

# Macroscopic descriptions of rarefied gases from the elimination of fast variables

Paul J. Dellar\*

*Department of Mathematics, Imperial College London, London SW7 2AZ, United Kingdom*<sup>†</sup>

(Dated: 29 January 2007, revised 15 July 2007, accepted 24 July 2007 by *Physics of Fluids*)

The Boltzmann equation describing a dilute monatomic gas is equivalent to an infinite hierarchy of evolution equations for successive moments of the distribution function. The five moments giving the macroscopic mass, momentum, and energy densities are unaffected by collisions between atoms, while all other moments naturally evolve on a fast collisional timescale. We show that the macroscopic equations of Chen, Rao, and Spiegel [*Phys. Lett. A*, **271**, 87], like the familiar Navier–Stokes–Fourier equations, emerge from using a systematic procedure to eliminate the higher moments, leaving closed evolution equations for the five moments unaffected by collisions. The two equation sets differ through their treatment of contributions from the temperature to the momentum and energy fluxes. Using moment equations offers a definitive treatment of the Prandtl number problem using model collision operators, greatly reduces the labor of deriving equations for different collision operators, and clarifies the rôle of solvability conditions applied to the distribution function. The original Chen–Rao–Spiegel approach offers greatly improved agreement with experiments for the phase speed of ultrasound, but when corrected to match the Navier–Stokes–Fourier equations at low frequencies it then under-estimates the phase speed at high frequencies. Our introduction of a translational temperature, as in the kinetic theory of polyatomic gases, motivates a distinction in the energy flux between advection of internal energy and the work done by the pressure. Exploiting this distinction yields macroscopic equations that offer further improvement in agreement with experimental data, and arise more naturally as an approximation to the infinite hierarchy of evolution equations for moments.

## I. INTRODUCTION

The derivation of suitable descriptions for the behavior of rarefied gases in practical applications is a long-standing problem. The underlying kinetic theory is formulated using a distribution function to specify the number density of atoms or molecules moving with a given velocity at a given point in space and time. The distribution function thus evolves in a six-dimensional phase space.<sup>1–3</sup> Boltzmann’s equation describes the evolution of the distribution function for a dilute monatomic gas, but even this is too unwieldy for many practical applications, especially those requiring more than one spatial dimension. Early applications were primarily in the area of high altitude aeronautics and hypersonic flow, but much recent work is motivated by the development of micro-electro-mechanical devices (MEMs) operating at room temperatures and pressures. In both cases, a simplified description exploits the separation between the scales that characterize collisions between atoms or molecules and the, typically much larger, scales of the device in question. This separation is quantified by the smallness of a dimensionless parameter, the Knudsen number  $Kn$ .

A straightforward expansion of the distribution function in Knudsen number leads inevitably to the Hilbert expansion,<sup>4</sup> which becomes disordered after times of  $O(1/Kn)$  when deviations from ideal fluid dynamics become appreciable. Descriptions valid over long timescales are therefore based on expanding the equations that describe the solution, rather than expanding the solution itself.<sup>4</sup> More precisely, the Chapman–Enskog expansion<sup>1,3</sup> yields closed evolution equations for the five quantities – mass, three components of momentum, and energy – that are conserved by collisions between atoms. The momentum and energy fluxes are expressed as series in these five quantities and their spatial derivatives. The Chapman–Enskog expansion yields the compressible Euler equations at leading order, and the Navier–Stokes–Fourier equations as the first corrections at  $O(Kn)$ . Although widely used, the Navier–Stokes–Fourier equations become inadequate for rarefied flows with  $Kn \gtrsim 0.01$ . For example, they predict a phase speed for ultrasound that grows arbitrarily large for sufficiently high frequencies (sufficiently large  $Kn$ ). Continuing the Chapman–Enskog expansion to higher order yields the Burnett and super-Burnett equations at  $O(Kn^2)$  and  $O(Kn^3)$  respectively. These equations have met with limited success at describing physical phenomena, since they lead to ill-posed initial value problems, and require additional boundary conditions.

The Chapman–Enskog expansion has usually been presented, since the 1960s, as a multiple-scales expansion of both the distribution function and the time derivative in powers of the Knudsen number.<sup>5,6</sup> The ordering of this double expansion does survive over long times, but at the price of requiring order-by-order solvability conditions on the expansion of the distribution function. Recent work by Chen, Rao, and Spiegel<sup>7–9</sup> discarded the multiple-scales expansion of the time derivative, with its associated order-by-order solvability conditions, in favor of solvability conditions imposed only upon the expansion as a whole. By thus retaining various higher order terms involving time derivatives of macroscopic quantities they obtained a description that sometimes offers greatly improved agreement with experiment, notably for the phase speed of ultrasound over the whole range of Knudsen numbers, for only a modest increase in complexity over the Navier–Stokes–Fourier equations.

In this paper we show that the Chen–Rao–Spiegel equations, like the Navier–Stokes–Fourier equations, may be derived using a general procedure for the elimination of fast variables proposed by van Kampen.<sup>10,11</sup> The Boltzmann equation is equivalent to an infinite hierarchy of evolution equations for successive moments of the distribution function with respect to the particle velocity.

---

\*Email: paul.dellar@na-net.ornl.gov

<sup>†</sup>Now at: OCIAM, Mathematical Institute, 24–29 St Giles’, Oxford OX1 3LB, United Kingdom.

The moments giving the mass, momentum, and energy densities evolve only through spatial gradients of higher moments, with no contributions from collisions between atoms. These five moments are therefore slow variables in van Kampen’s terminology, since the hydrodynamic timescale  $T$  associated with evolution due to spatial gradients is typically much longer than the timescale  $\tau$  characteristic of collisions between atoms. All other moments, notably the momentum and energy fluxes, naturally evolve on the fast collisional timescale. The slow variables are left unexpanded in van Kampen’s procedure, while the fast variables are expanded in powers of  $\epsilon = \tau/T$ . Solving order-by-order for the fast variables leads to closed evolution equations for the slow variables that remain valid over long times.<sup>10,11</sup>

The slow variables are uniquely determined by the structure of the equations, in this case by the collision operator, but to quote van Kampen: “*the fast variables are not unique but can be contaminated with an arbitrary amount of slow terms*”.<sup>10</sup> Different choices of fast variables lead to different, albeit asymptotically equivalent, evolution equations for the slow variables at each order of approximation. We show that the Chen–Rao–Spiegel and Navier–Stokes–Fourier equations arise from different decompositions of the momentum and energy fluxes between fast and slow variables. In the notation described below, the Navier–Stokes–Fourier equations arise from decomposing the momentum flux  $\Pi$  and energy flux  $\mathcal{F}$  into

$$\Pi = \rho \mathbf{u} \mathbf{u} + \rho \theta \mathbf{1} + \tilde{\mathbf{P}}, \quad \mathcal{F} = \frac{1}{2} \rho |\mathbf{u}|^2 \mathbf{u} + \tilde{\mathbf{P}} \cdot \mathbf{u} + \frac{5}{2} \rho \theta \mathbf{u} + \tilde{\mathbf{q}}, \quad (1)$$

while the Chen–Rao–Spiegel equations arise from decomposing the same fluxes into

$$\Pi = \rho \mathbf{u} \mathbf{u} + \mathbf{P}, \quad \mathcal{F} = \frac{1}{2} \rho |\mathbf{u}|^2 \mathbf{u} + \tilde{\mathbf{P}} \cdot \mathbf{u} + \mathbf{q}. \quad (2)$$

The slightly different set of equations introduced in this paper arise from separating the advection of internal energy from the work done by the pressure, and writing

$$\Pi = \rho \mathbf{u} \mathbf{u} + \mathbf{P}, \quad \mathcal{F} = \left( \frac{1}{2} \rho |\mathbf{u}|^2 + \frac{3}{2} \rho \theta \right) \mathbf{u} + \mathbf{P} \cdot \mathbf{u} + \tilde{\mathbf{q}}. \quad (3)$$

Thus  $\mathbf{P}$  denotes the complete pressure tensor, while  $\tilde{\mathbf{P}} = \mathbf{P} - \rho \theta \mathbf{1}$  is commonly called the deviatoric pressure. Similarly,  $\tilde{\mathbf{q}}$  would be the conductive heat flux in the Navier–Stokes–Fourier equations, while  $\tilde{\mathbf{q}}$  is an energy flux that also includes advection of internal energy and work done by pressure. Precise definitions are given in equations (11) and (12) of §II.

The fluid density  $\rho$ , velocity  $\mathbf{u}$ , and temperature  $\theta$  are slow variables, being conserved under collisions, while all other variables are fast. It is worth emphasizing that the decompositions in (2) and (3) lead to extra terms involving time derivatives of the slow variables  $\rho$ ,  $\mathbf{u}$ ,  $\theta$ . In contrast to Grad’s method of moments,<sup>2,12</sup> or the method known as extended irreversible thermodynamics,<sup>13–15</sup> we do not introduce time derivatives for the pressure tensor, energy flux, or any other quantity. Additional time derivatives of the temperature also appear in a modified form of the super-Burnett equations proposed by Slemrod.<sup>16</sup>

Besides clarifying the rôle of solvability conditions as undoing any expansion of the slow variables inherited from expanding the distribution function, proceeding from a system of moment equations offers a definitive treatment of the Prandtl number issue that improves agreement with experiment, and greatly reduces the labor (as contrasted with Ref. 17) of deriving the macroscopic equations that result from different microscopic collision operators. We also draw connections between previously unrelated earlier work. For instance, the Chen–Rao–Spiegel pressure tensor appeared previously in work by Ikenberry and Truesdell,<sup>18</sup> using a procedure they called “Maxwellian iteration” to approximate an infinite hierarchy of moment equations. Maxwellian iteration has since been revisited,<sup>19–21</sup> but always using the equations for  $\tilde{\mathbf{P}}$  and  $\tilde{\mathbf{q}}$  that lead to the familiar Navier–Stokes–Fourier equations. Van Kampen’s general theory, and its iterative extension by Warn *et al.*,<sup>22</sup> justifies the various assumptions that Ikenberry and Truesdell themselves regarded as questionable – these assumptions are necessary to suppress secular terms that would otherwise disorder the approximation after long times. Unlike van Kampen’s own work on kinetic theory, we make an explicit decomposition into fast and slow variables by working with a system of moments instead of the distribution function.

The next few sections establish notation and derive the necessary hierarchy of moment equations. We then describe van Kampen’s elimination procedure and its relation to the Chapman–Enskog expansion, both the original formulation and the more recent reinterpretation as a multiple-scales expansion. Results appear in §VI onwards.

## II. THE BOLTZMANN EQUATION AND ITS CONSERVATION LAWS

The Boltzmann equation describing the evolution of a dilute monatomic gas is commonly written as

$$\partial_t f + \boldsymbol{\xi} \cdot \nabla f = C[f, f]. \quad (4)$$

The distribution function  $f(\mathbf{x}, \boldsymbol{\xi}, t)$  gives the number density of particles (atoms) moving with velocity  $\boldsymbol{\xi}$  at a particular point  $\mathbf{x}$  in space at time  $t$ . The right hand side  $C[f, f]$  denotes Boltzmann’s collision operator, a multiple integral over pairs of particle velocities that describes binary collisions between particles. The first few moments of  $f$  with respect to  $\boldsymbol{\xi}$  give the macroscopic mass, momentum, and energy densities respectively,

$$\rho = \int f d\boldsymbol{\xi}, \quad \rho \mathbf{u} = \int \boldsymbol{\xi} f d\boldsymbol{\xi}, \quad \mathcal{E} = \frac{1}{2} \int |\boldsymbol{\xi}|^2 f d\boldsymbol{\xi}. \quad (5)$$

The energy density is  $\mathcal{E} = \frac{1}{2}\rho|\mathbf{u}|^2 + \frac{3}{2}\rho\theta$  in terms of the fluid density  $\rho$ , velocity  $\mathbf{u}$ , and temperature  $\theta$ . These quantities are all functions of  $\mathbf{x}$  and  $t$  only, due to the integrations over  $\boldsymbol{\xi}$ . We absorb the particle mass into  $\rho$ , and absorb Boltzmann's constant by measuring temperature in so-called energy units, so that  $\theta$  has dimensions of velocity squared. The adiabatic sound speed is then  $(\gamma\theta)^{1/2}$ , with adiabatic exponent  $\gamma = 5/3$  for monatomic gases. The specific heats are  $C_v = 3/2$  at constant volume, and  $C_p = 5/2$  at constant pressure.

