

On the high Mach number shock structure singularity caused by overreach of Maxwellian molecules

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The high Mach number shock structure singularity arising in moment equations of the Boltzmann equation was investigated. The source of the singularity is shown to be the unbalanced treatment between two high order kinematic and dissipation terms caused by the overreach of Maxwellian molecule assumption. In compressive gaseous flow, the high order stress-strain coupling term of quadratic nature will grow far faster than the strain term, resulting in an imbalance with the linear dissipation term and eventually a blow-up singularity in high thermal nonequilibrium. On the other hand, the singularity arising from unbalanced treatment does not occur in the case of velocity shear and expansion flows, since the high order effects are cancelled under the constraint of the free-molecular asymptotic behavior. As an alternative method to achieve the balanced treatment, Eu's generalized hydrodynamics, consistent with the second law of thermodynamics, was revisited. After introducing the canonical distribution function in exponential form and applying the cumulant expansion to the explicit calculation of the dissipation term, a natural platform suitable for the balanced treatment was derived. The resulting constitutive equation with the nonlinear factor was then shown to be well-posed for all regimes, effectively removing the high Mach number shock structure singularity. © 2014 AIP Publishing LLC. [<http://dx.doi.org/10.1063/1.4875587>]

I. INTRODUCTION

The physics and thermodynamics of fluids in high thermal nonequilibrium remains a fundamental research topic in various disciplines, from gaseous motion in rarefied micro- and nano-scale conditions, to electron transport in semi-conductor devices, and non-Newtonian viscoelastic fluids found in daily life, such as polymer solutions and complex fluids.¹⁻¹² Studying these mesoscopic fluids is mathematically difficult, because it involves microscopic collisional interactions among fluid particles and their interplay with the kinematic motion of particles in the macroscopic framework. This challenge is vividly illustrated by the celebrated classical problem known as the high Mach number shock singularity problem in gas dynamics.^{3, 13-15}

Over time there have been enormous efforts to solve the problem from various perspectives, not only by physicists and mathematicians, but engineers and also chemists. The trend reflects the inherent difficulties and subtleties associated with the nonlinear nature of the problem. The approaches adopted by researchers with different backgrounds and training are quite diverse. And as an inevitable consequence of the diversity, misconceptions and confusions have arisen, which have impeded development of a clear picture of the issue, resulting in inconsistency among the conclusions obtained by various works. The most obvious is the interpretation of the degree of thermal nonequilibrium; its clear definition is essential to understanding the fundamentals of fluid flows in high thermal nonequilibrium.

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Traditionally, the Knudsen number was considered the sole parameter for classifying the gaseous flow regimes; continuum, slip, transitional, and free-molecular. The rationale behind this common practice is simple; the ratio of the collision term to the kinematic term in the Boltzmann equation is nothing but the Knudsen number as given below

$$\mathbf{v} \cdot \nabla f = \frac{1}{Kn} C[f, f_2]. \quad (1.1)$$

However, this seemingly indisputable method was put into question when microscale gas flows with *high* Knudsen number were solved accurately by the linear Navier-Stokes-Fourier theory with slip boundary conditions. The same linear theory does not produce accurate results in the case of hypersonic rarefied gas flows with *low* Knudsen number. This inconsistency can be only resolved by revisiting the initial step of how fluid motions are described in the macroscopic world. It is straightforward to show that, owing to the statistical average procedure introduced in the Boltzmann kinetic equation to obtain the continuum conservation laws, there are three, instead of two, terms in the conservation law of momentum: convective, pressure, and viscous terms. The reduction of information from the microscopic description in phase space to the macroscopic description in thermodynamic space is the ultimate reason for this disparity—two terms in the microscopic description and three terms in the macroscopic description. Thus, at least two non-dimensional parameters—for example, the Reynolds and Mach (or Knudsen and Mach) numbers—are necessary to classify the regimes fully:

$$\rho \mathbf{u} \mathbf{u} + \frac{1}{\gamma M^2} p \mathbf{I} + \frac{1}{Re} \mathbf{\Pi} = 0. \quad (1.2)$$

Also, the degree of thermal nonequilibrium in thermodynamic space can be best represented by a dimensionless number defined as the ratio of the viscous force to the thermodynamic pressure, Π/p , since the viscous force is a direct consequence of the thermal nonequilibrium effect. The ratio can further be expressed as a composite number $Kn \cdot M$, not the Knudsen number alone. This explains why most microscale gas flows, with proper slip boundary conditions, can be described by the linear theory; according to the new composite parameter, the very low Mach number typical in microscale devices yields the relatively low level in thermal nonequilibrium.

Another instance—far more serious in its implication—can also be found in the interpretation of Maxwellian gas molecules and Bhatnagar-Gross-Krook (BGK) approximations commonly employed in the mathematical development of gas kinetic theory. The Maxwellian gas molecule assumption results in the disappearance of velocity dependence on the collision kernel in the Boltzmann equation.^{1,2,5} Since virtually all the mathematical difficulties related to the nonlinear Boltzmann equation and subsequent moment equations come from the nonlinear collision integral, the assumption simplifies the mathematical problem tremendously. In similar spirit, the so-called BGK approximation can be introduced to the Boltzmann collision integral for all types of molecules. Based on these simplifications, many interesting results, otherwise intractable, can be obtained. Therefore, it is natural to anticipate that most results of Maxwellian molecules will carry over to the general molecules since the physical system embedded in the Boltzmann equation must be continuous for the type of molecules. This explains why there were strong temptations in the past to generalize insights gained from these simplified models into general real molecules.

However, there are caveats associated with this shortcut. The most serious is an inconsistency: while the results for Maxwellian molecules are *mathematically exact* in treating the dissipation term involving the collision integral, the BGK results are *approximate* for all types of molecules including Maxwellian molecules. Then, the immediate question arises: how is it nonetheless possible to have *exactly* the same final results? Something must be missing in this logic.

While this insight is put aside in a moment, there are many useful results in these simplified models, though significant portions of them may be unjustified in the end. For example, it becomes possible to claim that the Navier-Stokes (NS) (or Chapman-Enskog) viscosity is exactly equal to the true viscosity in the case of Maxwellian molecules. According to this argument, the following

constitutive equation of the shear stress is exact to the original Boltzmann equation:

$$\begin{aligned} \rho \frac{d(\boldsymbol{\Pi}/\rho)}{dt} + 2[\boldsymbol{\Pi} \cdot \nabla \mathbf{u}]^{(2)} + 2p[\nabla \mathbf{u}]^{(2)} &= -\frac{p}{\mu_{NS}} \boldsymbol{\Pi}, \\ \text{or } \frac{d\hat{\Pi}}{d\hat{t}} - \hat{\Pi}\hat{\Pi}_{NS} - \hat{\Pi}_{NS} &= -\hat{\Pi} \text{ in 1-d compression and expansion problem,} \\ \text{where } \hat{t} \equiv \frac{t}{\mu_{NS}/p}, \hat{\Pi} \equiv \frac{\boldsymbol{\Pi}}{p}, \Pi_{NS} &\equiv -\frac{4}{3}\mu_{NS}\frac{\partial u}{\partial x}. \end{aligned} \quad (1.3)$$

Furthermore, one may jump to the conclusion that the same relation, the linear viscosity in the dissipation term, must be valid in general molecules as well. By proceeding further, it may be concluded that, for Maxwellian molecules, the BGK form is correct even if the distribution function is far from thermal equilibrium, suggesting that the BGK model may be a legitimate approximation to the collision term in higher moment systems.

In this paper, the inconsistency in the interpretation of Maxwellian gas molecules and BGK approximations is revisited. It will be demonstrated that some of the unsolved problems in gas kinetic theory, notably, the mathematical singularity in shock structure at high Mach numbers, are caused by the overreach of Maxwellian gas molecules and BGK approximations. In essence, it will be shown that the commonly accepted claim, the equivalence of the linear viscosity and the true physical viscosity in the case of Maxwellian molecules, is incorrect, and that realization of this critical point holds the key to resolving the shock singularity problem. Then, a more accurate method—in the sense that all the approximations are deferred as late as possible in derivation—is presented on the basis of Eu's theory,^{6,7,16} the gist of which—a nonlinear factor $q(|\boldsymbol{\Pi}|/p)$ —can be summarized: in the case of a one-dimensional problem,^{17,18} it is

$$\begin{aligned} \frac{d\hat{\Pi}}{d\hat{t}} - \hat{\Pi}\hat{\Pi}_{NS} - \hat{\Pi}_{NS} &= -\hat{\Pi}q(|\hat{\Pi}|), \\ \text{where } q(|\hat{\Pi}|) &\equiv \frac{\sinh|\hat{\Pi}|}{|\hat{\Pi}|}. \end{aligned} \quad (1.4)$$

The key steps of deriving the nonlinear factor are described in detail with special emphasis on explaining Eu's original theory^{6,7}—published mostly in the chemistry community—in close connection with Grad's theory,^{2,3} which is familiar in physics and mathematics communities.

This paper is organized as follows. Section II discloses the source of the overreach of the Maxwellian molecule approximation and its consequence in the shock structure singularity problem. Subsequently, the reason why such an overreach does not cause the same kind of mathematical singularity for velocity shear and expansion cases is explained. Section III presents a more balanced treatment method for approximating the kinematic high order and dissipation terms based on the second law of thermodynamics and uncovers the role of the second law in removing the shock structure singularity. Summary and concluding remarks are given in Sec. IV. In Appendices A and B, detailed derivation of exact moment equations and the cumulant expansion in Eu's theory are explained in detail in order to help readers unfamiliar with these topics.

