Regularized 13 moment equations for hard sphere molecules: Linear bulk equations

Henning Struchtrup[1,a)] and Manuel Torrilhon[2,b)]

[1]*Department of Mechanical Engineering, University of Victoria, Victoria, British Columbia V8W 2Y2, Canada*
[2]*Department of Mathematics, RWTH Aachen, Germany*

The regularized 13 moment equations of rarefied gas dynamics are derived for a monatomic hard sphere gas in the linear regime. The equations are based on an extended Grad-type moment system, which is systematically reduced by means of the Order of Magnitude Method [H. Struchtrup, "Stable transport equations for rarefied gases at high orders in the Knudsen number," Phys. Fluids **16**(11), 3921–3934 (2004)]. Chapman-Enskog expansion of the final equations yields the linear Burnett and super-Burnett equations. While the Burnett coefficients agree with literature values, this seems to be the first time that super-Burnett coefficients are computed for a hard sphere gas. As a first test of the equations the dispersion and damping of sound waves is considered. © *2013 AIP Publishing LLC*. [http://dx.doi.org/10.1063/1.4802041]

I. INTRODUCTION

Whether gas flows can be described by the classical equations of hydrodynamics—the Navier-Stokes and Fourier laws—depends on the Knudsen number ε of the flow.[1–3] The Knudsen number is defined as the ratio between the mean free path of the gas molecules and the typical length scale under consideration. Classical hydrodynamics is applicable only for Knudsen numbers below 0.05 or so. For larger Knudsen numbers non-local transport due to relatively large mean free path requires more detailed equations that are able to picture the non-locality. A fully detailed description of the gas flow at all Knudsen numbers is offered by the Boltzmann equation, which solves for the microscopic distribution function of the gas.[1,2] For many technical applications, in particular those in the so-called transition regime where, roughly, $0.05 \leq \varepsilon \leq 2$, the solution of the Boltzmann equation is rather costly, and provides far more detail than necessary. For flows with large Knudsen numbers the Boltzmann equation is indispensable, but for flows in the transition regime models of extended hydrodynamics offer an alternative.[3,4]

The present paper deals with an extension of a model that we have developed over the last decade, the regularized 13 moment (R13) equations.[5–9] The R13 equations are closely related to Grad's classical moment method,[10,11] which provides extended sets of equations for rarefied gases. In Grad's original method the Knudsen number is not used for model reduction, and therefore it is difficult to know which sets of moments one should consider for a given process. Our derivation of the Grad equations and of the R13 equations in Refs. 7 and 8 by means of the *Order of Magnitude Method* closed this gap, as it provided a clear relation between Knudsen number and the appropriate moment set to consider. The analysis showed that Grad's 13 moment equations are appropriate to order $\mathcal{O}(\varepsilon^2)$, while the regularized 13 moment equations are of order $\mathcal{O}(\varepsilon^3)$. Other authors have extended the method to R26 moments,[12] which should be of order[3] $\mathcal{O}(\varepsilon^5)$.

Boundary conditions for moments were already discussed by Grad, but systematic solutions of boundary value problems for (regularized) moment equations were studied only recently.[9,13]

---

a)struchtr@uvic.ca. URL: http://www.engr.uvic.ca/~struchtr/
b)mt@mathcces.rwth-aachen.de

In several papers it was shown that for flows with moderate Knudsen numbers the R13 equations provide accurate predictions in agreement to solutions of the Boltzmann equation, see, e.g., Refs. 14–19.

Burnett-type equations are an alternative to moment models. These equations are obtained from the Boltzmann equation by Chapman-Enskog expansion[1,20,21] as the second order (Burnett) and third order (super-Burnett) correction to the equations of hydrodynamics. An alternative approach to their derivation is the Chapman-Enskog expansion of larger moment systems.[22,23] While the Burnett-type equations can describe rarefaction effects in gas flows, they suffer from instabilities that hinder their use as a predictive tool.[24,25] Some authors suggested stabilized variants.[26,27] Especially the method presented in Refs. 28 and 29 has been extensively studied, for example in Refs. 30–32. However, at present, there is no complete theory of wall boundary conditions available for any of the Burnett-type equations.