The corresponding five moments of Boltzmann's collision operator vanish,  $\int C[f, f]d\boldsymbol{\xi} = 0$  etc. This is the mathematical statement that mass, momentum, and energy are all conserved by elastic collisions between atoms. However, collisions relax the distribution function  $f$  towards a Maxwell–Boltzmann distribution,

$$f^{(0)} = \frac{\rho}{(2\pi\theta)^{3/2}} \exp\left(-\frac{|\boldsymbol{\xi} - \mathbf{u}|^2}{2\theta}\right), \quad (6)$$

with parameters  $\rho$ ,  $\mathbf{u}$ ,  $\theta$  in  $f^{(0)}$  determined by conservation of mass, momentum, and energy. These essential properties are shared by the much simpler single-relaxation-time, Bhatnagar–Gross–Krook (BGK),<sup>23</sup> or Welander<sup>24</sup> collision operator,

$$\partial_t f + \boldsymbol{\xi} \cdot \nabla f = -\frac{1}{\tau}(f - f^{(0)}). \quad (7)$$

It is understood that the quantities  $\rho$ ,  $\mathbf{u}$ , and  $\theta$  appearing in  $f^{(0)}$  are computed from  $f$  using (5). Equation (7) explicitly shows the distribution function relaxing towards equilibrium with timescale  $\tau$ , but the implicit dependence of  $f^{(0)}$  on  $f$  through  $\rho$ ,  $\mathbf{u}$ ,  $\theta$  ensures that these five quantities only evolve on a (much slower) hydrodynamic timescale. The standard Chapman–Enskog expansion leading from (4) to the Navier–Stokes–Fourier equations may be applied equally well to the BGK approximation (7). However, the BGK approximation gives an incorrect Prandtl number, the ratio of viscosity to thermal conductivity. We return to this point in the next section.

Taking moments of the Boltzmann equation (4), or the BGK equation (7), with respect to 1,  $\boldsymbol{\xi}$ , and  $\frac{1}{2}|\boldsymbol{\xi}|^2$  therefore gives conservation laws for the five macroscopic quantities defined above,

$$\partial_t \rho + \nabla \cdot (\rho \mathbf{u}) = 0, \quad \partial_t (\rho \mathbf{u}) + \nabla \cdot \boldsymbol{\Pi} = 0, \quad \partial_t \left( \frac{1}{2} \rho |\mathbf{u}|^2 + \frac{3}{2} \rho \theta \right) + \nabla \cdot \mathcal{F} = 0. \quad (8)$$

The vanishing right hand sides reflect the microscopic conservation of mass, momentum, and energy under collisions. The momentum flux tensor  $\boldsymbol{\Pi}$  and energy flux vector  $\mathcal{F}$  are given by higher moments of the distribution function with respect to  $\boldsymbol{\xi}$ ,

$$\boldsymbol{\Pi} = \int \boldsymbol{\xi} \boldsymbol{\xi} f d\boldsymbol{\xi}, \quad \mathcal{F} = \frac{1}{2} \int |\boldsymbol{\xi}|^2 \boldsymbol{\xi} f d\boldsymbol{\xi}. \quad (9)$$

However, in kinetic theory it is conventional to use moments with respect to the peculiar velocity  $\mathbf{c} = \boldsymbol{\xi} - \mathbf{u}$ , the deviation of the particle velocity  $\boldsymbol{\xi}$  from its local average  $\mathbf{u}$  defined by (5). Multiplication by  $\mathbf{c}$  does not commute with either  $\partial_t$  or  $\boldsymbol{\xi} \cdot \nabla$ , since  $\mathbf{u}$  is a function of  $\mathbf{x}$  and  $t$ , but the conservation laws (8) may still be rewritten as

$$\partial_t \rho + \nabla \cdot (\rho \mathbf{u}) = 0, \quad (10a)$$

$$\partial_t (\rho \mathbf{u}) + \nabla \cdot (\rho \mathbf{u} \mathbf{u} + \mathbf{P}) = 0, \quad (10b)$$

$$\partial_t \left( \frac{1}{2} \rho |\mathbf{u}|^2 + \frac{3}{2} \rho \theta \right) + \nabla \cdot \left( \frac{1}{2} \rho |\mathbf{u}|^2 \mathbf{u} + \frac{3}{2} \rho \theta \mathbf{u} + \mathbf{P} \cdot \mathbf{u} + \tilde{\mathbf{q}} \right) = 0, \quad (10c)$$

using a pressure tensor  $\mathbf{P}$  and heat flux vector  $\tilde{\mathbf{q}}$  defined by

$$\mathbf{P} = \int \mathbf{c} \mathbf{c} f d\boldsymbol{\xi}, \quad \tilde{\mathbf{q}} = \frac{1}{2} \int |\mathbf{c}|^2 \mathbf{c} f d\boldsymbol{\xi}. \quad (11)$$

For future reference we define additional quantities  $\tilde{\mathbf{P}}$  and  $\mathbf{q}$  by

$$\tilde{\mathbf{P}} = \mathbf{P} - \rho \theta \mathbf{I}, \quad \mathbf{q} = \frac{5}{2} \rho \theta \mathbf{u} + \tilde{\mathbf{q}}. \quad (12)$$

The tilde on  $\tilde{\mathbf{P}}$  and  $\tilde{\mathbf{q}}$  denotes quantities that vanish when evaluated for the Maxwell–Boltzmann distribution (6). We show below that the Chen–Rao–Spiegel equations follow from applying van Kampen's elimination procedure to  $\mathbf{P}$  and  $\mathbf{q}$ , just as the Navier–Stokes–Fourier equations follow from applying the same procedure to  $\tilde{\mathbf{P}}$  and  $\tilde{\mathbf{q}}$ . The slightly modified equations derived in §IX arise from eliminating  $\mathbf{P}$  and  $\tilde{\mathbf{q}}$ . Comparing the definitions of the pressure tensor and the energy density establishes the consistency relations

$$\text{Tr } \mathbf{P} = \int |\mathbf{c}|^2 f d\boldsymbol{\xi} = 3\rho\theta, \quad \text{Tr } \tilde{\mathbf{P}} = 0. \quad (13)$$

These relations are satisfied exactly by the Navier–Stokes–Fourier constitutive relations, but are only satisfied in a consistent asymptotic sense by the Chen–Rao–Spiegel constitutive relations,<sup>8,25</sup> as described in §VIII below.

For many purposes it is useful to simplify the above conservation equations, eliminating time derivatives that are given by lower moments, to obtain

$$\frac{D\rho}{Dt} + \rho \nabla \cdot \mathbf{u} = 0, \quad \rho \frac{D\mathbf{u}}{Dt} + \nabla \cdot \mathbf{P} = 0, \quad \frac{3}{2} \rho \frac{D\theta}{Dt} + \mathbf{P} : \nabla \mathbf{u} + \nabla \cdot \tilde{\mathbf{q}} = 0. \quad (14)$$

Here  $D/Dt = \partial_t + \mathbf{u} \cdot \nabla$  denotes a Lagrangian, or material, time derivative moving with the macroscopic fluid velocity. Combining the continuity and temperature equations gives an evolution equation for the entropy,

$$\rho \theta \frac{D\beta}{Dt} + \tilde{\mathbf{P}} : \nabla \mathbf{u} + \nabla \cdot \tilde{\mathbf{q}} = 0, \quad (15)$$

where  $\beta = \frac{3}{2} \log(\theta \rho^{-2/3})$  is the thermodynamic entropy in our energy units. This quantity is commonly called just “entropy” in kinetic theory, even though  $\beta$  need not be proportional to Boltzmann’s entropy  $H = \int f \log f d\xi$  when the distribution function  $f$  differs from a Maxwellian.<sup>12</sup>

However, none of these sets of equations are closed until the momentum and energy fluxes are known. For this we turn again to the Boltzmann equation.

### III. HIGHER MOMENTS OF THE BOLTZMANN EQUATION

Maxwell’s equation of transfer determines the evolution of moments of the distribution function  $f$  with respect to arbitrary functions of the peculiar velocity  $\mathbf{c}$ .<sup>12,18,26</sup> The pressure tensor  $\mathbf{P}$  thus evolves according to

$$\partial_t P_{ij} + \partial_k (u_k P_{ij} + Q_{ijk}) + P_{ik} \frac{\partial u_j}{\partial x_k} + P_{kj} \frac{\partial u_i}{\partial x_k} = -\frac{1}{\tau} (P_{ij} - P_{ij}^{(0)}), \quad (16)$$

where the  $1/\tau$  factor on the right hand side comes directly from using the BGK collision operator. An effective  $\tau$  may be calculated for many other collision operators, as described below. The superscript (0) on  $P_{ij}^{(0)}$  on the right hand side denotes the quantity  $P_{ij}$  evaluated for the Maxwell–Boltzmann distribution  $f^{(0)}$ . The left hand side of (16) involves the divergence of a higher moment, the heat flow tensor  $\mathbf{Q}$  with components

$$Q_{ijk} = \int c_i c_j c_k f d\xi. \quad (17)$$

This moment in turn evolves under Maxwell’s equation of transport according to

$$\begin{aligned} \frac{\partial}{\partial t} Q_{klh} + \frac{\partial}{\partial x_i} (u_i Q_{klh} + R_{iklh}) + Q_{ilh} \frac{\partial u_k}{\partial x_i} + Q_{kih} \frac{\partial u_l}{\partial x_i} + Q_{kli} \frac{\partial u_h}{\partial x_i} \\ - \frac{1}{\rho} \left( P_{lh} \frac{\partial P_{ik}}{\partial x_i} + P_{hk} \frac{\partial P_{il}}{\partial x_i} + P_{kl} \frac{\partial P_{ih}}{\partial x_i} \right) = -\frac{\sigma}{\tau} (Q_{klh} - Q_{klh}^{(0)}), \end{aligned} \quad (18)$$

which involves the divergence of the fourth moment of the distribution function,

$$R_{ijkl} = \int c_i c_j c_k c_l f d\xi. \quad (19)$$

The heat flux vector  $\tilde{\mathbf{q}}$  results from contracting  $\mathbf{Q}$  on two of its three indices,  $\tilde{q}_k = \frac{1}{2} Q_{iik}$  in the conventional notation. Contracting (18) on two indices gives an evolution equation for  $\tilde{\mathbf{q}}$ ,

$$\partial_t \tilde{\mathbf{q}} + \nabla \cdot (\mathbf{u} \tilde{\mathbf{q}}) + \mathbf{Q} : \nabla \mathbf{u} + \tilde{\mathbf{q}} \cdot \nabla \mathbf{u} - \frac{1}{2\rho} (\text{Tr } \mathbf{P}) \nabla \cdot \mathbf{P} - \frac{1}{\rho} (\nabla \cdot \mathbf{P}) \cdot \mathbf{P} + \frac{1}{2} \nabla \cdot \mathbf{R} = -\frac{\sigma}{\tau} (\tilde{\mathbf{q}} - \tilde{\mathbf{q}}^{(0)}), \quad (20)$$

where the second rank tensor  $\mathbf{R}$  is a contraction of  $R_{ijkl}$  on two indices, with components

$$R_{ij} = \int c_i c_j |\mathbf{c}|^2 f d\xi. \quad (21)$$

The coefficient  $\sigma$  on the right hand sides of (18) and (20) is the Prandtl number, the ratio of viscosity to thermal conductivity.

Particles with larger peculiar velocities make a larger contribution to transporting energy than they do to transporting momentum, because energy is proportional to the square of velocity and momentum is proportional to velocity. This is not captured by the BGK collision operator, which employs only a single relaxation time  $\tau$ . The BGK collision operator therefore gives the incorrect value  $\sigma = 1$ , in the standard kinetic theory definition of  $\sigma$  that absorbs a factor of  $C_p = 5/2$ . However, the evolution equations (16) and (20) given above may be derived equally well using the linearized Boltzmann collision operator for Maxwell molecules, those with a soft  $r^{-5}$  repulsive interaction, or the Fokker–Planck collision operator that describes many glancing collisions. These both give  $\sigma = 2/3$ , which is accurate to within 1% over the whole range of inter-molecular interactions, including the limiting case of hard spheres.<sup>27</sup> One may also use various “synthetic” collision operators that yield equations (16)

and (20) with any desired Prandtl number. These include the Gross–Jackson extended BGK models,<sup>28</sup> the Shakhov S-model,<sup>29</sup> and the ellipsoidal statistics equilibrium.<sup>30–32</sup>

The linearized Boltzmann and Fokker–Planck collision operators are singular linear operators, and isotropic second rank tensors lie in their kernels. In other words, these collision operators enforce the consistency relation  $\frac{1}{3}\text{Tr} \mathbf{P} = \rho\theta$ . One should therefore reformulate equation (16) for the *traceless* part  $\tilde{\mathbf{P}} = \mathbf{P} - \rho\theta\mathbf{I}$  of the pressure tensor if using these collision operators. The resulting evolution equation for  $\tilde{\mathbf{P}}$ , equation (34) in §VI, then exactly preserves the consistency relation since  $\partial_t \text{Tr} \tilde{\mathbf{P}} = 0$ . However, we show below that if one accepts (16) as written for the complete pressure tensor, at worst the expression for  $\mathbf{P}$  computed up to and including terms of  $O(\tau)$  violates the consistency relation by  $O(\tau^2)$ .<sup>8,25</sup> Further discussion may be found in §VIII.