II. OVERREACH OF MAXWELLIAN MOLECULE ASSUMPTION

The Boltzmann equation can be transformed into the moment equations by introducing the statistical average in velocity space $\langle \cdot \rangle$; after some manipulation (summarized in detail in (A6) of Appendix A), it is reduced to

$$\begin{aligned} \rho \frac{d(\boldsymbol{\Pi}/\rho)}{dt} + \nabla \cdot (\langle m\mathbf{c}\mathbf{c}\mathbf{c}f \rangle - \langle m\text{Tr}(\mathbf{c}\mathbf{c}\mathbf{c})f \rangle \mathbf{I}/3) + 2[\boldsymbol{\Pi} \cdot \nabla \mathbf{u}]^{(2)} + 2p[\nabla \mathbf{u}]^{(2)} &= \boldsymbol{\Lambda}^{(\Pi)}, \\ \rho \frac{d(\mathbf{Q}/\rho)}{dt} + \nabla \cdot (\langle mc^2\mathbf{c}\mathbf{c}f/2 \rangle - C_p T(p\mathbf{I} + \boldsymbol{\Pi})) + \langle m\mathbf{c}\mathbf{c}\mathbf{c}f \rangle : \nabla \mathbf{u} + \frac{d\mathbf{u}}{dt} \cdot \boldsymbol{\Pi} + \mathbf{Q} \cdot \nabla \mathbf{u} + \boldsymbol{\Pi} \cdot C_p \nabla T \\ + pC_p \nabla T &= \boldsymbol{\Lambda}^{(Q)}. \end{aligned} \quad (2.1)$$

The $\Lambda^{(\Pi)}$, $\Lambda^{(Q)}$ in the right-hand side represent the dissipation terms of shear stress and heat flux. The general form of the dissipation terms is defined by $\Lambda^{(n)} \equiv \langle h^{(n)} C[f, f_2] \rangle$, where $h^{(n)}$ denotes the molecular expressions for moment. Since the mathematical structure of the constitutive equation of heat flux is essentially the same as that of the constitutive equation of shear stress, it is enough to consider the constitutive equation of shear stress only. Then it can be expressed as follows, after the dissipation term in the right-hand side, $\Lambda^{(\Pi)}$, is explicitly calculated for the Maxwellian molecules ($B_1^{(\Pi)}$ being constant^{2,5}):

$$\rho \frac{d(\Pi/\rho)}{dt} + \nabla \cdot \Psi^{(\Pi)} + 2[\Pi \cdot \nabla \mathbf{u}]^{(2)} + 2p[\nabla \mathbf{u}]^{(2)} = -\frac{6}{m} B_1^{(\Pi)} \rho \Pi, \quad (2.2)$$

$$\Psi^{(\Pi)} \equiv \langle m \mathbf{c} \mathbf{c} \mathbf{c} f \rangle - \langle m \text{Tr}(\mathbf{c} \mathbf{c} \mathbf{c}) f \rangle \mathbf{I}/3.$$

When the Navier-Stokes or 1st order approximation (meaning near equilibrium) is introduced, or equivalently, when the first three terms of the left-hand side are ignored, the constitutive equation is simplified into

$$-2\mu_{NS} [\nabla \mathbf{u}]^{(2)} = \Pi, \text{ where } \mu_{NS} \equiv \frac{mRT}{6} \frac{1}{B_1^{(\Pi)}}, \quad (2.3)$$

which is called the Navier-Stokes (approximate) constitutive relation. With the definition of the linear viscosity μ_{NS} in (2.3), Eq. (2.2) can be expressed as another and yet still exact equation to the original Boltzmann equation:

$$\rho \frac{d(\Pi/\rho)}{dt} + \nabla \cdot \Psi^{(\Pi)} + 2[\Pi \cdot \nabla \mathbf{u}]^{(2)} + 2p[\nabla \mathbf{u}]^{(2)} = -\frac{p}{\mu_{NS}} \Pi. \quad (2.4)$$

Here the explanation of physical meaning of various terms is in order; the five terms represent the material time derivative, open high order, explicit high order (elastic stress-strain coupling), force (or strain), and dissipation (or production) effects, respectively.

A. Source of mathematical singularity in the shock structure problem

The open high order term $\nabla \cdot \Psi^{(\Pi)}$ must now be treated in order to close the system (2.4). Since it vanishes in the limit of thermal equilibrium, it may be assumed to be zero as an approximation. Then the exact equation (2.4) becomes

$$\rho \frac{d(\Pi/\rho)}{dt} + 2[\Pi \cdot \nabla \mathbf{u}]^{(2)} + 2p[\nabla \mathbf{u}]^{(2)} = -\frac{p}{\mu_{NS}} \Pi. \quad (2.5)$$

In the past, Eq. (2.5) was often treated as the exact consequence of the Boltzmann equation. Obviously Eq. (2.5) is not exact since the closure $\nabla \cdot \Psi^{(\Pi)} = 0$, which is basically not exact in nature, has already been introduced in the left-hand side. However, there is a more compelling reason why it should not be; in order for Eq. (2.5) to be accepted as the exact consequence of the Boltzmann equation, it must be well-posed in *all* flow situations, which will be shown to not be the case.

The essential mathematical property of Eq. (2.5) can be investigated by considering one-dimensional flow cases; for example, gaseous expansion and compression (forming the shock structure for supersonic upstream). Equation (2.5) is then transformed into

$$\rho \frac{\mu_{NS}}{p^2} \frac{d(\Pi/\rho)}{dt} - \hat{\Pi} \hat{\Pi}_{NS} - \hat{\Pi}_{NS} = -\hat{\Pi}, \text{ where } \hat{\Pi} \equiv \frac{\Pi}{p}, \Pi_{NS} \equiv -\frac{4}{3} \mu_{NS} \frac{\partial u}{\partial x}. \quad (2.6)$$

Here the positive value of $\hat{\Pi}_{NS}$ represents the compression (shock) case, while its negative value represents the expansion case. Note also that the material derivative is $d/dt = \partial/\partial t + u\partial/\partial x$ in general, but, due to Galilean invariance, the convective derivative $u\partial/\partial x$ does not affect the mathematical property of Eq. (2.6). Then Eq. (2.6), without losing the essence of mathematical property, can be rewritten as an ordinary differential equation of $\hat{\Pi}$ with respect to dimensionless time \hat{t} :

$$\frac{d\hat{\Pi}}{d\hat{t}} = \hat{\Pi} \hat{\Pi}_{NS} + \hat{\Pi}_{NS} - \hat{\Pi}, \text{ where } \hat{t} \equiv \frac{t}{\mu_{NS}/p}. \quad (2.7)$$

Equation (2.7) shows the nature of the constitutive equation in general; it provides information of how the stress $\hat{\Pi}$ is determined in the form of $\hat{\Pi}(\hat{t}, \hat{\Pi}_{NS})$ for a given input $\hat{\Pi}_{NS}$ and initial condition $\hat{\Pi}(\hat{t} = 0)$. The general solution of the ordinary differential equation (2.7) is

$$\hat{\Pi}(\hat{t}) = \frac{\hat{\Pi}_{NS}}{1 - \hat{\Pi}_{NS}} + \left[\hat{\Pi}(\hat{t} = 0) - \frac{\hat{\Pi}_{NS}}{1 - \hat{\Pi}_{NS}} \right] \exp[-(1 - \hat{\Pi}_{NS})\hat{t}]. \quad (2.8)$$

When time asymptotic behavior—in either steady-state or fast relaxation of shear stress—is concerned, the solution becomes

$$\lim_{\hat{t} \rightarrow \infty} \hat{\Pi}(\hat{t}) \rightarrow \frac{\hat{\Pi}_{NS}}{1 - \hat{\Pi}_{NS}} \quad (2.9)$$

$$\text{with } -1 < \hat{\Pi} \text{ and } -\infty < \hat{\Pi}_{NS} < 1.$$

This steady-state constitutive relation is well-defined in the whole range of gaseous expansion (negative $\hat{\Pi}_{NS}$), but only in a small portion of gaseous compression ($0 \leq \hat{\Pi}_{NS} < 1$). In fact, there is a mathematical singularity in the compressive shock case near $\hat{\Pi}_{NS} = 1$, where the shear stress $\hat{\Pi}$ becomes infinity and across which the shear stress $\hat{\Pi}$ abruptly changes its sign.

This kind of high Mach number shock singularity in a high order constitutive equation was first identified by Grad in 1952.³ Since then, it has remained as a major stumbling block to researchers studying gas dynamics in high thermal nonequilibrium and its ultimate origin is still elusive up to the present. Since it is improbable to think that the Boltzmann equation itself contains the singularity or that the one-dimensional assumption used in (2.6) creates the singularity, the only possible cause is when Eq. (2.5) is derived from the exact equation (2.4) by applying the closure for the high order term $(\nabla \cdot \Psi^{(1)})_{xx}$. The key observation is that the closure itself is not the problem, but the number of places of approximation—just one in the case of Eq. (2.4) of the Maxwellian molecules—is the problem. The reason why the number does matter is simple; the equation will eventually blow up in a high nonequilibrium shock structure case unless one approximation is balanced by another approximation. Specifically, in the constitutive equation $-\hat{\Pi}\hat{\Pi}_{NS} - \hat{\Pi}_{NS} = -\hat{\Pi}$ with the closure (or approximation) applied to the left-hand side, the high order stress-strain coupling term $|\hat{\Pi}\hat{\Pi}_{NS}|$ of quadratic nature will grow far faster than the force term $|\hat{\Pi}_{NS}|$, resulting in an imbalance with the right-hand side term $|\hat{\Pi}|$ and eventually a blow-up singularity $\lim_{\hat{\Pi}_{NS} \rightarrow 1} \hat{\Pi} \rightarrow \infty$. (It must be noted

that such a singularity will not appear when the sign of $\hat{\Pi}_{NS}$ is negative, since two terms in the left-hand side have the opposite sign.)

Once the source of the singularity is uncovered, it is straightforward to develop a method to resolve the singularity. There are basically two directions: (1) developing a very accurate treatment for the high order term in the left-hand side to keep up with the right-hand side; (2) making room for another approximate treatment and naturally achieving a balance between two places of approximation. The former basically requires inclusion of a greater number of high order moments beyond the conventional shear stress tensor and heat flux vector. However, the benefit gained from adding more moments turns out so far to be minimal at best,¹³ which is expected from the inherent limitation involved in closing non-closable higher order terms. On the other hand, the latter is conceptually simple, practical, more natural in handling general types of molecules, and, first of all, does not demand an insurmountable task like accurately closing open high order terms.