All equations of extended hydrodynamics, whether stemming from the moment method or the Chapman-Enskog expansion, are derived as approximations to the Boltzmann equation. With the order of magnitude method and the Chapman-Enskog method relying on the Knudsen number as smallness parameter, it is clear that the agreement between solutions of extended hydrodynamics and the Boltzmann equation will be better at smaller Knudsen numbers, and not as good for processes at larger Knudsen number. There is no clear cut-off for agreement, as differences grow continuously with the Knudsen number. Our experience so far suggests good quantitative agreement of the—third order—R13 equations for Knudsen numbers up to $\varepsilon \simeq 0.4$, where $\varepsilon^3 = 0.064 \ll 1$, while qualitative agreement extends to somewhat higher Knudsen numbers.

In the present paper, see also Ref. 33, we discuss another important factor of influence, which until now did not receive much attention, namely the influence of the molecular interaction potential on the transport equations. So far, the R13 equations were developed only for Maxwell molecules and the BGK model, for which the derivation of moment equations is particularly simple, since the moments of the Boltzmann collision term can be computed without a model for the distribution function.[1,3,34] For numerical solutions of the Boltzmann equation, one often considers hard sphere molecules, since for these the numerics of the collision term are easier to handle. Quite often, again for simpler access, the Boltzmann collision term is replaced by kinetic models such as the BGK model,[35] the ES-BGK model that corrects the Prandtl number deficiency of the original BGK model,[36] and the Shakov model which essentially is a linearized from of the ES-BGK model.[37]

On the hydrodynamic level, the main difference between the various models for the collision term in the Boltzmann equation is in the temperature dependence of the viscosity μ, with $\mu \sim T^{0.5}$ for hard spheres, $\mu \sim T$ for Maxwell molecules, and $\mu \sim T^\omega$ for other models (measured value for argon: $\omega = 0.81$). The Prandtl number—the dimensionless ratio of viscosity and heat conductivity—varies only slightly, with a value of $\mathrm{Pr} = \frac{2}{3}$ for Maxwell molecules, and $\mathrm{Pr} = 0.661$ for hard spheres. It is an easy task to incorporate a different temperature dependence of viscosity and a different Prandtl number into the Boltzmann equation, the kinetic models, or the moment equations. Thus, one can mimic the leading order behavior of a gas quite well. However, viscosity and heat conductivity are not the only transport parameters relevant for a rarefied gas flow. This is best known from the Burnett equations, for which the transport coefficients for a variety of molecular interaction potentials are known.[3,23] It must be expected that differences in Burnett coefficients due to different molecular interaction potentials are accompanied by visible differences in the prediction of transport quantities. However, we are not aware of systematic studies of this.

The aim of the present paper is to obtain insight into the influence of the molecular interaction potential on the R13 equations. The interaction potential affects the derivation of the equations, on which the present paper focuses, as well as the boundary conditions and the solutions of boundary value problems, which will be considered elsewhere. As will be seen in the course of this paper, the derivation of the R13 equations for non-Maxwellian interaction potentials is rather cumbersome, and thus we present only the derivation of the linearized equations. The derivation of the theory is general, that is not restricted to a particular molecular interaction potential. The coefficients in the final equations depend in a complicated manner on the interaction potential, and in the present paper we shall evaluate them for the case of hard sphere molecules in comparison to Maxwell molecules.

The linearized Burnett and super-Burnett equations are obtained by Chapman-Enskog expansion of the R13 equations. It will be seen that the Burnett coefficients for hard spheres coincide with the literature values.[1,23] Up to now, the super-Burnett coefficients, linear or non-linear, were only known for Maxwell molecules.[3,21] Thus, this appears to be the first time that super-Burnett coefficients are given for non-Maxwellian molecules.