All the constitutive relations in this paper may also be derived from Grad’s 13 moment equations,<sup>2,12</sup> in which (16) and (20) are closed by postulating relations between  $\mathbf{R}$ ,  $\mathbf{Q}$  and the lower moments. Further details are given in the appendix.

#### IV. THE MODERN CHAPMAN–ENSKOG EXPANSION

In the previous two sections we derived evolution equations for the conserved mass, momentum, and energy densities, and also for the fluxes of momentum and energy. The five conserved quantities only evolve through spatial gradients, on a hydrodynamic timescale  $T$ , say, while the evolution equations for the fluxes contain  $O(1/\tau)$  terms due to collisions between particles. The Chapman–Enskog expansion exploits the separation between these two timescales to derive closed evolution equations for just the five conserved quantities. Closure is achieved by expressing the momentum and energy fluxes in terms of  $\rho$ ,  $\mathbf{u}$ ,  $\theta$  and their spatial derivatives.

In modern work,<sup>5,6</sup> the Chapman–Enskog expansion is usually presented as a multiple-scales expansion of the distribution function and time derivative in powers of a small parameter  $\epsilon = \tau/T$ , the ratio of timescales,

$$f = f^{(0)} + \epsilon f^{(1)} + \dots, \quad \partial_t = \partial_{t_0} + \epsilon \partial_{t_1} + \dots. \quad (22)$$

The expansion of the time derivative suppresses secular terms proportional to  $\epsilon t$  that would otherwise disorder the expansion of  $f$  after long times when  $t = O(1/\epsilon)$ . One may think of  $t_0$  and  $t_1 = \epsilon t_0$  as typical advective and diffusive timescales respectively.

To determine a unique expansion, it is then necessary to impose solvability conditions,

$$\int f^{(n)} d\xi = 0, \quad \int \xi f^{(n)} d\xi = 0, \quad \int |\xi|^2 f^{(n)} d\xi = 0, \quad \text{for } n = 1, 2, \dots, \quad (23)$$

such that  $f^{(1)}$  and higher do not contribute to the macroscopic mass, momentum, and energy densities. However, all other moments, notably the momentum and energy fluxes, inherit expansions in  $\epsilon$ . For example, the pressure tensor may be written as

$$\mathbf{P} = \mathbf{P}^{(0)} + \epsilon \mathbf{P}^{(1)} + \dots, \quad (24)$$

where each term is a moment of the corresponding  $f^{(n)}$ ,

$$\mathbf{P}^{(n)} = \int \mathbf{c} \mathbf{c} f^{(n)} d\xi, \quad \text{for } n = 0, 1, \dots \quad (25)$$

Although the definition  $\epsilon = \tau/T$  gives  $\epsilon$  the physical interpretation of a Knudsen number based on timescales instead of lengthscales, it is common practice in kinetic theory to introduce  $\epsilon$  as a formal small parameter, later set equal to unity, by replacing  $\tau$  with  $\epsilon\tau$  in the collision operator. This leads to powers of  $\tau$  appearing explicitly in the expressions for the higher terms in the expansions of the moments.

The compressible Euler equations arise at leading order, when the pressure tensor and energy flux are evaluated for the Maxwell Boltzmann distribution  $f^{(0)}$ ,

$$\partial_{t_0} \mathbf{u} + \mathbf{u} \cdot \nabla \mathbf{u} + \frac{1}{\rho} \nabla(\rho\theta) = 0, \quad \frac{3}{2} \rho (\partial_{t_0} \theta + \mathbf{u} \cdot \nabla \theta) + \rho \theta \nabla \cdot \mathbf{u} = 0. \quad (26)$$

The Navier–Stokes–Fourier equations result from computing the  $O(\epsilon)$  correction  $f^{(1)}$  to the equilibrium, and then eliminating time derivatives in favor of space derivatives using  $\partial_t = \partial_{t_0}$  to sufficient accuracy. Equivalently, one finds the  $O(\epsilon)$  corrections  $\mathbf{P}^{(1)}$  and  $\tilde{\mathbf{q}}^{(1)}$  by substituting the expansions of the moments into (16) and (20) and collecting the  $O(1)$  terms,

$$\partial_{t_0} P_{ij}^{(0)} + \partial_k (u_k P_{ij}^{(0)} + Q_{ijk}^{(0)}) + P_{ik}^{(0)} \frac{\partial u_j}{\partial x_k} + P_{kj}^{(0)} \frac{\partial u_i}{\partial x_k} = -\frac{1}{\tau} P_{ij}^{(1)}, \quad (27a)$$

$$\begin{aligned} \partial_{t_0} \tilde{\mathbf{q}}^{(0)} + \nabla \cdot (\mathbf{u} \tilde{\mathbf{q}}^{(0)}) + \mathbf{Q}^{(0)} : \nabla \mathbf{u} + \tilde{\mathbf{q}}^{(0)} \cdot \nabla \mathbf{u} - \frac{1}{2\rho} (\text{Tr} \mathbf{P}^{(0)}) \nabla \cdot \mathbf{P}^{(0)} \\ - \frac{1}{\rho} (\nabla \cdot \mathbf{P})^{(0)} \cdot \mathbf{P}^{(0)} + \frac{1}{2} \nabla \cdot \mathbf{R}^{(0)} = -\frac{\sigma}{\tau} \tilde{\mathbf{q}}^{(1)}. \end{aligned} \quad (27b)$$

The multiple-scales expansion permits the replacement of  $\partial_t$  by  $\partial_{t_0}$  at this order. One then evaluates  $\partial_{t_0} P_{ij}^{(0)} = \partial_{t_0} (\rho\theta) \delta_{ij}$  using the Euler equations (26) and the continuity equation. Since  $\tilde{\mathbf{q}}^{(0)} = 0$  there is no need to compute  $\partial_{t_0} \tilde{\mathbf{q}}^{(0)}$ , but one reaches exactly the same constitutive relations by considering the whole energy flux  $\mathcal{F}$  and computing  $\partial_{t_0} \mathcal{F}^{(0)} = \partial_{t_0} (\frac{5}{2} \rho \theta \mathbf{u} + \frac{1}{2} \rho |\mathbf{u}|^2 \mathbf{u})$ .

Chen, Rao, and Spiegel<sup>7,8</sup> omitted the multiple-scales expansion in time, and applied solvability conditions to the expansion as a whole, not order by order as in (23). Leaving the time derivatives as an unexpanded  $\partial_t$  in their analogs of (27), they obtained expressions for the momentum and energy fluxes involving time derivatives of  $\mathbf{u}$  and  $\theta$ . These expressions revert to the usual Navier–Stokes–Fourier forms if one evaluates the time derivatives using the Euler equations, as above, instead of the exact conservation laws from §II.

## V. CHAPMAN–ENSKOG AS THE ELIMINATION OF FAST VARIABLES

Although the above presentation using multiple scales is now widespread, Chapman and Enskog themselves used a different approach. They sought a special class of solutions in which each term in the expansion of the distribution function  $f$  depends on  $\mathbf{x}$  and  $t$  only through the unexpanded slow variables  $\rho$ ,  $\mathbf{u}$ ,  $\theta$  and their spatial derivatives. Like the multiple-scales expansion of  $\partial_t$  in (22), this special class of solutions was chosen to suppress secular terms proportional to  $\epsilon t$  that would otherwise disorder the expansion after long times.

van Kampen<sup>10,11</sup> showed that the Chapman–Enskog expansion is an application of a general procedure for approximating systems of evolution equations of the form

$$\frac{\partial \mathbf{s}}{\partial t} + \mathbf{S}(\mathbf{s}, \mathbf{f}, \epsilon) = 0, \quad \frac{\partial \mathbf{f}}{\partial t} + \frac{1}{\epsilon} \mathbf{F}(\mathbf{s}, \mathbf{f}, \epsilon) = 0. \quad (28)$$

Here  $\mathbf{s}$  and  $\mathbf{f}$  are vectors of slow and fast variables ( $\mathbf{f}$  should not be confused with the distribution function  $f$ ), and  $\epsilon$  a small parameter. The slow variables are determined uniquely by the absence of a  $1/\epsilon$  factor in the first of equations (28). The slow variables therefore evolve on an  $O(1)$  timescale, while the fast variables naturally evolve on a faster  $O(\epsilon)$  timescale.

van Kampen<sup>10,11</sup> showed that one may find reduced approximate descriptions of the system (28), valid for long times of  $O(1/\epsilon)$ , by expanding *only the fast variables* in powers of  $\epsilon$ ,

$$\mathbf{f} = \mathbf{f}^{(0)} + \epsilon \mathbf{f}^{(1)} + \epsilon^2 \mathbf{f}^{(2)} + \dots, \quad (29)$$

and leaving the slow variables  $\mathbf{s}$  unexpanded. The  $\epsilon \rightarrow 0$  limit of the fast equations determines the first approximation  $\mathbf{f}^{(0)}(\mathbf{s})$  that satisfies  $\mathbf{F}(\mathbf{s}, \mathbf{f}^{(0)}(\mathbf{s}), 0) = 0$ . Higher terms come from finding successively more accurate series solutions of the fast equations. Substituting into the slow equations yields successive sets of closed evolution equations for just the slow variables. The first two of these are

$$\frac{\partial \mathbf{s}}{\partial t} + \mathbf{S}(\mathbf{s}, \mathbf{f}^{(0)}, 0) = 0, \quad \frac{\partial \mathbf{s}}{\partial t} + \mathbf{S}(\mathbf{s}, \mathbf{f}^{(0)} + \epsilon \mathbf{f}^{(1)}, \epsilon) \Big|_{O(\epsilon)} = 0, \quad (30)$$

where the last expression denotes the expansion of  $\mathbf{S}(\mathbf{s}, \mathbf{f}^{(0)} + \epsilon \mathbf{f}^{(1)}, \epsilon)$  truncated after the  $O(\epsilon)$  terms.

The multiple-scales approach expands the whole distribution function in (22), and subsequently imposes solvability conditions (23) that leave the slow variables unaffected by the higher terms in the expansion. Van Kampen’s approach leaves the slow variables unexpanded in the first place, and expands only the fast variables. Either approach serves to suppress secular terms that would otherwise disorder the expansion. The question of whether to apply solvability conditions order-by-order, or to the expansion as a whole,<sup>7-9</sup> does not arise using van Kampen’s approach,<sup>10,11</sup> because the slow variables are not expanded.