The key idea of the latter approach can be developed by reexamining the initial stage of deriving the moment equations from the original Boltzmann equation. The exact form for general type of molecules can be written as

$$\rho \frac{d(\mathbf{\Pi}/\rho)}{dt} + \nabla \cdot (\langle m\mathbf{ccc}f \rangle - \langle m\text{Tr}(\mathbf{ccc})f \rangle \mathbf{I}/3) + 2[\mathbf{\Pi} \cdot \nabla \mathbf{u}]^{(2)} + 2p[\nabla \mathbf{u}]^{(2)} = \mathbf{\Lambda}^{(1)}. \quad (2.10)$$

There are two places for approximation: (1) the high order term $\nabla \cdot (\langle m\mathbf{ccc}f \rangle - \langle m\text{Tr}(\mathbf{ccc})f \rangle \mathbf{I}/3)$ and the dissipation term $\mathbf{\Lambda}^{(1)} (\equiv \langle m[\mathbf{cc}]^{(2)}C[f, f_2] \rangle)$. Note that they are the only terms in the constitutive equation that are directly connected to next level high order moments and the explicit form of the distribution function f or the collision integral $C[f, f_2]$. The latter approach is simply to impose the

same level of approximations on both places so that the resulting constitutive equation may remain balanced even in high nonequilibrium. For the general type of molecules, Eq. (2.10) can be written

$$\rho \frac{d(\mathbf{\Pi}/\rho)}{dt} + \nabla \cdot \mathbf{\Psi}^{(\Pi)} + 2[\mathbf{\Pi} \cdot \nabla \mathbf{u}]^{(2)} + 2p[\nabla \mathbf{u}]^{(2)} = -\frac{p}{\mu_{NS}} \mathbf{\Pi} F(p, T, \mathbf{\Pi} : \mathbf{\Pi}, \mathbf{Q} \cdot \mathbf{Q}, \dots). \quad (2.11)$$

In case of the Maxwellian molecules, $F = 1$, irrespective of the degree of thermal nonequilibrium. If the positive nonlinear scalar function F reduces to 1 near thermal equilibrium and its exact form is determined by the Boltzmann equation, then (2.11) is still exact. Then the latter approach requires the same level of approximation for $\nabla \cdot \mathbf{\Psi}^{(\Pi)}$ and F terms. For example, the crudest approximations are $\rho d(\mathbf{\Pi}/\rho)/dt + \nabla \cdot \mathbf{\Psi}^{(\Pi)} + 2[\mathbf{\Pi} \cdot \nabla \mathbf{u}]^{(2)} = 0$ and $F = 1$, which is nothing but the linear Navier-Stokes constitutive equation. The ultimate task in the latter method is then to find a proper form of the nonlinear viscosity factor F_{approx} corresponding to the next level approximation of closure for the high order term, for example, $\nabla \cdot \mathbf{\Psi}^{(\Pi)} = 0$:

$$\rho \frac{d(\mathbf{\Pi}/\rho)}{dt} + 2[\mathbf{\Pi} \cdot \nabla \mathbf{u}]^{(2)} + 2p[\nabla \mathbf{u}]^{(2)} = -\frac{p}{\mu_{NS}} \mathbf{\Pi} F_{approx}(p, T, \mathbf{\Pi} : \mathbf{\Pi}, \mathbf{Q} \cdot \mathbf{Q}, \dots). \quad (2.12)$$

Notice that Eq. (2.12) is also applicable to the Maxwellian molecules since the closure of the open high order term can be incorporated into the nonlinear factor F_{approx} in the dissipation term. That is, if a closure $\nabla \cdot \mathbf{\Psi}^{(\Pi)} = -p\mathbf{\Pi}(1 - F_{approx})/\mu_{NS}$ is applied to the equation of Maxwellian molecules (2.4), the resulting equation becomes the same form as (2.12). Therefore, in the latter method, all types of molecules can be treated within a single framework (2.12), which may be considered even better with respect to being mathematically well-posed, by continual dependence on the data.

B. Cancellation of nonlinear factor in the velocity shear problem

Equation (2.5), which was often mistaken as the exact consequence of the Boltzmann equation in the past, had been successfully applied to various gas flow problems, even though it suffered the shock structure singularity. At this stage, it is necessary to investigate the reason behind this disparity in the performance of the model. The constitutive equation (2.5) in the case of one-dimensional velocity shear flow is reduced into,¹⁹ under steady state condition,

$$\frac{1}{\mu_{NS}} \begin{bmatrix} 2\Pi_{xy}\Pi_{xyNS}/3 \\ -\Pi_{yy}\Pi_{xyNS} \end{bmatrix} - \frac{1}{\mu_{NS}} \begin{bmatrix} 0 \\ p\Pi_{xyNS} \end{bmatrix} = -\frac{p}{\mu_{NS}} \begin{bmatrix} \Pi_{yy} \\ \Pi_{xy} \end{bmatrix}, \text{ where } \Pi_{xyNS} \equiv -\mu_{NS} \frac{\partial u}{\partial y}. \quad (2.13)$$

On the other hand, the constitutive equation (2.12) becomes

$$\frac{1}{\mu_{NS}} \begin{bmatrix} 2\Pi_{xy}\Pi_{xyNS}/3 \\ -\Pi_{yy}\Pi_{xyNS} \end{bmatrix} - \frac{1}{\mu_{NS}} \begin{bmatrix} 0 \\ p\Pi_{xyNS} \end{bmatrix} = -\frac{p}{\mu_{NS}} \begin{bmatrix} \Pi_{yy} \\ \Pi_{xy} \end{bmatrix} F_{approx}. \quad (2.14)$$

It is straightforward to show that the solutions of (2.13) and (2.14) are, respectively,

$$\hat{\Pi}_{xy} = \frac{3\hat{\Pi}_{xyNS}}{3 + 2\hat{\Pi}_{xyNS}^2}, \quad \hat{\Pi}_{xy} = \frac{3\hat{\Pi}_{xyNS}}{3F_{approx} + 2\hat{\Pi}_{xyNS}^2/F_{approx}}. \quad (2.15)$$

Surprisingly, when the two components of equations in (2.13) and (2.14) are divided with each other, the nonlinear factor F_{approx} and the driving force Π_{xyNS} are cancelled out, leaving only a common stress constraint:

$$\hat{\Pi}_{xy}^2 = -\frac{3}{2} (1 + \hat{\Pi}_{yy}) \hat{\Pi}_{yy}. \quad (2.16)$$

From (2.15) and (2.16), it can be concluded, in the velocity shear problem, that both constitutive equations (2.5) and (2.12) produce qualitatively the same solutions and do not suffer any singularity.

In turn, this means that, owing to the cancellation, the nonlinear factor does not play any significant role in determining the mathematical property of the velocity shear problem. This point explains precisely why, in spite of its inherent mathematical singularity in the high Mach number shock structure problem, the over-reached model (2.5) based on the Maxwellian molecules was shown to successfully describe the velocity-shear dominated gas flow like micro flows.^{12,19}

In summary, when and where one applies the closure (or introduces an approximation) is critical in the study of moment equations because of the subtle interplay of the kinematic high order and dissipation terms. Obviously, postponing approximation as late as possible will always be better since it will reduce the possibility of accumulating errors. In addition, maintaining the same level of accuracy in closing high order and dissipation terms also reduces the possibility of producing a singularity in the constitutive equations.

III. BALANCED APPROXIMATIONS VIA THE SECOND LAW OF THERMODYNAMICS

From the study of the shock structure singularity in Sec. II, it appears a simple way to remove the singularity is to introduce some kind of nonlinear viscosity. Such a method was developed for the one-dimensional expansion and compression (shock structure) problem by Karlin *et al.* in 1997²⁰ by starting the Grad's moment equation of the Maxwellian molecules. After introducing the nonlinear viscosity F

$$\Pi = \Pi_{NS} F \left(\frac{\mu_{NS} \partial u / \partial x}{p} \right), \text{ where } \Pi_{NS} \equiv -\mu_{NS} \frac{\partial u}{\partial x}, \quad (3.1)$$

they calculated the time derivative of the normal stress $\partial \Pi / \partial t$; one from the Grad's constitutive equation and another from the definition of the nonlinear viscosity (3.1) and the conservation laws (A5). Then, after they collected the terms relevant to the effect $p \partial u / \partial x$ and equated them, they were able to derive an ordinary differential equation of the unknown factor F in terms of the dimensionless forcing parameter Π_{NS} / p . The solution of the differential equation is shown to remove the shock singularity. Even though their method is instructive in its own right, there are significant shortcomings; it does not cure the constitutive equation and, rather, it simply replaces the constitutive equation with another regularized equation through the nonlinear viscosity (3.1), resulting in complete abandonment of original Grad's constitutive equation. As a consequence, it is not apparent how to extend the method in a systematic way to the general case involving heat flux and multi-dimensionality.

However, there already exists a more general method, known in the literature as Eu's generalized hydrodynamics.¹⁶ Actively developed since 1980s, Eu's theory was primarily disseminated in the chemistry community, in the context of irreversible thermodynamics, and so has so far remained largely unnoticed by physicists, engineers, and mathematicians. His theory is also known to work not only for dilute gases, but also for liquids;⁸ for this reason, his theory is considered in detail here.