To derive the R13 equations for non-Maxwellian interaction potential we shall use the order of magnitude method,[7,8,38] which consists of the following steps:

1. Set-up of a Grad-type moment system for arbitrary choice and number of moments which approximates the infinite moment hierarchy similar to Refs. 22 and 23.
2. Chapman-Enskog expansion to determine the leading order of moments. Linear combination of moments to construct new moments such that the number of moments at a given Chapman-Enskog order is minimal. Repeat for the next order of magnitude.
3. Use of the established Chapman-Enskog orders to rescale the equations for the new moments, use of the scaling for model reduction to a given order of accuracy.

To increase readability and structure of the proceedings, we have split the paper into a relatively large number of sections and subsections. Since the application of the order of magnitude method is cumbersome, we prelude its development with a summary of the resulting equations and their coefficients for Maxwell molecules, BGK model, and hard spheres in Sec II. Section III presents, as an interesting first application of the equations, the dispersion and damping of high frequency sound waves with moment and Burnett-type models, comparing predictions for Maxwell molecules and hard spheres. With these introductory sections, we hope that the reader can appreciate the results of the paper before going through the lengthy details of the derivation. These commence in Sec. IV, where the foundations of kinetic theory and its moment equations with Grad closure are presented. The main part of the model reduction to the R13 equations is performed in Sec. V, which gives a step by step account of the procedure. This section also includes a very brief discussion of the derivation of the Burnett and super-Burnett equations. The paper closes with some final comments.

II. PRELUDE: TRANSPORT EQUATIONS UP TO THIRD ORDER IN THE KNUDSEN NUMBER

The bulk of this paper is concerned with the details of the derivation of the linearized transport equations for rarefied gas flows up to third order in the Knudsen number. Due to the abundance of detail necessary for the derivation, we believe it will be useful to first summarize the main outcome of this paper, that is the linear transport equations that arise at the different orders of the Knudsen number together with their coefficients for Maxwell molecules and hard sphere molecules.

The linearized equations describe transport in a rarefied gas when deviations from a rest state of given temperature and temperature are small. In dimensionless form, the variables are the deviations of density ρ and temperature θ from the rest state, the velocity vector v_i, the anisotropic stress tensor σ_{ij} and the heat flux vector q_i. The dimensionless pressure is given by the linearized ideal gas law $p = 1 + \rho + \theta$, and the dimensionless specific internal energy of the monatomic gas is $u = \frac{3}{2}(1 + \theta)$. The Knudsen number is defined as $\varepsilon = \frac{\mu_0 \sqrt{\theta_0}}{p_0 L}$, where μ_0 is the rest state viscosity, L is the reference length, p_0 is the reference pressure, and θ_0 is the reference temperature in specific energy units.

The conservation laws for mass, momentum, and energy read

$$\frac{\partial \rho}{\partial t} + \frac{\partial v_k}{\partial x_k} = 0,$$

$$\frac{\partial v_i}{\partial t} + \frac{\partial \rho}{\partial x_i} + \frac{\partial \theta}{\partial x_i} + \frac{\partial \sigma_{ik}}{\partial x_k} = G_i, \tag{1}$$

$$\frac{3}{2}\frac{\partial \theta}{\partial t} + \frac{\partial v_k}{\partial x_k} + \frac{\partial q_k}{\partial x_k} = 0,$$

where G_i is the dimensionless body force (e.g., gravity). The conservation laws must be furnished with equations for stress and heat flux, which depend on the Knudsen number order, and the method

of derivation. In zeroth order approximation, when the Knudsen number is effectively zero, we have $\sigma_{ij} = q_i = 0$, then (1) reduce to the linearized Euler equations.