Following Warn *et al.*<sup>22</sup> for the general procedure, one may also solve the second of equations (28) by iterating *only* on the fast variables, beginning with the zeroth iterate  $\mathbf{f}^{[0]} = \mathbf{f}^{(0)}(\mathbf{s})$  as before. The fast equations considered below have a particular structure reminiscent of the BGK collision operator,

$$\frac{\partial \mathbf{f}}{\partial t} + \mathbf{F}(\mathbf{s}, \mathbf{f}) = -\frac{1}{\epsilon} \left( \mathbf{f} - \mathbf{f}^{(0)}(\mathbf{s}) \right), \quad (31)$$

which motivates defining successive iterates  $\mathbf{f}^{[1]}, \mathbf{f}^{[2]}, \dots$  according to

$$\frac{\partial \mathbf{f}^{[n]}}{\partial t} + \mathbf{F}(\mathbf{s}, \mathbf{f}^{[n]}) = -\frac{1}{\epsilon} \left( \mathbf{f}^{[n+1]} - \mathbf{f}^{(0)}(\mathbf{s}) \right). \quad (32)$$

Substituting any one of these iterates  $\mathbf{f}^{[n]}$  into the slow evolution equations again yields closed evolution equations for the slow variables. In particular, the first iterative improvement  $\mathbf{f}^{[1]}$  coincides with the first two terms of the expansion (29) above,

$$\mathbf{f}^{[1]} = \mathbf{f}^{(0)} + \epsilon \mathbf{f}^{(1)} = \mathbf{f}^{(0)}(\mathbf{s}) - \epsilon \left( \frac{\partial \mathbf{f}^{(0)}}{\partial \mathbf{s}} \cdot \frac{\partial \mathbf{s}}{\partial t} + \mathbf{F}(\mathbf{s}, \mathbf{f}^{(0)}(\mathbf{s})) \right), \quad (33)$$

which is sufficient for the Navier–Stokes–Fourier and Chen–Rao–Spiegel equations. When applied to the moment equations from kinetic theory, this iterative approach is very similar to what Ikenberry and Truesdell termed “Maxwellian iteration”.<sup>18</sup> The justification, however, is due to van Kampen’s general theory,<sup>10,11</sup> and the iterative extension by Warn *et al.*<sup>22</sup>

## VI. NAVIER–STOKES–FOURIER EQUATIONS FROM ELIMINATION OF FAST VARIABLES

The consistency relation  $\text{Tr } \mathbf{P} = 3\rho\theta$  for the trace of the pressure tensor implies that  $\mathbf{P}$  contains a mixture of fast and slow behavior. Alternatively, the evolution of  $\text{Tr } \mathbf{P}$  is already known from the three conservation laws (8), so all that remains is to find an evolution equation for the traceless part of  $\mathbf{P}$ . Subtracting a multiple of the temperature equation (14) from the pressure equation (16), following Ikenberry and Truesdell<sup>18</sup> and Grad<sup>12</sup> gives an evolution equation for the quantity  $\tilde{\mathbf{P}} = \mathbf{P} - \rho\theta\mathbf{I}$ ,

$$\begin{aligned} \partial_t \tilde{P}_{ij} + \partial_k \left( \tilde{P}_{ij} u_k + Q_{ijk} - \frac{2}{3} \tilde{q}_k \delta_{ij} \right) + \rho\theta \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3} \frac{\partial u_k}{\partial x_k} \delta_{ij} \right) \\ + \tilde{P}_{ik} \frac{\partial u_j}{\partial x_k} + \tilde{P}_{jk} \frac{\partial u_i}{\partial x_k} - \frac{2}{3} (\tilde{\mathbf{P}} : \nabla \mathbf{u}) \delta_{ij} = -\frac{1}{\tau} \tilde{P}_{ij}. \end{aligned} \quad (34)$$

The quantity  $-\tilde{\mathbf{P}}$  is the deviatoric stress in hydrodynamic terminology, and the trace of equation (34) shows that  $\text{Tr } \tilde{\mathbf{P}} = 0$  is preserved by the evolution of  $\tilde{\mathbf{P}}$ . Since  $\tilde{\mathbf{P}}$  vanishes at equilibrium,  $\tilde{\mathbf{P}}^{(0)} = 0$ , no time derivatives appear in the equation for the first correction  $\tilde{\mathbf{P}}^{(1)}$  obtained using van Kampen's procedure. This agrees with the well-known observation that the Navier–Stokes–Fourier constitutive relations contain only spatial derivatives of the slow variables.

Following the iterative version of van Kampen's procedure, we find the first correction to equilibrium by substituting  $\tilde{\mathbf{P}} = \tilde{\mathbf{P}}^{(0)} = 0$  and  $\mathbf{Q} = \mathbf{Q}^{(0)} = 0$  into the left hand side of (34). The majority of terms vanish, leaving

$$\tilde{P}_{ij}^{(1)} = -\tau\rho\theta \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3} \frac{\partial u_k}{\partial x_k} \delta_{ij} \right). \quad (35)$$

This is the Navier–Stokes viscous stress for a dilute monatomic gas with shear viscosity  $\mu = \tau\rho\theta$ , and zero bulk viscosity. Equation (35) is commonly written as  $\tilde{\mathbf{P}}^{(1)} = -\tau\rho\theta\dot{\mathbf{E}}$ , where  $\dot{\mathbf{E}}$  denotes the symmetric, traceless part of the velocity gradient tensor in the notation of Chapman and Cowling.<sup>1</sup>

Turning to the heat flux  $\tilde{\mathbf{q}}$ , we rewrite its evolution equation (20) in terms of  $\tilde{\mathbf{P}}$  as

$$\begin{aligned} \partial_t \tilde{\mathbf{q}} + \nabla \cdot (\mathbf{u}\tilde{\mathbf{q}}) + \mathbf{Q} : \nabla \mathbf{u} + \tilde{\mathbf{q}} \cdot \nabla \mathbf{u} - \frac{1}{2\rho} (3\rho\theta + \text{Tr } \tilde{\mathbf{P}}) (\nabla(\rho\theta) + \nabla \cdot \tilde{\mathbf{P}}) \\ - \frac{1}{\rho} (\nabla(\rho\theta) + \nabla \cdot \tilde{\mathbf{P}}) \cdot (\theta\rho\mathbf{I} + \tilde{\mathbf{P}}) + \frac{1}{2} \nabla \cdot \mathbf{R} = -\frac{\sigma}{\tau} \tilde{\mathbf{q}}. \end{aligned} \quad (36)$$

Substituting  $\mathbf{Q} = \mathbf{Q}^{(0)} = 0$ ,  $\tilde{\mathbf{q}} = \tilde{\mathbf{q}}^{(0)} = 0$ ,  $\tilde{\mathbf{P}} = \tilde{\mathbf{P}}^{(0)} = 0$ , and

$$\mathbf{R}_{ij}^{(0)} = \int c_i c_j |\mathbf{c}|^2 f^{(0)} d\xi = 5\rho\theta^2 \delta_{ij}, \quad (37)$$

into the left hand side of (36) we obtain Fourier's heat flux

$$\tilde{\mathbf{q}}^{(1)} = -\frac{\tau}{\sigma} \left[ \nabla \cdot \left( \frac{5}{2} \rho\theta^2 \mathbf{I} \right) - \frac{3}{2} \theta \nabla(\rho\theta) - \theta \nabla(\rho\theta) \right] = -\frac{5}{2} \frac{\tau}{\sigma} \rho\theta \nabla\theta. \quad (38)$$

Equation (37) shows that  $\mathbf{R}$  also mixes fast and slow behavior. Before continuing the elimination to higher order, one might therefore choose to separate out the slow component by writing  $\mathbf{R} = 5\rho\theta^2 \mathbf{I} + \tilde{\mathbf{R}}$ , following the earlier rewriting of the pressure tensor as  $\mathbf{P} = \rho\theta\mathbf{I} + \tilde{\mathbf{P}}$ .

## VII. CHEN–RAO–SPIEGEL EQUATIONS FROM ELIMINATION OF FAST VARIABLES

We might equally well apply the same elimination procedure directly to equation (16) for the complete pressure tensor  $\mathbf{P}$ , which does not vanish at equilibrium. Substituting  $\mathbf{P} = \mathbf{P}^{(0)} = \rho\theta\mathbf{I}$  and  $\mathbf{Q} = \mathbf{Q}^{(0)} = 0$  into the left hand side of (16) gives an equation for the first iterative correction,

$$\partial_t (\rho\theta\delta_{ij}) + \partial_k (\rho\theta\delta_{ij}u_k) + \rho\theta\delta_{ik} \frac{\partial u_j}{\partial x_k} + \rho\theta\delta_{jk} \frac{\partial u_i}{\partial x_k} = -\frac{1}{\tau} \left( P_{ij}^{[1]} - \rho\theta\delta_{ij} \right), \quad (39)$$

that rearranges into the expression for the pressure tensor given by Chen, Rao, and Spiegel,<sup>7,8</sup>

$$P_{ij}^{[1]} = \rho\theta\delta_{ij} - \tau\rho \left[ \frac{D\theta}{Dt} + \frac{2}{3} \theta \nabla \cdot \mathbf{u} \right] \delta_{ij} - \tau\rho\theta \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3} \frac{\partial u_k}{\partial x_k} \delta_{ij} \right). \quad (40)$$

This expression may be written more compactly as<sup>8</sup>

$$\mathbf{P}^{[1]} = \rho\theta \left( 1 - \frac{2}{3} \tau \frac{D\beta}{Dt} \right) \mathbf{I} - \tau\rho\theta\dot{\mathbf{E}}, \quad (41)$$

using the evolution equation (15) for the entropy  $\beta = \frac{3}{2} \log(\theta \rho^{-2/3})$ . The same expression (41) was given by Ikenberry and Truesdell.<sup>18</sup> They advocated retention of the full pressure tensor  $\mathbf{P}$ , instead of a decomposition into an isotropic part  $\rho\theta\mathbf{I}$  and a traceless part  $\mathbf{P}$ , to preserve the correct transformation properties of the material time derivative of  $\mathbf{P}$  under rotations. Transformation under rotations becomes a contentious issue when the standard Chapman–Enskog expansion is continued to Burnett order.<sup>20,33,34</sup>

The Chen–Rao–Spiegel heat flux vector differs from the usual Fourier form (38) by terms involving the time derivative of the velocity, but not by terms involving the time derivative of the temperature. The latter already appears in the total energy flux through the rate of working of the pressure. The Chen–Rao–Spiegel heat flux therefore follows from introducing the entropy flux

$$\mathbf{h} = \frac{\mathbf{q}}{\theta} = \frac{\tilde{\mathbf{q}}}{\theta} + \frac{5}{2}\rho\mathbf{u} \quad (42)$$

as a fast variable. Recall that  $\mathbf{q} = \tilde{\mathbf{q}} + (5/2)\rho\theta\mathbf{u}$  as defined in equation (12) includes the contribution to the energy flux from macroscopic advection of the internal energy  $(3/2)\rho\theta$ , and also the contribution from the work done by the equilibrium pressure,  $\mathbf{u} \cdot \mathbf{P}^{(0)} = \rho\theta\mathbf{u}$ . For the earlier derivation Fourier’s law it made no difference whether one considered  $\tilde{\mathbf{q}}$  or  $\tilde{\mathbf{q}}/\theta$ , since the vanishing of the equilibrium term,  $\tilde{\mathbf{q}}^{(0)} = 0$ , eliminates any contribution from the time derivative of  $1/\theta$ . The reader who finds the introduction of  $\mathbf{h}$  contrived may prefer the approach given in §IX below.

The variable  $\mathbf{h}$  defined in (42) evolves according to

$$\begin{aligned} \partial_t \mathbf{h} + \left( \mathbf{h} - \frac{5}{2}\rho\mathbf{u} \right) \cdot \nabla \mathbf{u} + \frac{5}{2} \nabla \cdot \mathbf{P} - \frac{2}{3\rho\theta} \left( \mathbf{h} - \frac{5}{2}\rho\mathbf{u} \right) \left[ \mathbf{P} : \nabla \mathbf{u} + \nabla \cdot \left( \theta \mathbf{h} - \frac{5}{2}\rho\theta\mathbf{u} \right) \right] \\ + \frac{1}{\theta} \left[ 2\mathbf{Q} : \nabla \mathbf{u} - \frac{1}{2\rho} (\text{Tr } \mathbf{P}) \nabla \cdot \mathbf{P} - \frac{1}{\rho} (\nabla \cdot \mathbf{P}) \cdot \mathbf{P} + \frac{1}{2} \nabla \cdot \mathbf{R} \right] = -\frac{\sigma}{\tau} \left( \mathbf{h} - \frac{5}{2}\rho\mathbf{u} \right). \end{aligned} \quad (43)$$

Substituting the equilibrium values  $\mathbf{h}^{(0)} = (5/2)\rho\mathbf{u}$ ,  $\mathbf{P}^{(0)} = \rho\theta\mathbf{I}$ ,  $\mathbf{Q}^{(0)} = 0$ ,  $\mathbf{R}^{(0)} = 5\rho\theta^2\mathbf{I}$  gives

$$\partial_t \left( \frac{5}{2}\rho\mathbf{u} \right) + \nabla \cdot \left( \frac{5}{2}\rho\mathbf{u}\mathbf{u} + \frac{5}{2}\rho\theta\mathbf{I} \right) + \frac{5}{2}\rho\nabla\theta = -\frac{\sigma}{\tau} \left( \mathbf{h}^{[1]} - \frac{5}{2}\rho\mathbf{u} \right), \quad (44)$$

which rearranges into

$$\tilde{\mathbf{q}}^{[1]} = -\frac{5}{2}\frac{\tau}{\sigma}\rho\theta \left[ \nabla\theta + \left( \frac{D\mathbf{u}}{Dt} + \frac{1}{\rho}\nabla(\rho\theta) \right) \right]. \quad (45)$$

This coincides with the expression resulting from the Prandtl number adjustment used by Spiegel and Thiffeault.<sup>25</sup> However, the earlier general expression given by Chen, Rao, and Spiegel,<sup>7,9</sup>

$$\tilde{\mathbf{q}}^{[1]} = -\frac{5}{2}\tau\rho\theta \left[ \frac{1}{\sigma}\nabla\theta + \frac{D\mathbf{u}}{Dt} + \frac{1}{\sigma}\frac{1}{\rho}\nabla(\rho\theta) \right], \quad (46)$$

agrees with those above when  $\sigma = 1$ , but differs from Fourier’s law at  $O(\tau)$  when  $\sigma \neq 1$ . The leading order momentum equation has been broken into two parts, and only one part contains a factor of  $1/\sigma$ . This mismatch leads to an excessive attenuation of ultrasound at low frequencies, as shown in Fig. 2 below.