A. Resolving the shock structure singularity: Subtle interplay of kinematic and dissipation terms

Eu's theory^{6,7} starts from a crucial observation that the kinetic theory of fluids is intimately connected to irreversible thermodynamics. Once this insight is recognized, one can naturally arrive at the idea that the second law of thermodynamics may be used as a guiding principle for studying fluid motion, and in particular, in high thermal nonequilibrium. After all, the high Mach number shock structure problem—in which the kinetic energy of gas particles rapidly transforms into thermal energy—represents the most vivid example of irreversible thermodynamics. The starting point of this method is the balance equation for the calortropy $\hat{\Psi}$, which is in general different from the Boltzmann entropy,

$$\rho \hat{\Psi}(\mathbf{r}, t) = -k_B \left\langle \left[\ln f^c(\mathbf{v}, \mathbf{r}, t) - 1 \right] f(\mathbf{v}, \mathbf{r}, t) \right\rangle, \quad (3.2)$$

where the nonequilibrium canonical distribution function f^c represents the thermodynamic branch of the solution of the Boltzmann kinetic equation f .⁷ By differentiating the local calortropy density $\hat{\Psi}$ with time and combining it with the Boltzmann equation (A1), the following equation can be obtained:

$$\rho \frac{d\hat{\Psi}}{dt} + \nabla \cdot (-k_B \langle \mathbf{c} (\ln f^c - 1) f \rangle) + k_B \left\langle f \left(\frac{d}{dt} + \mathbf{c} \cdot \nabla \right) \ln f^c \right\rangle = \sigma_c \left(\equiv -k_B \langle \ln f^c C[f, f_2] \rangle \right). \quad (3.3)$$

In calculating the dissipation term the distribution function f may be written as $f = f^c + \Delta f$, where $\Delta f \equiv f - f^c$. If Δf is neglected, which is tantamount to neglecting fluctuations of distribution functions f from the thermodynamic branch of the distribution functions, the calortropy production σ_c , which is always positive, in the right-hand side can further be expressed as ($g_{12} \equiv |\mathbf{v} - \mathbf{v}_2|$)

$$\sigma_c = \frac{1}{4} k_B \int d\mathbf{v} \int d\mathbf{v}_2 \int_0^{2\pi} d\phi \int_0^\infty db b g_{12} \ln(f^{c*} f_2^* / f^c f_2^c) (f^{c*} f_2^* - f^c f_2^c) \geq 0. \quad (3.4)$$

Then, if the calortropy production σ_c is worked out first, instead of the dissipation term $\Lambda^{(n)}$ in the conventional approach, and if there is a direct relation between σ_c and $\Lambda^{(n)}$, a thermodynamically consistent form of $\Lambda^{(n)}$ can be obtained.

From the logarithmic form of the calortropy production in (3.3), $\ln f^c$, it will be convenient to write the distribution function f^c in the exponential form, instead of Grad's polynomial form:

$$f^c = \exp \left[-\beta \left(\frac{1}{2} m c^2 + \sum_{n=1}^{\infty} X^{(n)} h^{(n)} - N \right) \right], \quad (3.5)$$

$$\exp(-\beta N) = \frac{1}{n_d} \left\langle \exp \left[-\beta \left(\frac{1}{2} m c^2 + \sum_{n=1}^{\infty} X^{(n)} h^{(n)} \right) \right] \right\rangle, \quad \beta \equiv \frac{1}{k_B T}.$$

In this expression N is the normalization factor, n_d is the number density, and $X^{(n)}$, unknown macroscopic quantities, are the conjugate variables to the molecular expressions for moment, $h^{(n)}$. The advantage of this exponential form is obvious; in the physical sense it is the only form that satisfies the additive property of the calortropy and calortropy production, all of which are in the logarithmic form; in the mathematical sense it assures the non-negativity of the distribution function regardless of the level of approximations. It must also be noted that no finite approximation for moments is made in (3.5); that is, the number of moments goes to infinity as shown in $\sum_{n=1}^{\infty} X^{(n)} h^{(n)}$.

This is in contrast with a common practice in considering only the first 13 moments from the outset in the formulation of the theory. After the superscripts c in the distribution function f^c are dropped for simplicity and with a short notation for the exponent, the distribution function can be rewritten

$$f = f^{(0)} \exp(-x), \quad \text{where } x \equiv \beta \left(\sum_{n=1}^{\infty} X^{(n)} h^{(n)} - N \right). \quad (3.6)$$

With further introduction of notations and dimensionless variables (y being the post-collision value of x),

$$x_{12} = x_1 + x_2, \quad y_{12} = y_1 + y_2 = x_{12}^*,$$

$$\bar{\sigma}_c = \frac{\sigma_c}{k_B / g}, \quad g \equiv \frac{1}{n^2 d^2} \sqrt{\frac{m}{2k_B T}}, \quad (3.7a)$$

$$\bar{b} = \frac{b}{d}, \quad \bar{g}_{12} = g_{12} \sqrt{\frac{m}{2k_B T}},$$

$$\mathbf{w} = \mathbf{c} \sqrt{\frac{m}{k_B T}}, \quad \omega(\mathbf{w}) \equiv \frac{1}{(2\pi)^{3/2}} \exp\left(-\frac{1}{2} w^2\right), \quad \omega_{12}(\mathbf{w}, \mathbf{w}_2) \equiv \frac{1}{(2\pi)^3} \exp\left(-\frac{1}{2} w^2 - \frac{1}{2} w_2^2\right),$$

$$\langle A \rangle_c \equiv \int d\hat{\Gamma}_{12} \omega_{12}(\mathbf{w}, \mathbf{w}_2) A(\mathbf{w}, \mathbf{w}_2), \quad (3.7b)$$

$$\int d\hat{\Gamma}_{12} \cdots \equiv \int d\mathbf{w} \int d\mathbf{w}_2 \int_0^{2\pi} d\phi \int_0^\infty d\bar{b} \bar{b} \bar{g}_{12} \cdots,$$

$$\int d\Gamma_{12} \cdots \equiv \int d\mathbf{v} \int d\mathbf{v}_2 \int_0^{2\pi} d\phi \int_0^\infty db b g_{12} \cdots,$$

the calortropy production can be expressed as

$$\begin{aligned} \sigma_c &\equiv -k_B \langle \ln f C[f, f_2] \rangle = \frac{1}{T} \left\langle \left(\frac{1}{2} m c^2 + \sum_{n=1}^{\infty} X^{(n)} : h^{(n)} - N \right) C[f^{(0)} \exp(-x), f_2^{(0)} \exp(-x_2)] \right\rangle \\ &= \frac{1}{4} k_B \int d\mathbf{v} \int d\mathbf{v}_2 \int_0^{2\pi} d\phi \int_0^\infty db b g_{12} f^{(0)} f_2^{(0)} (x_{12} - y_{12}) [\exp(-y_{12}) - \exp(-x_{12})] \quad (3.8) \\ &= \frac{1}{4T} \int d\Gamma_{12} f^{(0)} f_2^{(0)} (x_{12} - y_{12}) [\exp(-y_{12}) - \exp(-x_{12})] \end{aligned}$$

or

$$\bar{\sigma}_c = \frac{1}{4} \langle (x_{12} - y_{12}) [\exp(-y_{12}) - \exp(-x_{12})] \rangle_c. \quad (3.9)$$

This form of mathematical equation is suitable for so-called cumulant expansion; from Appendix B, it can be written as

$$\begin{aligned} \bar{\sigma}_c &= \kappa_1^2 q(\kappa_1^{(\pm)}, \kappa_2^{(\pm)}, \dots), \quad \text{where } \kappa_1 \equiv \frac{1}{2} \{ \langle (x_{12} - y_{12})^2 \rangle_c \}^{1/2}, \\ q(\kappa_1^{(\pm)}, \kappa_2^{(\pm)}, \dots) &\equiv \frac{1}{2\kappa_1} \left\{ \exp \left[\sum_{l=1}^{\infty} \frac{(-1)^l}{l!} \kappa_l^{(+)} \right] - \exp \left[\sum_{l=1}^{\infty} \frac{(-1)^l}{l!} \kappa_l^{(-)} \right] \right\}. \quad (3.10) \end{aligned}$$

Note that this form guarantees the positivity of the calortropy production regardless of the level of approximations. In addition, when the distribution function (3.6) is inserted into the definition of calortropy production, the dissipation term $\Lambda^{(n)}$ is shown to be directly related to the calortropy production σ_c ,

$$\begin{aligned} \sigma_c &\equiv -k_B \langle \ln f C[f, f_2] \rangle = -k_B \left\langle -\beta \sum_{n=1}^{\infty} X^{(n)} h^{(n)} C[f, f_2] \right\rangle \\ &= \frac{1}{T} \sum_{n=1}^{\infty} X^{(n)} \langle h^{(n)} C[f, f_2] \rangle = \frac{1}{T} \sum_{n=1}^{\infty} X^{(n)} \Lambda^{(n)}. \quad (3.11) \end{aligned}$$

Now the explicit form of the dissipation term $\Lambda^{(n)}$ can be derived from (3.10) and (3.11) by calculating the first reduced collision integral κ_1 in terms of $X^{(n)}$; since x appearing in κ_1 consists of a sum of various moments, $x \equiv \beta \left(\sum_{n=1}^{\infty} X^{(n)} h^{(n)} - N \right)$, with the definition $\Delta h^{(n)} = h^{(n)} - h^{(n)*}$, etc., κ_1^2 may be expressed as a quadratic form of X and X_2 ,

$$\kappa_1^2 = \frac{1}{4} \sum_{n,l=1}^{\infty} \left\langle \left(X^{(n)} \Delta h^{(n)} + X_2^{(n)} \Delta h_2^{(n)} \right) \left(X^{(l)} \Delta h^{(l)} + X_2^{(l)} \Delta h_2^{(l)} \right) \right\rangle_c. \quad (3.12)$$

On rearrangement of the terms it may become

$$\kappa_1^2 = \sum_{n,l=1}^{\infty} X^{(n)} R_{12}^{(nl)} X_2^{(l)}, \quad (3.13)$$

where $R_{12}^{(nl)}$ are scalar coefficients made up of collision bracket integrals of $h^{(n)}$ and $h_2^{(l)}$ for an isotropic system of dilute gases. After comparing (3.10), (3.11) and (3.13),

$$\bar{\sigma}_c = \kappa_1^2 q(\kappa_1^{(\pm)}, \kappa_2^{(\pm)}, \dots) = \beta g \sum_{n=1}^{\infty} X^{(n)} \Lambda^{(n)} = \sum_{n,l=1}^{\infty} X^{(n)} R_{12}^{(nl)} X_2^{(l)} q(\kappa_1^{(\pm)}, \kappa_2^{(\pm)}, \dots), \quad (3.14)$$

the following dissipation term can be derived:

$$\Lambda^{(n)} = \frac{1}{\beta g} \sum_{l=1}^{\infty} R_{12}^{(nl)} X_2^{(l)} q(\kappa_1^{(\pm)}, \kappa_2^{(\pm)}, \dots). \quad (3.15)$$