For non-zero Knudsen numbers, the necessary equations depend on the Knudsen number order. For up to third order in the Knudsen number, the order of magnitude method gives the equations

$$\frac{\partial q_i}{\partial t} + a^{(1,1)} \frac{\partial \sigma_{ik}}{\partial x_k} - \underline{a^{(1,2)} \frac{\partial}{\partial x_k} \left[\sigma_{ik} + 2\varepsilon \frac{\partial v_{\langle i}}{\partial x_{k\rangle}} \right]}$$

$$\underline{\underline{- a^{(1,3)} \varepsilon \frac{\partial}{\partial x_k} \frac{\partial q_{\langle i}}{\partial x_{k\rangle}} - a^{(1,4)} \varepsilon \frac{\partial^2 q_k}{\partial x_i \partial x_k}}} = -\frac{1}{\varepsilon} a^{(1,0)} \left[q_i + \varepsilon \frac{5}{2\,\mathrm{Pr}} \frac{\partial \theta}{\partial x_i} \right], \tag{2}$$

$$\frac{\partial \sigma_{ij}}{\partial t} + a^{(2,1)} \frac{\partial q_{\langle i}}{\partial x_{j\rangle}} - \underline{a^{(2,2)} \frac{\partial}{\partial x_{\langle i}} \left[q_{j\rangle} + \varepsilon \frac{\kappa_1}{2} \frac{\partial \theta}{\partial x_{j\rangle}} \right]}$$

$$\underline{\underline{- a^{(2,3)} \varepsilon \frac{\partial}{\partial x_k} \frac{\partial \sigma_{\langle ij}}{\partial x_{k\rangle}} - a^{(2,4)} \varepsilon \frac{\partial^2 \sigma_{ij}}{\partial x_k \partial x_k}}} = -\frac{1}{\varepsilon} a^{(2,0)} \left[\sigma_{ij} + 2\varepsilon \frac{\partial v_{\langle i}}{\partial x_{j\rangle}} \right]. \tag{3}$$

Here, we have used underlining to distinguish terms of different order in ε. For first order in the Knudsen number it suffices to consider only the non-underlined terms on the rhs of the equations (that is the lhs is set to zero), which are, in fact, the laws of Navier-Stokes and Fourier. For second order in ε one has to add the single-underlined terms on the lhs, with which the equations become the generalization of Grad's 13 moment equations. For third order in ε the double-underlined terms must be considered as well, then the equations are the full R13 equations for non-Maxwellian molecules.

The Knudsen number ε is the dimensionless viscosity. The values of the coefficients $a^{(\alpha, \beta)}$ and the Prandtl number Pr depend on the molecular interaction potential, where the order of magnitude method gives the values in Table I, which are for Maxwell molecules,[3,7] the BGK model,[35] and hard spheres, respectively. The values for Maxwell molecules and BGK model are exact, but those for hard spheres depend somewhat on the size of the underlying Grad system. We note differences between the coefficients for Maxwell molecules and hard spheres of up to 25%.

The Burnett and super-Burnett equations resulting from the Chapman-Enskog expansion of Eqs. (2) and (3) read

$$q_i = -\frac{5}{2\,\mathrm{Pr}} \varepsilon \frac{\partial \theta}{\partial x_i} + \varepsilon^2 \underline{\left(\frac{\theta_4^B}{2} \frac{\partial^2 v_i}{\partial x_k \partial x_k} + \frac{2}{3} \left(\frac{\theta_4^B}{4} - \theta_2^B \right) \frac{\partial^2 v_k}{\partial x_k \partial x_i} \right)}$$

$$\underline{\underline{- \varepsilon^3 \left(\theta_1^{sB} \frac{\partial^3 \rho}{\partial x_i \partial x_k \partial x_k} + \theta_2^{sB} \frac{\partial^3 \theta}{\partial x_k \partial x_k \partial x_i} \right)}}, \tag{4}$$

$$\sigma_{ij} = -2\varepsilon \frac{\partial v_{\langle i}}{\partial x_{j\rangle}} - \varepsilon^2 \underline{\left(\varpi_2^B \frac{\partial^2 \rho}{\partial x_{\langle i} \partial x_{j\rangle}} + \left(\varpi_2^B - \varpi_3^B \right) \frac{\partial^2 \theta}{\partial x_{\langle i} \partial x_{j\rangle}} \right)}$$

$$\underline{\underline{+ \varepsilon^3 \left(\varpi_1^{sB} \frac{\partial^2}{\partial x_{\langle i} \partial x_{j\rangle}} \frac{\partial v_k}{\partial x_k} - \varpi_2^{sB} \frac{\partial^2}{\partial x_k \partial x_k} \frac{\partial v_{\langle i}}{\partial x_{j\rangle}} \right)}}. \tag{5}$$