## VIII. INTERPRETATION USING TRANSLATIONAL TEMPERATURE

The pressure tensor given by Ikenberry and Truesdell,<sup>18</sup> and by Chen, Rao, and Spiegel,<sup>7,8</sup> differs from the usual Navier–Stokes expression by an isotropic term proportional to the Lagrangian rate of entropy production  $D\beta/Dt$ ,

$$\mathbf{P}^{[1]} = \left[ \rho\theta\mathbf{I} - \tau\rho\theta\dot{\mathbf{E}} \right] - \frac{2}{3}\tau\rho\theta\frac{D\beta}{Dt}\mathbf{I}. \quad (47)$$

In particular, one third of the trace of the pressure tensor is no longer precisely equal to the thermodynamic pressure  $\rho\theta$ ,

$$\frac{1}{3}\text{Tr } \mathbf{P}^{[1]} = \rho\theta \left( 1 - \frac{2}{3}\tau\frac{D\beta}{Dt} \right) = \rho\theta + O(\tau^2), \quad (48)$$

but only up to and including terms of  $O(\tau)$ , which is consistent to the order of approximation of the theory. This feature is shared by other theories, such as the nonlocal theory of Woods.<sup>27</sup> The pressure tensor  $\mathbf{P}^{[2]}$  computed to  $O(\tau^2)$  by Spiegel and Thiffeault<sup>25</sup> satisfies  $\frac{1}{3}\text{Tr } \mathbf{P}^{[2]} = \rho\theta + O(\tau^3)$ , again a consistent approximation for the theory.

The consistency relation  $\frac{1}{3}\text{Tr } \mathbf{P} = \rho\theta$  should hold exactly for dilute monatomic gases. However, in the kinetic theory of polyatomic gases, the standard Chapman–Enskog expansion leads to a modified Navier–Stokes viscous stress that is no longer traceless,

$$\mathbf{P} = \rho\theta\mathbf{I} - \mu\dot{\mathbf{E}} - \mu'(\nabla \cdot \mathbf{u})\mathbf{I}. \quad (49)$$



The additional term  $-\mu'(\nabla\cdot\mathbf{u})\mathbf{I}$  is interpreted as a bulk viscous stress, with a coefficient of bulk viscosity  $\mu'$  analogous to the shear viscosity  $\mu$  previously given by  $\mu = \tau\rho\theta$ . The additional term arises because polyatomic gas molecules may absorb or release energy from their internal degrees of freedom. The expression  $\mathcal{E} = \frac{1}{2}\rho|\mathbf{u}|^2 + \frac{3}{2}\rho\theta$  therefore no longer coincides with the total energy density, and will not be conserved under collisions.

Alternatively, one may retain the previous expression for the viscous stress,<sup>35,36</sup>

$$\mathbf{P} = \rho\Theta\mathbf{I} - \mu\dot{\mathbf{E}}, \quad (50)$$

by defining a translational temperature  $\Theta$  such that  $\frac{1}{3}\text{Tr}\mathbf{P} = \rho\Theta$ . A bulk viscous effect then appears in the energy equation, as rewritten to express conservation of the total energy  $\mathcal{E}' = \frac{1}{2}\rho|\mathbf{u}|^2 + \frac{3}{2}\rho\Theta + \varepsilon$ . The energy density  $\varepsilon$  associated with the internal degrees of freedom takes the form  $\varepsilon = \varepsilon_0(\Theta) + \frac{3}{2}\mu'\nabla\cdot\mathbf{u}$  for small departures from an equilibrium between translational and internal degrees of freedom.<sup>35</sup> Bulk viscosity now enters through the relation between the conserved total energy and the isotropic part of the pressure,

$$\frac{1}{3}\text{Tr}\mathbf{P} = \rho\Theta = \frac{2}{3}\left(\mathcal{E}' - \frac{1}{2}\rho|\mathbf{u}|^2 - \frac{3}{2}\mu'\nabla\cdot\mathbf{u}\right). \quad (51)$$

The two approaches are entirely equivalent, but Kogan argues that effects caused by energy transferring to and from internal degrees of freedom belong more naturally in the energy equation than the momentum equation.<sup>35,36</sup>

By analogy with the second approach to polyatomic gases, the pressure tensor (47) may be interpreted as defining a translational temperature  $\Theta$  for which the pressure tensor takes its usual form  $\mathbf{P} = \rho\Theta\mathbf{I} - \mu\dot{\mathbf{E}}$ ,

$$\Theta = \theta\left(1 - \frac{2}{3}\tau\frac{D\beta}{Dt}\right). \quad (52)$$

This may be rewritten with the aid of the continuity equation as

$$\Theta = \theta\left(1 - \frac{2}{3}\tau\nabla\cdot\mathbf{u} - \tau\frac{D}{Dt}\log\theta\right). \quad (53)$$

The combination  $\rho\Theta = \rho\theta(1 - \frac{2}{3}\tau\nabla\cdot\mathbf{u})$  is the mechanical pressure, or trace of the pressure tensor, as modified by bulk viscosity. However, the Ikenberry–Truesdell and Chen–Rao–Spiegel mechanical pressure is modified by a further term involving the Lagrangian derivative of temperature. Unlike bulk viscosity, no additional dissipation is caused by an *adiabatic* convergence or divergence,  $\nabla\cdot\mathbf{u} \neq 0$  but  $D\beta/Dt = 0$ ,

In summary, the deviation of  $\frac{1}{3}\text{Tr}\mathbf{P}$  from the thermodynamic pressure  $\rho\theta$  may be interpreted as a model, or parametrization, for the transfer of excitations to and from higher moments of the distribution function that do not appear explicitly in the theory. The complete pressure tensor takes the standard Navier–Stokes form  $\mathbf{P} = \Theta\mathbf{I} - \mu\dot{\mathbf{E}}$  when written using the translational temperature, but  $\Theta$  deviates from the thermodynamic temperature  $\theta$  by an  $O(\tau^2)$  amount proportional to  $D\beta/Dt$ , the Lagrangian rate of entropy production, that is itself  $O(\tau)$ .

## IX. ALTERNATIVE APPROACH

In this section we derive a slightly modified expression for the heat flux that arises more naturally from a system of moment equations. As an added benefit, the resulting dispersion relation offers further gains in agreement with experiment. We write the conservation laws for momentum and energy as

$$\partial_t(\rho\mathbf{u}) + \nabla\cdot(\rho\mathbf{u}\mathbf{u} + \mathbf{P}) = 0, \quad \partial_t\mathcal{E} + \nabla\cdot(\mathcal{E}\mathbf{u} + \mathcal{F}') = 0, \quad (54)$$

where  $\mathcal{E} = \frac{1}{2}\rho|\mathbf{u}|^2 + \frac{3}{2}\rho\theta$  is the (total) energy density as before. In other words, we decompose the total energy flux  $\mathcal{F}$  into an advection of the energy density plus a correction,

$$\mathcal{F} = \mathcal{E}\mathbf{u} + \mathcal{F}' = \mathcal{E}\mathbf{u} + \mathbf{u}\cdot\mathbf{P} + \tilde{\mathbf{q}}, \quad (55)$$

just as we previously decomposed the momentum flux into an advection of momentum plus a correction by writing  $\mathbf{\Pi} = \rho\mathbf{u}\mathbf{u} + \mathbf{P}$ . Neither correction need be small.

We now formulate an evolution equation for  $\mathcal{F}'$  by using

$$\partial_t\mathcal{F}' = (\partial_t\mathbf{u})\cdot\mathbf{P} + \mathbf{u}\cdot\partial_t\mathbf{P} + \partial_t\tilde{\mathbf{q}}. \quad (56)$$

Combining the evolution equations for  $\mathbf{P}$  and  $\tilde{\mathbf{q}}$  derived using Maxwell's equation of transfer in §III gives

$$\begin{aligned} & \left[ \frac{D\mathbf{u}}{Dt} + \frac{1}{\rho}\nabla\cdot\mathbf{P} \right] \cdot \mathbf{P} + \mathbf{u} \cdot \left[ \partial_t\mathbf{P} + \nabla\cdot(\mathbf{u}\mathbf{P} + \mathbf{Q}) + \mathbf{P}\cdot\nabla\mathbf{u} + (\mathbf{P}\cdot\nabla\mathbf{u})^\top + \frac{1}{\tau}(\mathbf{P} - \mathbf{P}^{(0)}) \right] \\ & + \left[ \partial_t\tilde{\mathbf{q}} + \nabla\cdot(\mathbf{u}\tilde{\mathbf{q}}) + \mathbf{Q}:\nabla\mathbf{u} + \tilde{\mathbf{q}}\cdot\nabla\mathbf{u} - \frac{1}{2\rho}(\text{Tr}\mathbf{P})\nabla\cdot\mathbf{P} - \frac{1}{\rho}(\nabla\cdot\mathbf{P})\cdot\mathbf{P} + \frac{1}{2}\nabla\cdot\mathbf{R} + \frac{\sigma}{\tau}(\tilde{\mathbf{q}} - \tilde{\mathbf{q}}^{(0)}) \right] = 0. \end{aligned} \quad (57)$$

The second expression in square brackets  $[\partial_t \mathbf{P}^{(0)} + \dots]$  is equation (16) for  $\partial_t P_{ij}$  rewritten in vector notation.

Following the iterative approach to the elimination of fast variables, we replace  $\mathbf{P}$ ,  $\mathbf{Q}$ , and  $\tilde{\mathbf{q}}$  by their equilibrium values everywhere except in the collision terms that contain factors of  $1/\tau$ ,

$$\begin{aligned} & \left[ \frac{D\mathbf{u}}{Dt} + \frac{1}{\rho} \nabla \cdot \mathbf{P}^{(0)} \right] \cdot \mathbf{P}^{(0)} + \mathbf{u} \cdot \left[ \partial_t \mathbf{P}^{(0)} + \nabla \cdot (\mathbf{u} \mathbf{P}^{(0)} + \mathbf{Q}^{(0)}) + \mathbf{P}^{(0)} \cdot \nabla \mathbf{u} + (\mathbf{P}^{(0)} \cdot \nabla \mathbf{u})^\top + \frac{1}{\tau} (\mathbf{P}^{[1]} - \mathbf{P}^{(0)}) \right] \\ & + \left[ \partial_t \tilde{\mathbf{q}}^{(0)} + \nabla \cdot (\mathbf{u} \tilde{\mathbf{q}}^{(0)}) + \mathbf{Q}^{(0)} : \nabla \mathbf{u} + \tilde{\mathbf{q}}^{(0)} \cdot \nabla \mathbf{u} \right. \\ & \left. - \frac{1}{2\rho} (\text{Tr } \mathbf{P}^{(0)}) \nabla \cdot \mathbf{P}^{(0)} - \frac{1}{\rho} (\nabla \cdot \mathbf{P}^{(0)}) \cdot \mathbf{P}^{(0)} + \frac{1}{2} \nabla \cdot \mathbf{R}^{(0)} + \frac{\sigma}{\tau} (\tilde{\mathbf{q}}^{[1]} - \tilde{\mathbf{q}}^{(0)}) \right] = 0. \end{aligned} \quad (58)$$

The whole of the second expression in square brackets  $[\partial_t \mathbf{P}^{(0)} + \dots]$  exactly cancels, through the definition of  $\mathbf{P}^{[1]}$  as the solution to

$$\partial_t \mathbf{P}^{(0)} + \nabla \cdot (\mathbf{u} \mathbf{P}^{(0)} + \mathbf{Q}^{(0)}) + \mathbf{P}^{(0)} \cdot \nabla \mathbf{u} + (\mathbf{P}^{(0)} \cdot \nabla \mathbf{u})^\top + \frac{1}{\tau} (\mathbf{P}^{[1]} - \mathbf{P}^{(0)}) = 0. \quad (59)$$

The third expression in square brackets  $[\partial_t \tilde{\mathbf{q}}^{(0)} + \dots]$  simplifies as described in §VI. This just leaves a correction to Fourier's law from the leading order momentum equation in the first term of (58),

$$\tilde{\mathbf{q}}^{[1]} = -\frac{\tau}{\sigma} \left[ \frac{5}{2} \rho \theta \nabla \theta + \rho \theta \left( \frac{D\mathbf{u}}{Dt} + \frac{1}{\rho} \nabla \cdot (\rho \theta) \right) \right]. \quad (60)$$

Notice that this expression differs from those given earlier, even in the BGK approximation with  $\sigma = 1$ , because the factor of  $5/2$  only multiplies the temperature gradient.