In the meantime, the unknown conjugate variables $X^{(n)}$, which were first introduced in (3.5) of the distribution function, need to be determined in terms of macroscopic variables, consistent with the laws of thermodynamics. One way to achieve this is to generalize the equilibrium Gibbs ensemble theory—providing the relationship between thermodynamic variables and the partition functions—to nonequilibrium processes. Such nonequilibrium generalization was developed by Eu⁷ and the main result relevant to the present work can be summarized as

$$\langle h^{(n)} f \rangle / \rho = -k_B T \left(\frac{\partial}{\partial X^{(n)}} \ln Z \right), \text{ where } Z \equiv \frac{1}{n_d} \left\langle \exp \left[-\frac{1}{k_B T} \left(\frac{1}{2} m c^2 + \sum_{n=1}^{\infty} X^{(n)} h^{(n)} \right) \right] \right\rangle. \quad (3.16)$$

Then the $X^{(n)}$ can be determined in terms of the macroscopic flux $\langle h^{(n)} f \rangle$ by solving the differential equation (3.16). The leading order approximate solutions are known to be

$$X^{(1)} = -\frac{\mathbf{\Pi}}{2p}, \quad X^{(2)} = -\frac{\mathbf{Q}}{pC_p T}. \quad (3.17)$$

Finally, the moment equation for general type of molecules (2.1) can be rewritten as ($n = 2$ for shear stress); *still exact to the original Boltzmann equation*,

$$\rho \frac{d(\mathbf{\Pi}/\rho)}{dt} + \nabla \cdot \Psi^{(\Pi)} + 2[\mathbf{\Pi} \cdot \nabla \mathbf{u}]^{(2)} + 2p[\nabla \mathbf{u}]^{(2)} = \frac{1}{\beta g} \sum_{l=1}^{\infty} R_{12}^{(2l)} X_2^{(l)} q(\kappa_1^{(\pm)}, \kappa_2^{(\pm)}, \dots). \quad (3.18)$$

This equation is now suitable for balanced treatment in approximating the kinematic high order term in the left-hand side, $\nabla \cdot \Psi^{(\Pi)}$, and the dissipation term in the right-hand side, $\sum_{l=1}^{\infty} R_{12}^{(2l)} X_2^{(l)} q(\kappa_1^{(\pm)}, \kappa_2^{(\pm)}, \dots)$. The simplest approximation in next level to the linear Navier-Stokes in the left-hand side would be $\nabla \cdot \Psi^{(\Pi)} = 0$, while the leading order approximation of the dissipation term in the right-hand side would be $R_{12}^{(21)} X_2^{(1)} q(\kappa_1^{(\pm)})$. Then, the resulting equation can be expressed as the following, after the Chapman-Enskog collision integral approximation, Eq. (3.17), and the first order cumulant expansion $q(\kappa_1^{(\pm)})$ are applied,

$$\rho \frac{d(\mathbf{\Pi}/\rho)}{dt} + 2[\mathbf{\Pi} \cdot \nabla \mathbf{u}]^{(2)} + 2p[\nabla \mathbf{u}]^{(2)} = -\frac{p}{\mu_{NS}} \mathbf{\Pi} q(\kappa_1), \quad (3.19)$$

$$q(\kappa_1) \equiv \frac{\sinh \kappa_1}{\kappa_1}, \quad \kappa_1 \equiv \frac{(mk_B)^{1/4} T^{1/4}}{\sqrt{2}d} \left(\frac{\mathbf{\Pi} : \mathbf{\Pi}}{\mu_{NS}} + \frac{\mathbf{Q} \cdot \mathbf{Q}/T}{k_{NS}} \right)^{1/2}.$$

Notice that the first-order cumulant expansion takes a form of hyperbolic sine function whose argument is given in terms of basically a Rayleigh dissipation function.^{6,10} When (3.19) is compared with (2.12), the nonlinear factor is equal to

$$F_{approx}(p, T, \mathbf{\Pi} : \mathbf{\Pi}, \mathbf{Q} \cdot \mathbf{Q}, \dots) = q(\kappa_1). \quad (3.20)$$

This is believed to remove the shock singularity because of its balanced approximations. In order to confirm it, the one-dimensional shock structure problem studied in Subsection II A is again

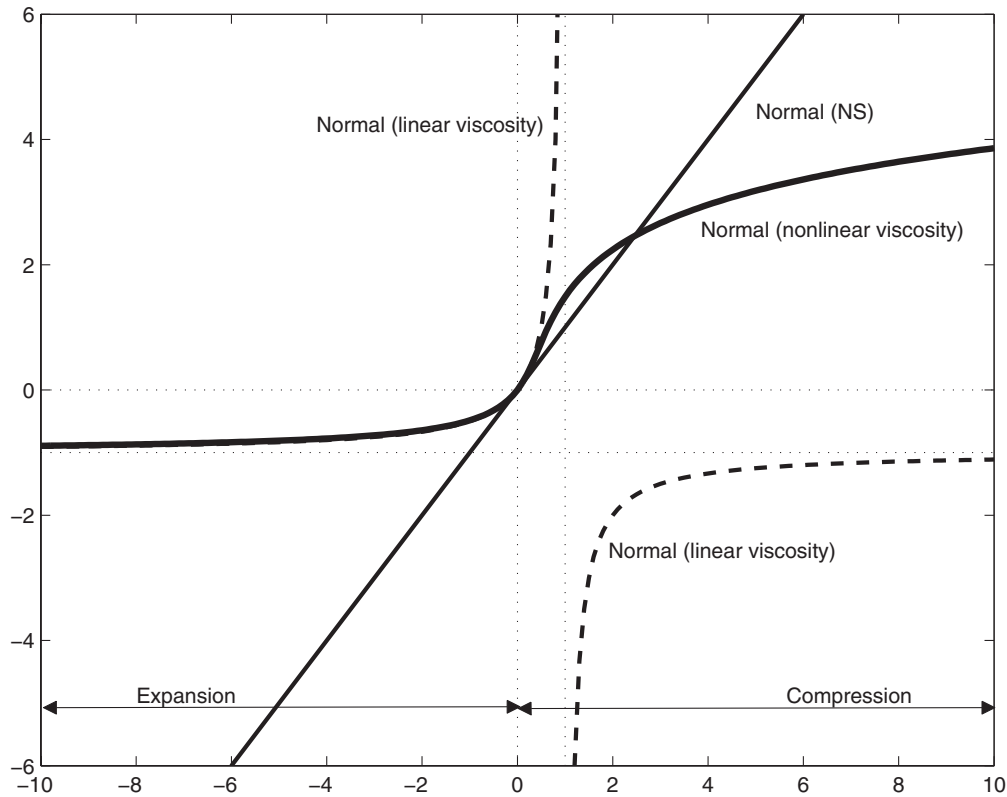


FIG. 1. Solutions of the constitutive equation with nonlinear viscosity (3.21) and the ill-posed constitutive equation (2.9) in the case of Maxwellian molecules. The horizontal and vertical axes represent the strain (force) term $\hat{\Pi}_{NS}$ and the normal stress $\hat{\Pi}$, respectively. The gas is expanding in the range of $\hat{\Pi}_{NS} < 0$, whereas the gas is compressed in the range of $\hat{\Pi}_{NS} > 0$.

considered. In steady-state condition, (3.19) reduces to

$$-\hat{\Pi}\hat{\Pi}_{NS} - \hat{\Pi}_{NS} = -\hat{\Pi}q(c|\hat{\Pi}|) \left(= -\hat{\Pi} - \frac{1}{3!}\hat{\Pi}(c\hat{\Pi})^2 - \frac{1}{5!}\hat{\Pi}(c\hat{\Pi})^4 - \dots \right). \quad (3.21)$$

Here the coefficient c is a positive value, close to 1, dependent on the type of gas molecules; for example, it is 1.0138, and 1.1908 for Maxwellian and hard sphere molecules, respectively.¹⁷

The general solution of the constitutive equation with nonlinear viscosity (3.21) is plotted in Fig. 1 along with the ill-posed equation (2.9) in the case of Maxwellian molecules. It must be noted that (3.21) is a mathematically implicit type due to the form of $q(c|\hat{\Pi}|)$. The implicitness is spawned since the dependent quantity (normal stress) $\hat{\Pi}$ appears in two places and one resides in the exponent of the exponential form. Therefore, the solution of (3.21) in Fig. 1 should be solved by the method of iterations. In contrast with the ill-posed equation (2.9), Eq. (3.21) is indeed well-posed (existence, uniqueness, and continuous dependence on the data) for all inputs $\hat{\Pi}_{NS}$, removing the shock structure singularity completely. The reason behind the removal of the blow-up singularity is simple: with (near-equilibrium) pivot terms $-\hat{\Pi}_{NS}$, $-\hat{\Pi}$ in the left-hand and right-hand sides, the presence of the term $q(c|\hat{\Pi}|)$ makes the $-\hat{\Pi}\hat{\Pi}_{NS}$ in the left-hand side balanced by the high order term like $-\hat{\Pi}(c\hat{\Pi})^2$. The solutions also show asymptotic behavior with the increasing degree of expansion, satisfying the free-molecular limit $\hat{\Pi} \rightarrow -1$ or $\Pi + p \rightarrow 0$.

