riemann solvers.

It should be remarked that care must be taken in differencing the moment equations so as to recover the correct Navier–Stokes behavior in the fluid dynamical regime.[24] This is because that behavior results from asymptotic balances in the moment equations for small mean free path that must be maintained by the numerical approximation. Algorithms naively based on splitting the convective and collisional terms will generally not work. Approaches that address this problem are found in ref. 24 and references therein.

Practical implementation of the above theory also requires the specification of boundary conditions. Of course, reflecting boundary conditions are easily imposed. Moreover, one can also impose in-flow or out-flow boundary conditions by simply specifying an external state and determining the flux at the boundary by (approximately) solving the Riemann problem. This is exactly what most Euler simulations do now. It is not clear that this treatment gives the correct boundary conditions in the Navier–Stokes approximation. The development of more sophisticated boundary conditions based on asymptotic boundary layer analyses requires a perturbative reformulation of the systematics presented here. This is being explored for the Gaussian closure in ref. 19.

Questions regarding the nature of the approximations in the above theory fall into two general areas—namely, those relating to the modification of the collision operator given by (6.31) and those relating to the form of $\mathcal{M}(\alpha)$ given by (4.10). The most basic question regarding the collisional approximation is the validity of replacing the true collision operator with a generalized BGK operator of the form (6.31). This question should be investigated in the context of Maxwell molecules. In that case the linearizations about a Maxwellian of both the Boltzmann collision operator and its generalized BGK approximation are diagonal with respect to the Hermite polynomials, and can therefore be made to agree rather well by a proper choice of the eigenvalues ν_k in (6.33). One can then focus on the approximation in the transition regime. For more general molecules it is clear that the nature of the approximation is more violent even near a local equilibrium. In that case one could hope that the ν_k could be systematically chosen so as to, for example, match terms in the corresponding Burnett and super-Burnett equations.

The closure strategy does not depend on the specific form of the modified collision operator proposed in (6.31). Other forms that satisfy the general properties put forth in Section 2 should also be considered,

although it is not clear what those forms might be. For example, if operators of the form (6.31) work well near local equilibria but not so well in the transition regime, then one could. consider allowing the η_k to be functionally dependent on more than just ρ and θ. On the other hand, if the form (6.31) does not work well near local equilibria, then a more dramatic revision is needed.

Deeper questions exist regarding the justification for the chosen form of $\mathcal{M}(\alpha)$ given by (4.10). This choice was guided only by entropy dissipation and conservation properties; no other knowledge about the dynamics was used. In particular, the specific form of the entropy dissipation rate (2.6) was not used. It would be natural to consider the role this functional might play in an alternative closure strategy.

Finally, we turn to the mathematical foundations of the above theory. Of course, being a symmetric hyperbolic system, the moment equations inherit a local existence theory of classical solutions for initial data in the Sobolev space H^s for any $s > D/2 + 1$ (for example, see refs. 25 and 30). One question to be addressed is whether the presence of collisional terms allows one to establish global existence for classical solutions that are close to a homogeneous equilibrium.[1] Within the context of classical solutions, one could also try to establish the validity of fluid dynamical approximations.[2] A natural question also arises as to the sense in which solutions of the hierarchy of moment equations approximate a solution of, say, the Boltzmann equation. While it may be that one could prove something in this direction, given our limited knowledge of classical solutions for the Boltzmann equation, such a result could prove to be a bit academic.

Any theory of global weak solutions for the moment equations would contain such a theory for the Euler equations of gas dynamics as a special case. Because the latter question is open, so is the former; however, they are likely of equal difficulty. Of course, given such a result, it is then natural to ask the sense in which weak solutions of the hierarchy of moment equations approximate DiPerna–Lions solutions of the Boltzmann equation. Fluid dynamical limits should be reexamined in this context, too.

A less ambitious program would be to investigate special solutions to the moment equations. The most important example of such would be the shock profile. For the weak shock profile one should at least be able to prove what is known for the Boltzmann equation. On the other hand, the existence of the strong shock profile is an open problem for the Boltzmann equation that may be more tractable for the moment equations because there it reduces to a question, albeit nontrival, about ordinary differential equations. Indeed, while the entropy flux acts as a formal Lyapunov function for those equations, it is not bounded from below. Therefore, any result on the existence of the strong shock profile would be interesting.

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