Heuristically, the  $(5/2)\rho\theta\mathbf{u}$  term in the equilibrium energy flux (1) combines  $(3/2)\rho\theta\mathbf{u}$  from the advection of the internal energy with a further  $\rho\theta\mathbf{u}$  from the work done by the equilibrium pressure. The earlier treatments by Spiegel and coworkers assign a finite response time to the whole  $(5/2)\rho\theta\mathbf{u}$  term, not just the contribution to the energy flux from the pressure. This leads to an overestimate of the reduction in phase speed of ultrasound at high frequencies, as shown below.

## X. PROPAGATION OF ULTRASOUND

The customary first test of a reduced description of rarefied gases is a comparison between the dispersion relation for linear plane waves and experimental measurements of the propagation of ultrasound.<sup>4,9,25,37-39</sup> These measurements were obtained using a column of gas confined between transmitting and receiving transducers.<sup>40,41</sup> The transmitter was excited at a prescribed frequency  $\omega$ , while varying the distance between transmitter and receiver. Assuming a plane-wave disturbance of the form  $\exp[i(\omega t - kz)]$ , the real and imaginary parts of the complex wave number  $k$  may be inferred from the variation in the phase and amplitude of the signal at the receiver with distance. Further details may be found in a review by Greenspan.<sup>38</sup> The extent to which the experimental disturbances may be described by plane waves, as opposed to solutions of a boundary value problem, has been subject to debate,<sup>39</sup> as described below.

The experimental data are commonly plotted using the dimensionless variables  $r$  and  $\mathcal{K}$  defined by<sup>38,40</sup>

$$r = \frac{c_0^2 \rho}{\gamma \omega \mu} = \frac{1}{\omega \tau}, \quad \mathcal{K} = \frac{k c_0}{\omega} = \frac{c_0}{c}. \quad (61)$$

Greenspan's rarefaction parameter  $r$  corresponds to an effective Reynolds number divided by the adiabatic exponent  $\gamma$ , and  $\omega\tau$  is the natural dimensionless combination for relaxation models containing an explicit timescale  $\tau$ . The dimensionless wavenumber  $\mathcal{K}$  also equals the dimensionless inverse phase speed, scaled using the adiabatic sound speed  $c_0 = (\gamma p/\rho)^{1/2}$  of low frequencies ( $r \rightarrow \infty$ ). The adiabatic exponent is  $\gamma = 5/3$  for a monatomic gas, so  $c_0 = (5\theta/3)^{1/2}$  with temperature  $\theta$  in energy units. In experiments, one typically fixes  $\omega$  at the resonant frequency of the two transducers, and varies  $\tau$  and  $r$  by varying the gas density.<sup>38</sup> However, it is useful to think of  $r \rightarrow 0$  as the high frequency limit, and  $r \rightarrow \infty$  as the low frequency limit. Low frequencies correspond to continuum behavior, as described by the Navier–Stokes–Fourier equations, while rarefied effects become significant at high frequencies. It is conventional to plot the real and imaginary parts of  $\mathcal{K}$  against  $r$ , as in Figs. 1 and 2 respectively.

Turning to the dispersion relations, we seek solutions of the various hydrodynamic equations with perturbations proportional to  $\exp[i(\omega t - kz)]$ . This follows the convention in more recent work,<sup>25,39</sup> but other conventions for signs and factors of  $i$  are widely used.<sup>9,37,38,40</sup> Throughout this section we take the Prandtl number to be  $\sigma = 2/3$ , as for Maxwell molecules. The dispersion relation for the Navier–Stokes–Fourier equations is then<sup>37,38</sup>

$$-\mathcal{K}^4 \left( i \frac{9}{10} \frac{1}{r} + \frac{6}{5} \frac{1}{r^2} \right) + \mathcal{K}^2 \left( i \frac{23}{10} \frac{1}{r} - 1 \right) + 1 = 0. \quad (62)$$

This is a quadratic equation for  $\mathcal{K}^2$  in terms of  $r$ . The low frequency (continuum) limit  $r \rightarrow \infty$  is a singular limit, because  $\mathcal{K}^4$  is multiplied by small terms of  $O(r^{-1})$  and  $O(r^{-2})$ . One pair of solutions gives the dispersion relation for acoustic waves,

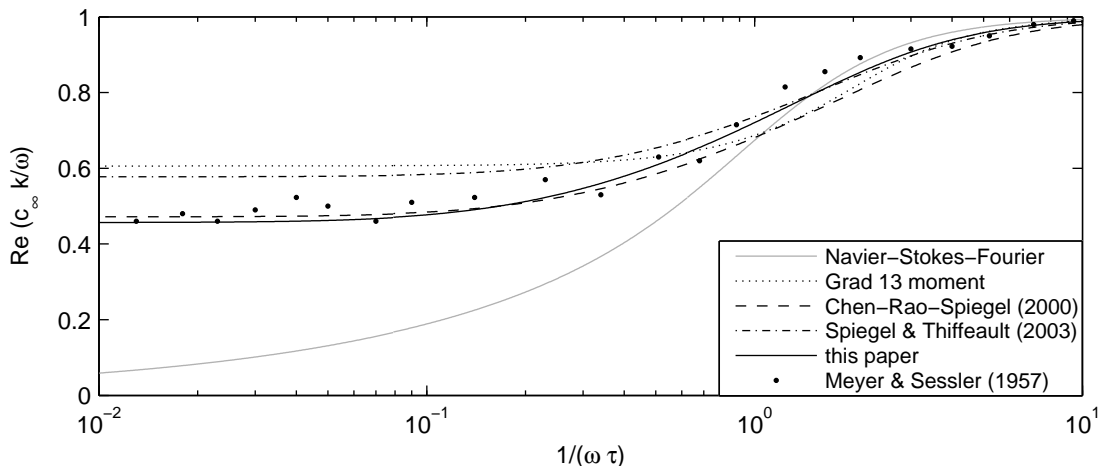


FIG. 1: Dimensionless inverse phase speed of ultrasound. The Chen–Rao–Spiegel theory,<sup>7–9</sup> the first order theory of Spiegel and Thiffeault,<sup>25</sup> and the theory from §IX of this paper, are compared with the experimental data of Meyer and Sessler,<sup>41</sup> the Grad 13 moment equations, and the Navier–Stokes–Fourier equations.<sup>37</sup>

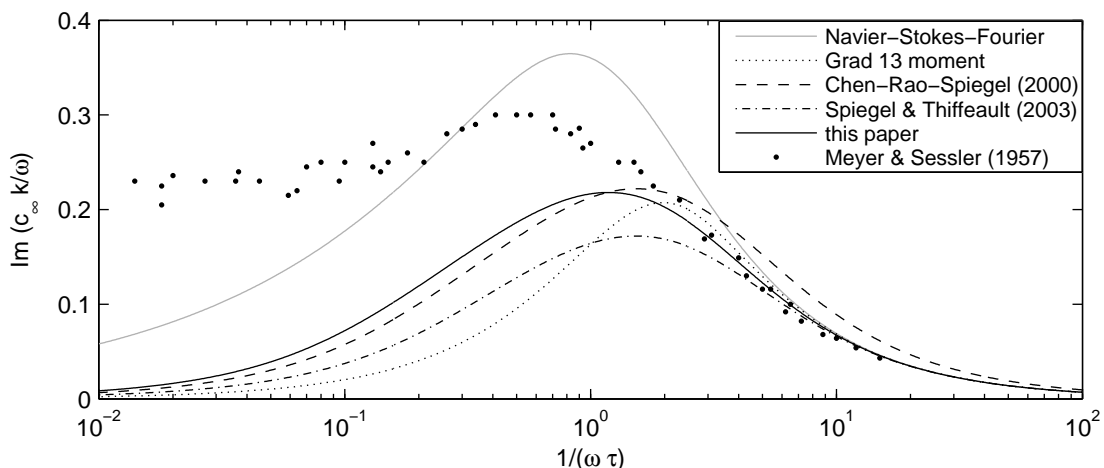


FIG. 2: Dimensionless attenuation rate of ultrasound with distance. The constitutive relations from §IX and Grad’s 13 moment equations are both in reasonable agreement with experiment for  $\omega\tau \lesssim 0.3$ , although all the theories shown predict a vanishing attenuation rate as  $\omega\tau \rightarrow \infty$ . The Chen–Rao–Spiegel theory systematically over-predicts the attenuation in the  $\omega\tau \rightarrow 0$  limit, while all the other theories converge to Navier–Stokes–Fourier behavior.

and is distinguished by  $\mathcal{K}^2 \rightarrow 1$  as  $r \rightarrow \infty$ . This is the branch of the dispersion relation that we compare with experimental measurements. The other pair of solutions correspond to thermal waves, and are distinguished by  $\mathcal{K} \sim \pm(\sqrt{5}/3)(1+i)r^{1/2}$  becoming large as  $r \rightarrow \infty$ . The phase speed, proportional to  $\mathcal{K}^{-1}$ , thus vanishes in the continuum limit. We therefore recover the purely diffusive behavior of thermal disturbances given by the Navier–Stokes–Fourier equations.

The acoustic branch of the Navier–Stokes–Fourier dispersion relation gives  $\mathcal{K} \rightarrow 0$  in the high frequency limit ( $r \rightarrow 0$ ). In other words, the phase speed tends to infinity at high frequencies, as shown in Fig. 1. The rate of attenuation with distance tends to zero, as shown in Fig. 2, having previously reached a maximum when  $r = O(1)$ . Neither the phase speed nor the attenuation rate given by the Navier–Stokes–Fourier equations is physically reasonable at high frequencies.

The dispersion relation for the Chen–Rao–Spiegel equations with  $\sigma = 2/3$  is<sup>9</sup>

$$-\mathcal{K}^4 \left( i \frac{9}{10} \frac{1}{r} + \frac{9}{2} \frac{1}{r^2} \right) + \mathcal{K}^2 \left( i \frac{14}{5} \frac{1}{r} + \frac{1}{r^2} - 1 \right) + 1 = 0, \quad (63)$$

while the dispersion relation for the first order equations of Spiegel and Thiffeault is<sup>25</sup>

$$-\mathcal{K}^4 \left( i \frac{9}{10} \frac{1}{r} + \frac{9}{2} \frac{1}{r^2} \right) + \mathcal{K}^2 \left( i \frac{23}{10} \frac{1}{r} + \frac{3}{2} \frac{1}{r^2} - 1 \right) + 1 = 0. \quad (64)$$

The additional  $O(\mathcal{K}^2/r^2)$  terms appearing in (63) and (64) limit the phase speed to finite values in the high frequency limit ( $r \rightarrow 0$ ). However, the different numerical coefficient, 14/5 rather than 23/10, of the  $i\mathcal{K}^2/r$  term in the dispersion relation for the Chen–Rao–Spiegel equations means that the attenuation rate of ultrasound exceeds that given by the Navier–Stokes–Fourier equations, even in the low frequency limit ( $r \rightarrow \infty$ ). This discrepancy is readily apparent from the comparison of

attenuation rates shown in Fig. 2. The alternative ‘‘Prandtl number fix’’ adopted by Spiegel and Thiffeault<sup>25</sup> leads to the same coefficient  $23/10$  as the Navier–Stokes–Fourier equations, but they did not remark on the misbehavior of the earlier equations in the continuum limit.