Another important point is that the constitutive equation without and with the nonlinear viscosity yields essentially the same solution in the case of expansion (negative $\hat{\Pi}_{NS}$). This clearly indicates that the behaviors of the constitutive equations are extremely complex and highly problem-dependent. In summary, accuracy and physical relevancy of constitutive equations can be assessed only *a posteriori* after painstakingly solving all possible basic flow situations—notably,

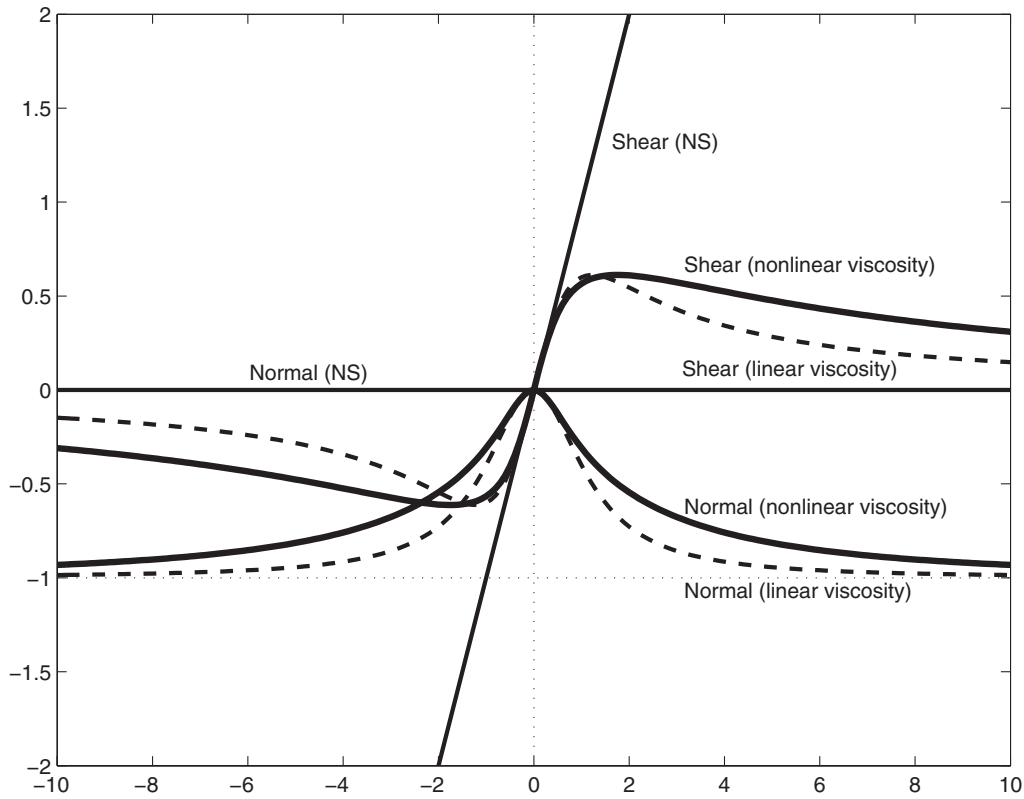


FIG. 2. Solutions of the constitutive equation with nonlinear viscosity (3.22) and the constitutive equation with linear viscosity, $\hat{\Pi}_{xy} = 3\hat{\Pi}_{xyNS}/(3 + 2\hat{\Pi}_{xyNS}^2)$, in the case of velocity shear flow. The horizontal and vertical axes represent the strain (force) term $\hat{\Pi}_{xyNS}$ and the shear and normal stresses $\hat{\Pi}_{xy}$, $\hat{\Pi}_{yy}$, respectively.

compression (shock), expansion, and velocity-shear—and ultimately after comparing with direct computer simulations of the Boltzmann equation and experimental observation.

B. Non-essential role of dissipation terms in the velocity shear problem

The negligible role of the nonlinear viscosity factor F_{approx} due to its cancellation in the velocity shear case was already demonstrated in (2.14)–(2.16) of Subsection II B. Since an explicit form of the nonlinear factor, $q(\kappa_1)$, was derived in Subsection III A, the solution of the constitutive equation can now be written as

$$\hat{\Pi}_{xy} = \frac{3\hat{\Pi}_{xyNS}}{3q(c|\hat{R}|) + 2\hat{\Pi}_{xyNS}^2/q(c|\hat{R}|)}, \text{ where } \hat{R}^2 \equiv 2\hat{\Pi}_{yy}(\hat{\Pi}_{yy} - 1), \hat{\Pi}_{xy}^2 = -\frac{3}{2}(1 + \hat{\Pi}_{yy})\hat{\Pi}_{yy}. \quad (3.22)$$

This highly nonlinear algebraic equation of stresses can be solved by the method of iterations and its solution is plotted in Fig. 2 along with the solution of the constitutive equation with the linear viscosity, $\hat{\Pi}_{xy} = 3\hat{\Pi}_{xyNS}/(3 + 2\hat{\Pi}_{xyNS}^2)$. Similar to the expansion case, the constitutive equation without and with the nonlinear viscosity yields qualitatively the same solution; the shear thinning and free-molecular behaviors for the shear and normal stresses, Π_{xy} , Π_{yy} , respectively. This non-intuitive result explains why the constitutive equation based on the overreach of the Maxwellian molecule assumption, in spite of its inherent weakness, successfully described the velocity-shear dominated flows like low-speed micro flows in the past.

IV. SUMMARY AND CONCLUDING REMARKS

The source of the high Mach number shock structure singularity in gas dynamics and its regularization were investigated in detail. For such an undertaking, four strategies were employed: interpreting the solution of constitutive equation as a relation to determine the unknown high order flux (like the stress) for a given input (like strain or velocity gradient); the one-dimensional flow assumption; the Galilean invariance; and deferring approximations to the last stage of the analysis in order to minimize any chance of accumulated error.

The ultimate source of the singularity turns out to be an unbalanced treatment among two open kinematic high order and dissipation terms, and its consequence is magnified in blow-up fashion, in a high compressive shock structure problem. As a method to achieve the balanced treatment, Eu's generalized hydrodynamics, consistent with the second law of thermodynamics, were considered. After introducing the canonical distribution function in exponential form, and by applying the nonequilibrium generalization of the Gibbs ensemble theory and the cumulant expansion to the explicit calculation of the dissipation term, a natural platform (3.18) suitable for the balanced treatment was derived. Then the constitutive equation (3.21) derived by the balanced treatment was shown to be well-posed for all input data, removing the blow-up shock singularity completely.

The present analysis strongly indicates that the constitutive equation (2.12) with the nonlinear viscosity factor, instead of the commonly used constitutive equation (2.5) with the linear viscosity, should be used for general types of molecule including the Maxwellian molecules. The difference between the two equations is shown to be negligible in the case of expansion and velocity-shear flows, since the nonlinear high order effects are cancelled under the constraint of the free-molecular

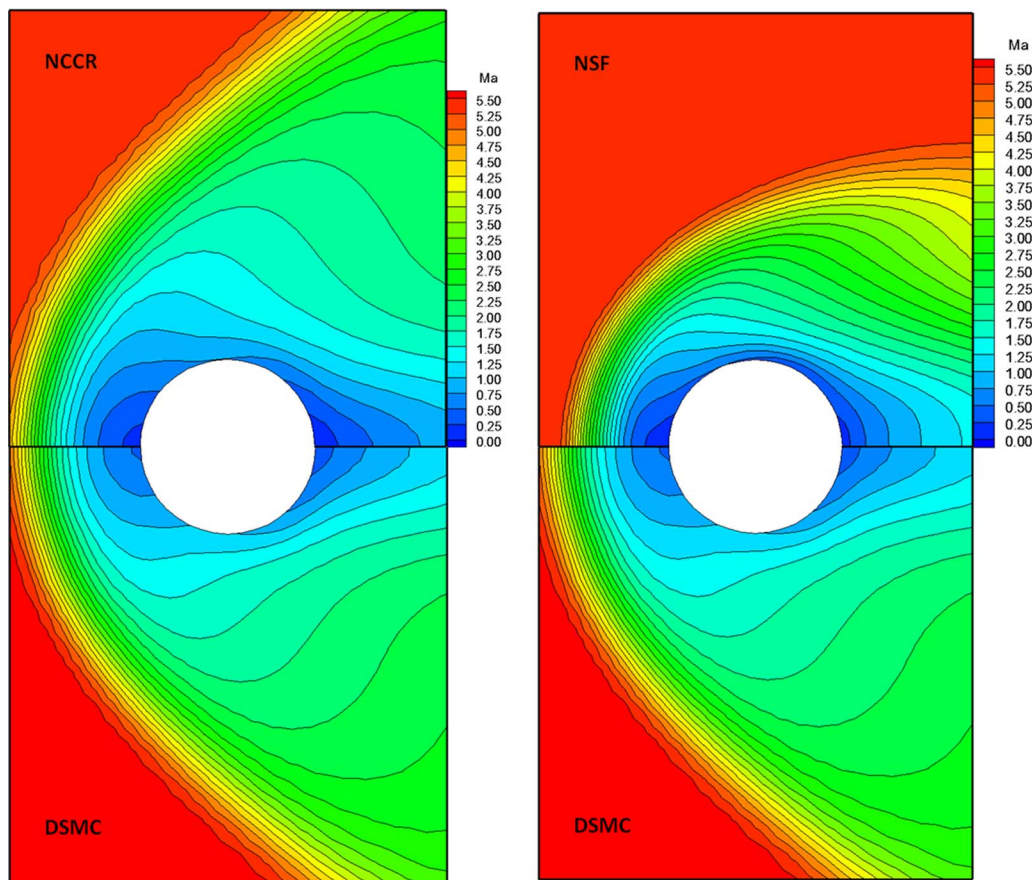


FIG. 3. Mach number contours of the hypersonic case (argon gas), $M = 5.48$ and $Kn = 0.5$: (a) constitutive equation with the nonlinear factor $q(\kappa_1)$ (NCCR; nonlinear coupled constitutive relation) and DSMC, and (b) NSF and DSMC.