The notation for Burnett coefficients follows the literature convention.[1] Again, we have used underlining to distinguish terms of different orders: The non-underlined terms are the laws of Navier-Stokes

TABLE I. R13 coefficients for Maxwell molecules, BGK model, and hard spheres.

	Pr	$a^{(1,0)}$	$a^{(1,1)}$	$a^{(1,2)}$	$a^{(1,3)}$	$a^{(1,4)}$	$a^{(2,0)}$	$a^{(2,1)}$	$a^{(2,2)}$	$a^{(2,3)}$	$a^{(2,4)}$
MM	2/3	2/3	1.0	0.0	2.4	2.0	1.0	0.8	0.0	2.0	0.0
BGK	1.0	1.0	1.0	0.0	2.8	1.33333	1.0	0.8	0.0	3.0	0.0
HS	0.66085	0.65006	0.78694	0.18661	2.10417	1.47742	0.98632	0.63125	0.09256	2.15033	-0.10259

TABLE II. Burnett and super-Burnett coefficients for Maxwell molecules, BGK model, and hard spheres.

	θ_2^B	θ_4^B	ϖ_2^B	ϖ_3^B	θ_1^{sB}	θ_2^{sB}	ϖ_1^{sB}	ϖ_2^{sB}
MM	5.625	3.0	2.0	3.0	0.625	9.8125	1.66667	1.33333
BGK	2.5	2.0	2.0	2.0	-1.0	4.16667	-0.66667	2.0
HS	5.81945	2.42113	2.02774	2.42113	2.23673	5.81182	0.49378	1.16695

and Fourier, the single-underlined terms are the Burnett corrections, and the double-underlined terms are the super-Burnett terms. Also the Burnett coefficients depend on the interaction potential. The values for Maxwell molecules are exact, but those for hard spheres depend on the size of the underlying Grad system. For Maxwell molecules, the BGK model, and hard spheres we find the values given in Table II. There are noticeable differences in the coefficients between the two molecule types.

The discussion of dispersion and damping of waves in Sec. III will show that the differences in coefficients lead to differences in the predictions on the behavior of moderately rarefied gas flows.

The equation summarized here will be derived in the Secs. IV and V, which consider moments in general, the Grad closure, and the reduction of moment equations by the order of magnitude method, respectively.

III. LINEAR WAVE ANALYSIS

In this section we discuss the behavior of linear waves as predicted in the new regularized 13-moment equations for hard sphere molecules and compare to existing models. To study linear waves we make the harmonic wave ansatz,

$$u_A(x, t) = \hat{u}_A \exp\left[i\left(\omega t - kx\right)\right], \tag{6}$$

where ω is the frequency, k is the wave number, and $\hat{u}_A$ is the complex amplitude. Inserting the wave ansatz (6) into the linearized and one-dimensional form of the transport equations and performing all derivatives gives an algebraic equation $A_{AB}(\omega, k)\hat{u}_B = 0$, which only has non-trivial solutions $\hat{u}_B$ for the complex amplitudes if the determinant of the matrix A_{AB} vanishes. Due to the polynomial structure of the complex matrix, its determinant is a polynomial both in k and ω with different degrees for different models. Solution of the solvability condition $\det A = 0$ gives the dispersion relation relating k and ω.