However, the high frequency limit  $\mathcal{K} \rightarrow \sqrt{2}/3 = 0.4714\dots$  as  $r \rightarrow 0$ , given by balancing the  $O(1/r^2)$  terms in the Chen–Rao–Spiegel equations,<sup>9</sup> is in remarkably good agreement with the limiting value  $\mathcal{K} \rightarrow 0.47$  derived from the collisionless Boltzmann equation by Kahn and Mintzer.<sup>37</sup> Both values are in good agreement with experiments, which give  $\mathcal{K} \rightarrow 0.45$  according to the interpretation of Kahn and Mintzer.<sup>37</sup> The corresponding limit  $\mathcal{K} \rightarrow 1/\sqrt{3} = .5773\dots$  for the first order Spiegel and Thiffeault theory is in noticeably poorer agreement with experiments. The limiting behavior of the second order theory comes closer, but lies below the range given by experiments.<sup>25</sup>

The dispersion relation arising from the alternative heat flux (60) is

$$-\mathcal{K}^4 \left( i \frac{9}{10} \frac{1}{r} + \frac{72}{25} \frac{1}{r^2} \right) + \mathcal{K}^2 \left( i \frac{23}{10} \frac{1}{r} + \frac{3}{5} \frac{1}{r^2} - 1 \right) + 1 = 0, \quad (65)$$

which agrees with the dispersion relations for the Navier–Stokes–Fourier and Spiegel–Thiffeault equations at  $O(r^0)$  and  $O(r^{-1})$ . However, the modifications to the  $O(r^{-2})$  terms lead to the high frequency limit

$$\mathcal{K} \rightarrow \sqrt{\frac{5}{24}} = 0.4564\dots \text{ as } r \rightarrow 0, \quad (66)$$

which is in much better agreement with Kahn and Mintzer’s interpretation of the experimental data for the phase velocity.<sup>37</sup>

All of the theories shown in Fig. 2 predict a vanishing of the attenuation rate at high frequencies ( $r \rightarrow 0$ ), while the experimental data show a trend towards a finite attenuation rate,  $\text{Im } \mathcal{K} \approx 0.2$  for  $r \ll 1$ . This is generally taken to be an aspect of the experiments that cannot be captured by theoretical studies of the dispersion relation for a single plane wave.<sup>37,39</sup> Particles leaving the transmitter might be expected to require several collisions before becoming organised into a single plane wave, and this cannot occur when the gas is sufficiently rarefied that the distance between transmitter and receiver is comparable to a mean free path. Mathematically, particles that do not undergo collisions contribute to the continuous spectrum of the linearised Boltzmann equation.<sup>42,43</sup> A continuous spectrum may exist in the linearised Boltzmann equation because it remains an integral equation in the particle velocity after assuming a plane wave behavior in  $\mathbf{x}$  and  $t$ . By contrast, finite systems of partial differential equations in just  $\mathbf{x}$  and  $t$ , like those derived in this paper, cannot possess continuous spectra. The amplitude of the modes in the continuous spectrum of the linearised Boltzmann equation is typically small compared with the amplitudes of the discrete modes, but the former decay more slowly with distance.

Buckner and Ferziger’s solution of a boundary value problem for the linearized Boltzmann equation using an eigenfunction expansion over a complete set of linear plane waves, including contributions from the continuous spectrum, gives excellent agreement with Schotter’s more recent experimental data over the whole range of  $r$ .<sup>44,45</sup> Schotter’s data show a smaller attenuation for  $r \approx 0.1$  that alleviates the disagreement between Buckner and Ferziger’s solution and earlier experiments.<sup>43</sup> In an alternative approach, Sirovich and Thurber<sup>46</sup> formulated a boundary value problem for the linearized Boltzmann equation in a half-space using Laplace transforms. Rather than solve this problem, though, they used analytic continuation of the dispersion relations obtained from the linearised, one-dimensional Boltzmann equation with Gross–Jackson collision operators using 3, 5, 8, or 11 moments. This approach captures the qualitative behavior over the whole range of  $r$  without explicitly formulating a boundary value problem, or considering the continuous spectrum. The phase speed and attenuation rate are both typically too large as  $r \rightarrow 0$ , but the precise details depend upon the number of moments retained in the Gross–Jackson collision operator, and whether their eigenvalues correspond to hard spheres or Maxwell molecules. An earlier review by Cercignani<sup>43</sup> favored the results of Sirovich and Thurber over those of Buckner and Ferziger, but Schotter’s more recent experimental data mentioned above favors the results of Buckner and Ferziger.<sup>45</sup> Kahn and Mintzer’s expansion about solutions of the collisionless Boltzmann equation appeared to work well even in the continuum limit,<sup>37</sup> but this was only due to an erroneous evaluation of certain integrals.<sup>47</sup> When corrected, the attenuation rate becomes negative in the near-continuum regime, where  $r$  is moderately large.<sup>47</sup>

In summary, the dispersion relation for the general purpose nonlinear theory presented in §IX gives the correct phase speed for ultrasound in both the continuum and highly rarefied limits, improving upon the earlier Chen–Rao–Spiegel and Spiegel–Thiffeault equations. The attenuation rate is in good agreement with experiment for  $r \gtrsim 3$ , but incorrectly vanishes in the highly rarefied limit  $r \rightarrow 0$ . The derivation of the general purpose theory is considerably simpler than that leading to the various linearised, one-dimensional theories mentioned above.<sup>37,44,46</sup>

## XI. CONCLUSION

The distribution function in Boltzmann’s equation evolves through a combination of two processes, spatial gradients and collisions between atoms, acting on two different timescales. Replacing Boltzmann’s equation by an equivalent hierarchy of moment equations leads to an explicit separation of timescales. The five moments that correspond to the macroscopic mass, momentum, and energy densities are unaffected by collisions, and evolve only slowly through spatial gradients. All higher moments, including the momentum and energy fluxes, tend to evolve on the faster timescale of collisions between atoms. Neither experimental measurements nor theoretical studies of the linearized Boltzmann collision operator show any evidence supporting a further separation of timescales between the higher moments.<sup>15</sup> Van Kampen’s theory for the elimination of fast variables,<sup>10,11</sup> and the center manifold theory of dynamical systems,<sup>48</sup> therefore motivate the formulation of approximate descriptions in the form of closed evolution equations for the five slowly evolving moments. These descriptions will remain valid over long timescales.

Exact conservation laws for the macroscopic mass, momentum, and energy densities follow from the corresponding moments of Boltzmann's equation, but these conservation laws are not closed because the momentum and energy fluxes involve the higher moments.

Closed evolution equations follow from expressing the instantaneous values of the higher moments in terms of the five slow moments and their derivatives. These expressions coincide with the constitutive relations that are postulated to complement the conservation laws in axiomatic approaches to continuum mechanics. The same distinction between (evolutionary) conservation laws and (instantaneous) constitutive relations was made in the original formulation of Chapman and Enskog, who postulated solutions in which the distribution function (and hence the higher moments) depend on space and time only through the five slow moments and their derivatives. All these approximate descriptions therefore lead to the so-called normal solutions of the Boltzmann equation, solutions in which the higher moments evolve on a slow hydrodynamic timescale, rather than on the fast collisional timescale characteristic of generic solutions.<sup>2</sup>

Maxwell's equation of transfer may be used to formulate evolution equations for the higher moments of the distribution function. The details specific to a number of different collision operators may be captured through an effective relaxation time  $\tau$  and Prandtl number  $\sigma$  in the evolution equations for the moments. The use of moment equations enables a systematic progression from kinetic theory to macroscopic equations without the subsequent alteration of coefficients or "Prandtl number fixes" found in Refs. 7,8,25. No solvability conditions are required, because the slow variables are left unexpanded.

The higher moments are known collectively as fast variables in van Kampen's theory. The five slow variables  $\rho$ ,  $\mathbf{u}$ ,  $\theta$  are uniquely identified by the collision operator, but any combination of fast and slow variables comprises another valid fast variable. Different fast variables lead to different, but asymptotically equivalent, evolution equations for the slow variables at each stage in van Kampen's procedure.<sup>10,11</sup> Although it is conventional to use moments with respect to the peculiar velocity in kinetic theory, the momentum flux  $\mathbf{\Pi}$  and energy flux  $\mathcal{F}$  may be written equally well as

$$\mathbf{\Pi} = \rho\mathbf{u}\mathbf{u} + \rho\theta\mathbf{I} + \tilde{\mathbf{P}}, \quad \mathcal{F} = \frac{1}{2}\rho|\mathbf{u}|^2\mathbf{u} + \tilde{\mathbf{P}} \cdot \mathbf{u} + \frac{5}{2}\rho\theta\mathbf{u} + \tilde{\mathbf{q}}, \quad (67)$$

or as

$$\mathbf{\Pi} = \rho\mathbf{u}\mathbf{u} + \mathbf{P}, \quad \mathcal{F} = \frac{1}{2}\rho|\mathbf{u}|^2\mathbf{u} + \tilde{\mathbf{P}} \cdot \mathbf{u} + \mathbf{q}, \quad (68)$$

or even as

$$\mathbf{\Pi} = \rho\mathbf{u}\mathbf{u} + \mathbf{P}, \quad \mathcal{F} = \left( \frac{1}{2}\rho|\mathbf{u}|^2 + \frac{3}{2}\rho\theta \right) \mathbf{u} + \mathbf{u} \cdot \mathbf{P} + \tilde{\mathbf{q}}. \quad (69)$$

Application of van Kampen's procedure,<sup>10,11</sup> or its iterative extension,<sup>22</sup> using any of these three pairs of expressions leads to constitutive relations for the momentum and energy fluxes in terms of the slow variables  $\rho$ ,  $\mathbf{u}$ ,  $\theta$  and their derivatives. The familiar Navier–Stokes–Fourier constitutive relations arise from eliminating the fast variables  $\tilde{\mathbf{P}}$  and  $\tilde{\mathbf{q}}$  appearing in (67).

However, we have shown that the Chen–Rao–Spiegel constitutive relations arise from applying exactly the same the procedure to eliminate  $\mathbf{P}$  and  $\mathbf{q}$  appearing in (68) instead. Since  $\mathbf{P}$  and  $\mathbf{q}$  do not vanish at equilibrium, the Chen–Rao–Spiegel constitutive relation are distinguished by the appearance of time derivatives of the leading order expressions  $\mathbf{P}^{(0)}$  and  $\mathbf{q}^{(0)}$ , or equivalently by time derivatives of the velocity and temperature. By contrast,  $\tilde{\mathbf{P}}^{(0)} = 0$  and  $\tilde{\mathbf{q}}^{(0)} = 0$ , so time derivatives only appear at second order when van Kampen's theory is applied to  $\tilde{\mathbf{P}}$  and  $\tilde{\mathbf{q}}$ .

The viscous stress that follows from writing  $\mathbf{\Pi} = \rho\mathbf{u}\mathbf{u} + \mathbf{P}$  may be interpreted as defining a translational temperature,<sup>35,36</sup>

$$\Theta = \theta \left( 1 - \frac{2}{3}\tau \frac{D\beta}{Dt} \right), \quad (70)$$

as in the kinetic theory of polyatomic gases. The pressure tensor then takes the standard Newtonian or Navier–Stokes form  $\mathbf{P} = \rho\Theta\mathbf{I} - \mu\dot{\mathbf{E}}$  with zero bulk viscosity, but the translational temperature deviates from the quantity  $\theta$  appearing in the energy equation by an amount proportional to the Lagrangian rate of entropy production  $D\beta/Dt$ . In physical terms, changes of internal energy caused by non-equilibrium (diabatic) processes are only reflected in the (mechanical) pressure after a delay comparable to the collision time. This interpretation motivates the rewriting of the energy flux in (69) to distinguish between the advection of internal energy and the work done by the pressure. Applying the usual elimination procedure leads to constitutive relations with slightly different coefficients in the heat flux,

$$\mathbf{P}^{[1]} = \rho\theta \left( 1 - \frac{2}{3}\tau \frac{D\beta}{Dt} \right) \mathbf{I} - \tau\rho\theta\dot{\mathbf{E}}, \quad \tilde{\mathbf{q}}^{[1]} = -\frac{\tau}{\sigma} \left[ \frac{5}{2}\rho\theta\nabla\theta + \rho\theta \left( \frac{D\mathbf{u}}{Dt} + \frac{1}{\rho}\nabla(\rho\theta) \right) \right], \quad (71)$$

and offers a modest further improvement in agreement with experiment, as shown in Figs. 1 and 2.