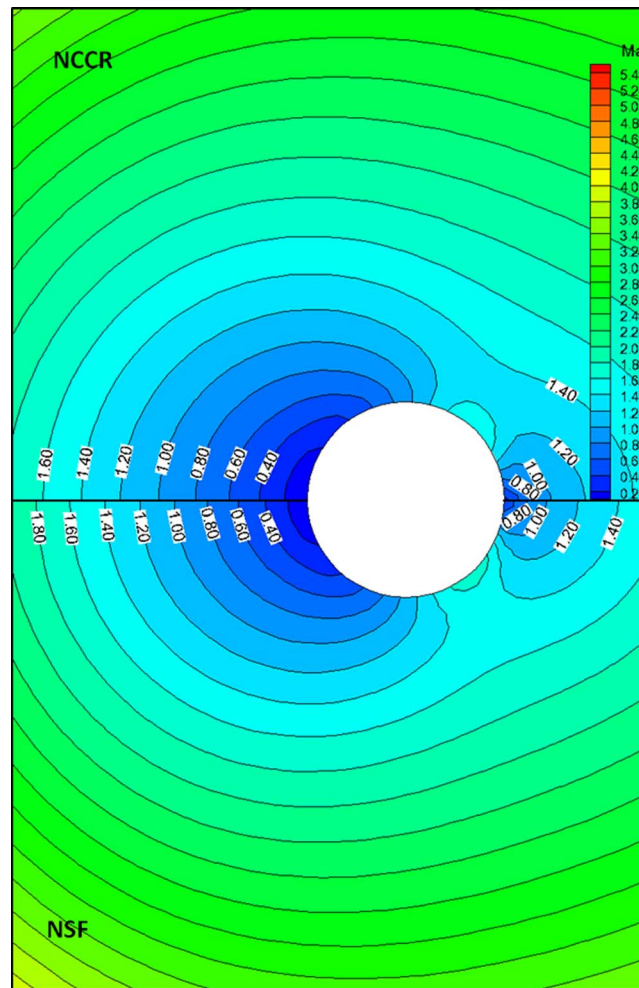


FIG. 4. Mach number contours of the hypersonic case (argon gas), $M = 5.48$ and $Kn = 5.0$: (a) constitutive equation with the nonlinear factor $q(\kappa_1)$ (NCCR; nonlinear coupled constitutive relation), and (b) NSF.

asymptotic behavior. However, the property ceases to be valid for compression, and consequently the nonlinear viscosity factor remains crucial. In this sense, the Maxwellian molecule model in the dissipation term is a nice-to-have mathematical coincidence, but if misplaced, becomes detached from the physics of general gas molecules. The conventional unbalanced treatment—the dissipation term being exact while the other high order term is non-exact—can mislead our understanding of constitutive equations of general gas molecules.

The practical application of the present theory is being actively undertaken at present. An example can be found in Figs. 3 and 4 of the computational simulation of high Mach number rarefied gas flows past a circular cylinder using an explicit triangular discontinuous Galerkin scheme of non-Newtonian implicit constitutive equations. The present model with the nonlinear factor $q(\kappa_1)$ term, presented in (3.19), is shown not only to work for all Mach numbers and high Knudsen numbers like $M = 5.48$ and $Kn = 0.5, 5.0$, but also to provide the results in close agreement with direct simulation Monte Carlo (DSMC).

The present study has been limited to a monatomic gas for its simplicity and historical significance in the development of kinetic theory. However, owing to the universal nature of the dissipation terms in a many-body problem, the same singularity problem may arise in non-Newtonian complex fluids like polymer solutions. Extension of the present line of investigation towards resolving the singularity problem in complex fluids will be reported in near future.

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APPENDIX A: DERIVATION OF EXACT MOMENT EQUATIONS

The Boltzmann kinetic equation of the distribution of monatomic gas particles f reads as follows:

$$\left(\frac{\partial}{\partial t} + \mathbf{v} \cdot \nabla \right) f(\mathbf{v}, \mathbf{r}, t) = C[f, f_2], \quad (\text{A1})$$

where the term $C[f, f_2]$ represents the Boltzmann collision integral of the interaction among the particles. The moment equations can be obtained by differentiating the statistical definition of the variable in question with time and later combining with the Boltzmann equation; it yields for molecular expressions of general moment $h^{(n)}$

$$\frac{\partial}{\partial t} \langle h^{(n)} f \rangle + \nabla \cdot (\mathbf{u} \langle h^{(n)} f \rangle) + \langle \mathbf{c} h^{(n)} f \rangle - \left\langle f \frac{d}{dt} h^{(n)} \right\rangle - \langle f \mathbf{c} \cdot \nabla h^{(n)} \rangle = \Lambda^{(n)} (\equiv \langle h^{(n)} C[f, f_2] \rangle). \quad (\text{A2})$$

The symbols $\mathbf{c}, \langle \rangle, \Lambda^{(n)}$ denote the peculiar velocity, the integral in velocity space, and the dissipation terms, respectively. For $h^{(1)} = [m\mathbf{c}\mathbf{c}]^{(2)}$, where $m, []^{(2)}$ denote the mass of gas molecule and the traceless symmetric part, the following constitutive equation of the shear stress tensor $\mathbf{\Pi} \equiv \langle m[\mathbf{c}\mathbf{c}]^{(2)} f \rangle$ can be derived:

$$\rho \frac{d(\mathbf{\Pi}/\rho)}{dt} + \nabla \cdot \mathbf{\Psi}^{(\mathbf{\Pi})} + 2[\mathbf{\Pi} \cdot \nabla \mathbf{u}]^{(2)} + 2p[\nabla \mathbf{u}]^{(2)} = \Lambda^{(\mathbf{\Pi})} (\equiv \langle h^{(1)} C[f, f_2] \rangle), \quad (\text{A3})$$

$$\mathbf{\Psi}^{(\mathbf{\Pi})} \equiv \langle m\mathbf{c}\mathbf{c}\mathbf{c} f \rangle - \langle m\text{Tr}(\mathbf{c}\mathbf{c}) f \rangle \mathbf{I}/3.$$

Note that Eq. (A3) is exactly the same as (5.15) in Grad's work.² Similarly, for the next term, $h^{(3)} = (mc^2/2 - mC_p T)\mathbf{c}$, C_p being the heat capacity per mass at constant pressure, the constitutive equation of the heat flux vector $\mathbf{Q} \equiv \langle mc^2 \mathbf{c} f / 2 \rangle$ can be obtained (assuming $\mathbf{J} \equiv \langle m\mathbf{c} f \rangle = 0$ in monatomic gas);

$$\rho \frac{d(\mathbf{Q}/\rho)}{dt} + \nabla \cdot \mathbf{\Psi}^{(\mathbf{Q})} + \langle m\mathbf{c}\mathbf{c}\mathbf{c} f \rangle : \nabla \mathbf{u} + \frac{d\mathbf{u}}{dt} \cdot \mathbf{\Pi} + \mathbf{Q} \cdot \nabla \mathbf{u} + \mathbf{\Pi} \cdot C_p \nabla T + pC_p \nabla T$$

$$= \Lambda^{(\mathbf{Q})} (\equiv \langle h^{(3)} C[f, f_2] \rangle), \quad (\text{A4})$$

$$\mathbf{\Psi}^{(\mathbf{Q})} \equiv \langle mc^2 \mathbf{c}\mathbf{c} f / 2 \rangle - C_p T (p\mathbf{I} + \mathbf{\Pi}).$$

Note that both of $\mathbf{\Psi}^{(\mathbf{\Pi})}$ and $\mathbf{\Psi}^{(\mathbf{Q})}$ vanish near equilibrium. Note also that the constitutive equation (A4) was not presented in Grad's work² since his 13-moment closure was already in place. In the derivation, the following relations are used:

$$\langle h^{(3)} f \rangle = \mathbf{Q} - C_p T \mathbf{J},$$

$$\langle \mathbf{c} h^{(3)} f \rangle = \langle \mathbf{c} (mc^2/2 - mC_p T) \mathbf{c} f \rangle = \langle mc^2 \mathbf{c}\mathbf{c} f / 2 \rangle - C_p T \mathbf{P},$$

$$\left\langle f \frac{\partial}{\partial t} h^{(3)} \right\rangle = \left\langle f \frac{\partial}{\partial t} (mc^2 \mathbf{c} / 2) \right\rangle - \left\langle f \frac{\partial}{\partial t} (C_p T) m\mathbf{c} \right\rangle - \left\langle m f C_p T \frac{\partial \mathbf{c}}{\partial t} \right\rangle = -\frac{\partial \mathbf{u}}{\partial t} \cdot \mathbf{P} - \rho E \mathbf{I} \cdot \frac{\partial \mathbf{u}}{\partial t}$$

$$- \mathbf{J} \frac{\partial}{\partial t} (C_p T) + \rho C_p T \frac{\partial \mathbf{u}}{\partial t} = -\frac{\partial \mathbf{u}}{\partial t} \cdot \mathbf{\Pi} - \mathbf{J} \frac{\partial}{\partial t} (C_p T),$$

$$\begin{aligned}
\langle f\mathbf{u} \cdot \nabla h^{(3)} \rangle &= \langle f\mathbf{u} \cdot \nabla (mc^2\mathbf{c}/2) \rangle - \langle mf\mathbf{u} \cdot \nabla (C_p T\mathbf{c}) \rangle = \langle fmc^2\mathbf{u} \cdot \nabla\mathbf{c}/2 \rangle + \langle fm(\mathbf{u} \cdot \nabla c^2)\mathbf{c}/2 \rangle \\
&\quad - \langle mf(\mathbf{u} \cdot \nabla C_p T)\mathbf{c} \rangle - \langle mfC_p T\mathbf{u} \cdot \nabla\mathbf{c} \rangle = -\rho E\mathbf{u} \cdot \nabla\mathbf{u} - \mathbf{u} \cdot \nabla\mathbf{u} \cdot \mathbf{P} - \mathbf{J}(\mathbf{u} \cdot \nabla C_p T) + \rho C_p T\mathbf{u} \cdot \nabla\mathbf{u}, \\
\langle f\mathbf{c} \cdot \nabla h^{(3)} \rangle &= \langle f\mathbf{c} \cdot \nabla (mc^2\mathbf{c}/2) \rangle - \langle mf\mathbf{c} \cdot \nabla (C_p T\mathbf{c}) \rangle = \langle fmc^2\mathbf{c} \cdot \nabla\mathbf{c}/2 \rangle + \langle fm(\mathbf{c} \cdot \nabla c^2)\mathbf{c}/2 \rangle \\
&\quad - \langle mf(\mathbf{c} \cdot \nabla C_p T)\mathbf{c} \rangle - \langle mfC_p T\mathbf{c} \cdot \nabla\mathbf{c} \rangle = -\mathbf{Q} \cdot \nabla\mathbf{u} - \psi^{(P)} : \nabla\mathbf{u} - \mathbf{P} \cdot \nabla C_p T + C_p T\mathbf{J} \cdot \nabla\mathbf{u}, \\
\psi^{(P)} &\equiv \langle m\mathbf{c}\mathbf{c}\mathbf{c}f \rangle, \rho E \equiv \langle mc^2 f/2 \rangle, C_p T = p/\rho + E, \mathbf{P} = p\mathbf{I} + \mathbf{\Pi}.
\end{aligned}$$

Finally, the following conservation laws and constitutive equations, all of which are an exact consequence of the Boltzmann equation, can be expressed in compact form:

$$\rho \frac{d}{dt} \begin{bmatrix} 1/\rho \\ \mathbf{u} \\ E_t \end{bmatrix} + \nabla \cdot \begin{bmatrix} -\mathbf{u} \\ p\mathbf{I} \\ p\mathbf{u} \end{bmatrix} + \nabla \cdot \begin{bmatrix} 0 \\ \mathbf{\Pi} \\ \mathbf{\Pi} \cdot \mathbf{u} + \mathbf{Q} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}, \quad (\text{A5})$$

$$\rho \frac{d}{dt} \begin{bmatrix} \mathbf{\Pi}/\rho \\ \mathbf{Q}/\rho \end{bmatrix} + \nabla \cdot \begin{bmatrix} \mathbf{\Psi}^{(\Pi)} \\ \mathbf{\Psi}^{(Q)} \end{bmatrix} + \begin{bmatrix} 2[\mathbf{\Pi} \cdot \nabla\mathbf{u}]^{(2)} \\ \psi^{(P)} : \nabla\mathbf{u} + \frac{d\mathbf{u}}{dt} \cdot \mathbf{\Pi} + \mathbf{Q} \cdot \nabla\mathbf{u} + \mathbf{\Pi} \cdot C_p \nabla T \end{bmatrix} + \begin{bmatrix} 2p[\nabla\mathbf{u}]^{(2)} \\ C_p p \nabla T \end{bmatrix} = \begin{bmatrix} \mathbf{\Lambda}^{(\Pi)} \\ \mathbf{\Lambda}^{(Q)} \end{bmatrix}. \quad (\text{A6})$$

APPENDIX B: CUMULANT EXPANSION FOR CALORTROPY PRODUCTION

After the canonical distribution function is inserted into the calortropy balance equation, the calortropy production term can be expressed in terms of exponential function as follows:^{6,7}

$$\bar{\sigma}_c \equiv -g \langle \ln f C[f, f_2] \rangle = \frac{1}{4} \langle (x_{12} - y_{12}) [\exp(-y_{12}) - \exp(-x_{12})] \rangle_c. \quad (\text{B1})$$

This form of mathematical equation is suitable for so-called cumulant expansion. It can further be cast into

$$\begin{aligned}
\bar{\sigma}_c &= \frac{1}{4} [R^{(+)}(\lambda) - R^{(-)}(\lambda)]_{\lambda=1}, \\
R^{(+)}(\lambda) &\equiv \langle (x_{12} - y_{12}) [\exp(-\lambda y_{12}) - 1] \rangle_c, \quad R^{(-)}(\lambda) \equiv \langle (x_{12} - y_{12}) [\exp(-\lambda x_{12}) - 1] \rangle_c.
\end{aligned} \quad (\text{B2})$$

Here the parameter λ is introduced as a bookkeeping index. After expansion in series of $R^{(\pm)}(\lambda)$, it will be set $\lambda = 1$. A description of the cumulant expansion will be helpful here. Let $f(x)$ be the probability distribution of x . The l th moment of this probability distribution is defined as the expectation value of x^l :

$$\langle x^l \rangle = \int x^l f(x) dx, \quad (\text{B3})$$

and the moment-generated function as the expectation value of $e^{\lambda x}$

$$\langle e^{\lambda x} \rangle = \int f(x) e^{\lambda x} dx. \quad (\text{B4})$$

The following relations hold for the power series and derivatives:

$$\langle e^{\lambda x} \rangle = \sum_{l=0}^{\infty} \frac{\lambda^l}{l!} \int f(x) x^l dx = \sum_{n=0}^{\infty} \frac{\lambda^n}{n!} \langle x^n \rangle \text{ or } \langle x^l \rangle = \left[\frac{d^l}{d\lambda^l} \langle e^{\lambda x} \rangle \right]_{\lambda=0}. \quad (\text{B5})$$

The logarithm of the characteristic function is called the cumulant-generating function and its series coefficients $\kappa_l^{(+)}$ in the Taylor expansion for λ are called cumulants of the variable x :

$$\ln \langle e^{\lambda x} \rangle = \sum_{l=0}^{\infty} \frac{\lambda^l}{l!} \kappa_l^{(+)} \text{ or } \kappa_l^{(+)} = \left[\frac{d^l}{d\lambda^l} \ln \langle e^{\lambda x} \rangle \right]_{\lambda=0}. \quad (\text{B6})$$

Expressions for cumulants in terms of moments may be obtained directly from the definition and Eq. (B5), for example,

$$\begin{aligned}\kappa_1^{(+)} &= \left[\frac{d}{d\lambda} \ln \langle e^{\lambda x} \rangle \right]_{\lambda=0} = \left[\frac{1}{\langle e^{\lambda x} \rangle} \frac{d}{d\lambda} \langle e^{\lambda x} \rangle \right]_{\lambda=0} = \left[\frac{d}{d\lambda} \langle e^{\lambda x} \rangle \right]_{\lambda=0} = \langle x \rangle, \\ \kappa_2^{(+)} &= \left[\frac{d^2}{d\lambda^2} \ln \langle e^{\lambda x} \rangle \right]_{\lambda=0} = \left[-\frac{1}{\langle e^{\lambda x} \rangle^2} \left(\frac{d}{d\lambda} \langle e^{\lambda x} \rangle \right)^2 + \frac{1}{\langle e^{\lambda x} \rangle} \frac{d^2}{d\lambda^2} \langle e^{\lambda x} \rangle \right]_{\lambda=0} = \langle x^2 \rangle - \langle x \rangle^2, \dots\end{aligned}\quad (\text{B7})$$

It should be noted that $\langle e^{\lambda x} \rangle = 1$ for $\lambda = 0$. Then the relationship between moments and cumulants may be summarized as follows:

$$\langle e^{\lambda x} \rangle = \sum_{l=0}^{\infty} \frac{\lambda^l}{l!} \langle x^l \rangle = \exp \left[\sum_{l=0}^{\infty} \frac{\lambda^l}{l!} \kappa_l^{(+)} \right]. \quad (\text{B8})$$

When this is applied to $R^{(\pm)}(\lambda)$ in (B2), the following cumulant expansion can be obtained:

$$R^{(\pm)}(\lambda) = \{ \langle (x_{12} - y_{12})^2 \rangle_c \}^{1/2} \left\{ \exp \left[\sum_{l=1}^{\infty} \frac{(-\lambda)^l}{l!} \kappa_l^{(\pm)} \right] - 1 \right\}. \quad (\text{B9})$$

In this step, since there is a term $(x_{12} - y_{12})$ in (B2), it is convenient to introduce a pre-factor $\{ \langle (x_{12} - y_{12})^2 \rangle_c \}^{1/2}$ in the front and then define subsequent cumulants. With such a factor the cumulants are constructed systematically by expansion and the resulting leading (1st-mean, 2nd-variance, 3rd-skewness) cumulants $\kappa_{1,2,3}^{(\pm)}$ are given by the moments of reduced collision integrals $\kappa_{1,2,3}$

$$\kappa_1^{(\pm)} = \mp \kappa_1, \kappa_2^{(\pm)} = \mp \frac{\kappa_2}{\kappa_1} - \kappa_1^2, \kappa_3^{(\pm)} = \mp \frac{\kappa_3}{\kappa_1} - 3\kappa_2 \mp 2\kappa_1^3, \quad (\text{B10})$$

where

$$\kappa_1 = \frac{1}{2} \{ \langle (x_{12} - y_{12})^2 \rangle_c \}^{1/2}, \kappa_2 = \frac{1}{4} \{ \langle (x_{12} - y_{12})(x_{12}^2 - y_{12}^2) \rangle_c \}, \kappa_3 = \frac{1}{4} \{ \langle (x_{12} - y_{12})(x_{12}^3 - y_{12}^3) \rangle_c \}. \quad (\text{B11})$$

The cumulant expansion may be regarded as a partial resummation of the expansion of the Boltzmann collision integral in a series of the parameter $\text{Kn} \cdot \text{M}$, and as such, it takes into account highly nonlinear irreversible processes to infinite order. Finally, the calortropy production can be written as

$$\begin{aligned}\bar{\sigma}_c &= \kappa_1^2 q(\kappa_1^{(\pm)}, \kappa_2^{(\pm)}, \dots), \\ \kappa_1 &\equiv \frac{1}{2} \{ \langle (x_{12} - y_{12})^2 \rangle_c \}^{1/2}, \\ q(\kappa_1^{(\pm)}, \kappa_2^{(\pm)}, \dots) &= \frac{1}{2\kappa_1} \left\{ \exp \left[\sum_{l=1}^{\infty} \frac{(-1)^l}{l!} \kappa_l^{(+)} \right] - \exp \left[\sum_{l=1}^{\infty} \frac{(-1)^l}{l!} \kappa_l^{(-)} \right] \right\}.\end{aligned}\quad (\text{B12})$$

Using three leading cumulants given in (B11) the expanded form can be expressed as

$$\begin{aligned}\bar{\sigma}_c &= \frac{\kappa_1}{2} \left\{ \exp \left[\kappa_1 - \frac{1}{2} \left(\frac{\kappa_2}{\kappa_1} + \kappa_1^2 \right) + \frac{1}{3!} \left(\frac{\kappa_3}{\kappa_1} + 3\kappa_2 + 2\kappa_1^3 \right) + \dots \right] \right. \\ &\quad \left. - \exp \left[-\kappa_1 + \frac{1}{2} \left(\frac{\kappa_2}{\kappa_1} - \kappa_1^2 \right) - \frac{1}{3!} \left(\frac{\kappa_3}{\kappa_1} - 3\kappa_2 + 2\kappa_1^3 \right) + \dots \right] \right\}.\end{aligned}\quad (\text{B13})$$

Notice that the source of different sign of the exponent is traced to the calortropy production, $\ln(f^* f_2^*/f f_2)(f^* f_2^* - f f_2)$, in (3.4). Finally, if the first-order cumulant approximation is applied, it reduces to

$$\bar{\sigma}_c = \kappa_1^2 q(\kappa_1) = \kappa_1 \sinh \kappa_1. \quad (\text{B14})$$

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