In conclusion, no solvability conditions are necessary in a derivation of closed macroscopic equations using moments, because the slow variables are explicitly identified and left unexpanded. The explicit freedom to choose fast variables in van Kampen's theory leads in principle to a continuum of possible constitutive relations, all equally valid within this theory, and all asymptotically equivalent to the Navier–Stokes–Fourier relations at first order in Knudsen number. Our introduction of a translational temperature, as in the kinetic theory of polyatomic gases, motivates a distinction in the energy flux between advection of internal energy and the work done by the pressure. Combining this distinction with a finite adjustment time for the pressure, comparable to the mean free time, yields a set of macroscopic equations that are similar in spirit to those of Chen, Rao, and Spiegel<sup>7–9</sup>

and Spiegel and Thiffeault.<sup>17,25</sup> However, the equations presented in this paper improve upon the earlier equations by giving the correct phase speeds for ultrasound in both the continuum and highly rarefied limits. The attenuation of ultrasound with distance is in good agreement with experiment in the continuum and moderately rarefied regimes. This improves slightly upon the equations of Spiegel and Thiffeault, and corrects a systematic error in the attenuation arising from the Chen–Rao–Spiegel equations in the continuum limit. All these sets of equations are much simpler than the specialised treatments of the linearised, one-dimensional Boltzmann equation summarised in §X.

### Acknowledgments

The author thanks Ed Spiegel, Rick Salmon, and Russ Caflisch for useful conversations. Jean-Luc Thiffeault kindly supplied the experimental data from Ref. 41 in tabulated form. Some of these interactions took place during travel supported by NSF grant OCE–0100868, and by the 2004 New Zealand Mathematics in Industry Study Group organized by Graeme Wake.

### APPENDIX A: RELATION TO GRAD’S MOMENT EQUATIONS

When eliminating fast variables as above, the contracted fourth moment  $R$  appearing in (20), and the heat flow tensor  $Q$ , were both approximated by their values at equilibrium. These approximations led to the various closed systems of equations described above. Grad proposed an alternative closure that expresses the complete fourth moment  $R_{ijkl}$  in terms of lower moments,<sup>2,12,26</sup>

$$R_{ijkl} = P_{ij}P_{kl} + P_{ik}P_{jl} + P_{il}P_{jk} - \tilde{P}_{ij}\tilde{P}_{kl} - \tilde{P}_{ik}\tilde{P}_{jl} - \tilde{P}_{il}\tilde{P}_{jk}. \quad (\text{A1})$$

There is no explicit requirement that any of the moments be close to their equilibrium values.

Inserting (A1) into (18) gives a closed system of equations for  $\rho$ ,  $\mathbf{u}$ ,  $\theta$ ,  $\tilde{P}$ , and  $Q$ , known as the 20 moment equations since there are 20 independent degrees of freedom. The more commonly used 13 moment equations result from a further approximation,

$$Q_{ijk} = \frac{2}{5} (q_i\delta_{jk} + q_j\delta_{ki} + q_k\delta_{ij}), \quad (\text{A2})$$

that restricts the heat flow tensor  $Q$  to just three degrees of freedom. Equations (A1) and (A2) were motivated by orthogonality relations among the tensor Hermite polynomials. They therefore hold exactly for the equilibrium Maxwell–Boltzmann distribution, for which  $P_{ij}^{(0)} = \rho\theta\delta_{ij}$ ,  $Q_{ijk}^{(0)} = 0$ , and  $R_{ij}^{(0)} = 5\rho\theta^2\delta_{ij}$  as used previously. All the constitutive relations derived in this paper may thus be derived from Grad’s 13 or 20 moment equations, as well as directly from the unclosed equations of transfer (16) and (18).

- 
- <sup>1</sup> S. Chapman and T. G. Cowling, *The Mathematical Theory of Non-Uniform Gases* (Cambridge University Press, Cambridge, 1970), 3rd ed.
  - <sup>2</sup> H. Grad, *Principles of the kinetic theory of gases*, in *Thermodynamik der Gase*, edited by S. Flügge (Springer-Verlag, Berlin, 1958), vol. 12 of *Handbuch der Physik*, pp. 205–294.
  - <sup>3</sup> G. E. Uhlenbeck and G. W. Ford, *Lectures in Statistical Mechanics*, vol. 1 of *Lectures in Applied Mathematics* (American Mathematical Society, Providence, 1963).
  - <sup>4</sup> H. Grad, *Asymptotic theory of the Boltzmann equation*, *Phys. Fluids* **6**, 147 (1963).
  - <sup>5</sup> J. E. McCune, T. F. Morse, and G. Sandri, *On the relaxation of gases towards continuum flow*, in *Proceedings of the Third International Symposium on Rarefied Gases*, edited by J. Laurmann (Academic Press, New York, 1963), vol. 1, pp. 115–135.
  - <sup>6</sup> C. Cercignani, *Mathematical Methods in Kinetic Theory* (MacMillan, London, 1969).
  - <sup>7</sup> X. Chen, H. Rao, and E. A. Spiegel, *Macroscopic equations for rarefied gas dynamics*, *Phys. Lett. A* **271**, 87 (2000).
  - <sup>8</sup> X. Chen, H. Rao, and E. A. Spiegel, *Continuum description of rarefied gas dynamics. I. Derivation from kinetic theory*, *Phys. Rev. E* **64**, 046308 (2001).
  - <sup>9</sup> X. Chen, H. Rao, and E. A. Spiegel, *Continuum description of rarefied gas dynamics. II. The propagation of ultrasound*, *Phys. Rev. E* **64**, 046309 (2001).
  - <sup>10</sup> N. G. van Kampen, *Elimination of fast variables*, *Phys. Rept.* **124**, 69 (1985).
  - <sup>11</sup> N. G. van Kampen, *Chapman–Enskog as an application of the method for eliminating fast variables*, *J. Statist. Phys.* **46**, 709 (1987).
  - <sup>12</sup> H. Grad, *On the kinetic theory of rarefied gases*, *Commun. Pure Appl. Math.* **2**, 331 (1949).
  - <sup>13</sup> D. Jou, J. Casas-Vázquez, and G. Lebon, *Extended irreversible thermodynamics*, *Rep. Prog. Phys.* **51**, 1105 (1988).
  - <sup>14</sup> D. Jou, J. Casas-Vázquez, and G. Lebon, *Extended irreversible thermodynamics revisited (1988–98)*, *Rep. Prog. Phys.* **62**, 1035 (1999).
  - <sup>15</sup> R. M. Velasco and L. S. García-Colín, *The kinetic foundation of extended irreversible thermodynamics revisited*, *J. Statist. Phys.* **69**, 217 (1992).
  - <sup>16</sup> M. Slemrod, *Constitutive relations for monatomic gases based on a generalized rational approximation to the sum of the Chapman–Enskog expansion*, *Arch. Ratl. Mech. Anal.* **150**, 1 (1999).
  - <sup>17</sup> E. A. Spiegel and J.-L. Thiffeault, *Continuum equations for stellar dynamics*, in *Stellar Astrophysical Fluid Dynamics*, edited by M. J. Thompson and J. Christensen-Dalsgaard (Cambridge University Press, Cambridge, 2003), pp. 377–391, eprint astro-ph/0210185.
  - <sup>18</sup> E. Ikenberry and C. Truesdell, *On the pressures and the flux of energy in a gas according to Maxwell’s kinetic theory, I*, *J. Ratl. Mech. Anal.* **5**, 1 (1956).

- <sup>19</sup> H. Struchtrup, *Some remarks on the equations of Burnett and Grad*, in *Transport in Transition Regimes*, edited by N. Ben Abdallah, A. Arnold, P. Degond, I. M. Gamba, R. T. Glassey, C. D. Levermore, and C. Ringhofer (Springer, New York, 2003), vol. 135 of *IMA Volume Series*, pp. 265–278.
- <sup>20</sup> I. Müller, *On the frame dependence of stress and heat flux*, *Arch. Ratl. Mech. Anal.* **45**, 241 (1972).
- <sup>21</sup> S. Reinecke and G. Kremer, *Burnett's equations from a (13+9N)-field theory*, *Continuum Mech. Thermodyn.* **8**, 121 (1996).
- <sup>22</sup> T. Warn, O. Bokhove, T. G. Shepherd, and G. K. Vallis, *Rossby number expansions, slaving principles, and balance dynamics*, *Quart. J. Roy. Meteor. Soc.* **121**, 723 (1995).
- <sup>23</sup> P. L. Bhatnagar, E. P. Gross, and M. Krook, *A model for collision processes in gases. I. Small amplitude processes in charged and neutral one-component system*, *Phys. Rev.* **94**, 511 (1954).
- <sup>24</sup> P. Welander, *On the temperature jump in a rarefied gas*, *Arkiv Fysik* **7**, 507 (1954).
- <sup>25</sup> E. A. Spiegel and J.-L. Thiffeault, *Higher-order continuum approximation for rarefied gases*, *Phys. Fluids* **15**, 3558 (2003).
- <sup>26</sup> T. I. Gombosi, *Gaskinetic Theory* (Cambridge University Press, Cambridge, 1994).
- <sup>27</sup> L. C. Woods, *Transport processes in dilute gases over the whole range of Knudsen numbers. Part 1. General theory*, *J. Fluid Mech.* **93**, 585 (1979).
- <sup>28</sup> E. P. Gross and E. A. Jackson, *Kinetic models and the linearized Boltzmann equation*, *Phys. Fluids* **2**, 432 (1959).
- <sup>29</sup> E. M. Shakhov, *Generalization of the Krook kinetic relaxation equation*, *Fluid Dynam.* **3**, 95 (1968).
- <sup>30</sup> A. M. Kogan, *Derivation of Grad's type equations and study of their relaxation properties by the method of maximization of entropy*, *J. Appl. Math. Mech.* **29**, 130 (1965).
- <sup>31</sup> L. H. Holway, *New statistical models for kinetic theory: Methods of construction*, *Phys. Fluids* **9**, 1658 (1966).
- <sup>32</sup> C. Cercignani and G. Tironi, *Nonlinear heat transfer between two parallel plates according to a model with correct Prandtl number*, in *Rarefied Gas Dynamics: Proceedings of the Fifth International Symposium*, edited by C. L. Brundin (Academic Press, New York, 1967), pp. 441–451.
- <sup>33</sup> L. C. Woods, *Frame-indifferent kinetic theory*, *J. Fluid Mech.* **136**, 423 (1983).
- <sup>34</sup> D. D. Joseph and L. Preziosi, *Addendum to the paper "Heat waves"*, *Rev. Mod. Phys.* **62**, 375 (1990).
- <sup>35</sup> M. N. Kogan, *Molecular gas dynamics*, *Annu. Rev. Fluid Mech.* **5**, 383 (1973).
- <sup>36</sup> M. N. Kogan, *Kinetic theory in aerothermodynamics*, *Progr. Aerospace Sci.* **29**, 271 (1992).
- <sup>37</sup> D. Kahn and D. Mintzer, *Kinetic theory of sound propagation in rarefied gases*, *Phys. Fluids* **8**, 1090 (1965).
- <sup>38</sup> M. Greenspan, *Transmission of sound waves in gases at very low pressures*, in *Physical Acoustics*, edited by W. P. Mason (Academic Press, New York, 1965), vol. IIA, pp. 1–45.
- <sup>39</sup> L. C. Woods and H. Troughton, *Transport processes in dilute gases over the whole range of Knudsen numbers. Part 2. Ultrasonic sound waves*, *J. Fluid Mech.* **100**, 321 (1980).
- <sup>40</sup> M. Greenspan, *Propagation of sound in five monatomic gases*, *J. Acoust. Soc. America* **28**, 644 (1956).
- <sup>41</sup> E. Meyer and G. Sessler, *Schallausbreitung in Gasen bei hohen Frequenzen und sehr niedrigen Drucken*, *Z. Physik* **149**, 15 (1957), in German.
- <sup>42</sup> H. Grad, *High frequency sound according to the Boltzmann equation*, *SIAM J. Appl. Math.* **14**, 935 (1966).
- <sup>43</sup> C. Cercignani, *Theory and application of the Boltzmann equation* (Scottish Academic Press, Edinburgh, 1975).
- <sup>44</sup> J. K. Buckner and J. H. Ferziger, *Linearized boundary value problem for a gas and sound propagation*, *Phys. Fluids* **9**, 2315 (1966).
- <sup>45</sup> R. Schotter, *Rarefied gas acoustics in the noble gases*, *Phys. Fluids* **17**, 1163 (1974).
- <sup>46</sup> L. Sirovich and J. K. Thurber, *Propagation of forced sound waves in rarefied gasdynamics*, *J. Acoust. Soc. America* **37**, 329 (1965).
- <sup>47</sup> F. B. Hanson and T. F. Morse, *Free-molecule expansion polynomials and sound propagation in rarefied gases*, *Phys. Fluids* **12**, 1564 (1969).
- <sup>48</sup> J. Carr, *Applications of Centre Manifold Theory* (Springer, Berlin, 1981).