A. Temporal stability

Temporal stability of the waves is investigated by assuming a perturbation with given real wave number k and solving the dispersion relation for complex modes $\omega^{(j)}(k) = \omega_r^{(j)} + i\omega_i^{(j)}$, $j = 1, 2,$ $\dots N$, where N is the number of evolution equations in the model considered. The growth rate of the amplitude of the perturbation is given by the imaginary part of $\omega^{(j)}$, such that linear stability is given if $\omega_i^{(j)} > 0$ for all modes j. It is well known that Burnett models suffer from instabilities at high wave numbers k, while the regularized 13-moment equations obtained from Maxwell molecules show stability.[5, 26] The same is true for the new R13 system for hard sphere particles. Figure 1 shows the damping coefficients for all modes. One of the sound modes occurs with double multiplicity. For all modes the damping is positive, hence the figure demonstrates linear stability of the system for all frequencies.

B. Sound experiments

Dispersion and damping can be measured.[39, 40] For high frequency waves one observes distinct deviations form the prediction of classical hydrodynamics, i.e., the Navier-Stokes-Fourier equations, due to gas rarefaction. For waves the Knudsen number must be formed as the ratio of mean free
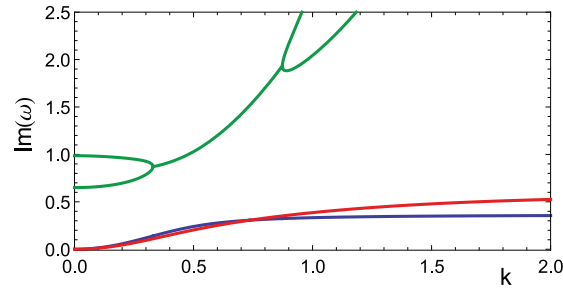
FIG. 1. Damping coefficients of the five modes $\omega^{(j)}(k)$, $j = 1, 2, 3, 4, 5$ of the new regularized 13-moment equations for hard-sphere potentials plotted over the perturbation wave number k.

path to wave length, and since wave length is inversely proportional to frequency, the Knudsen number for high frequency waves is not sufficiently small for the Navier-Stokes-Fourier theory to be valid. We shall not go into much detail of the computation, which was outlined, for the case of Maxwell molecules, in, e.g., Refs. 3, 5, and 19. We shall compare damping and dispersion for the following sets of equations: (a) Navier-Stokes-Fourier (NSF), (b) Grad 13 moment equations (G13), (c) regularized 13 moment equations (R13), (d) Burnett equations, and (e) super-Burnett equations.

For the solution for a periodically driven boundary we assume the frequency ω to be given and compute a complex wave number $k = k_r + ik_i$ from the dispersion relation. There exist ν branches for solutions of k of the dispersion relation

$$k^{(j)}(\omega), \quad j = 1, \ldots, \nu, \tag{7}$$

with $\nu = 4$ for NSF and G13, $\nu = 6$ for R13 and Burnett, and $\nu = 8$ for super-Burnett. The phase velocity of the wave is $v_{ph} = \frac{\omega}{k_r}$, and the damping is $(-k_i)$. For a wave with positive phase velocity (i.e., $k_r^{(j)} > 0$) one will expect a positive damping (i.e., $k_i^{(j)} < 0$). This is indeed the case for the R13 equations for hard sphere potentials.

While all modes can be induced in an experiment, in a sufficiently long apparatus only the mode with the weakest damping will be observed,[19] hence we show only these. Figure 2 shows the inverse dimensionless wave speed $\sqrt{\frac{5}{3}}\frac{1}{v_{ph}} = \sqrt{\frac{5}{3}}\frac{k_r}{\omega}$ and the reduced damping $\left(-\frac{k_i}{\omega}\right)$ as functions of the inverse frequency $\frac{1}{\omega}$ for Maxwell molecules (dashed lines) and hard sphere molecules (continuous lines), respectively. The dots are measurements by Meyer and Sessler.[39] For Burnett and super-Burnett equations there are discontinuities in phase speed, and (hardly visible) kinks in damping due to a switch in modes with lowest damping.

Burnett and super-Burnett equations have unphysical modes with negative damping, which appears in particular for high frequency waves, or waves with small wave lengths. This is well-known for Maxwell molecules,[3,19,24] and the same behavior is observed for the hard sphere gas. For the super-Burnett equations gaps in the curves for phase speeds occur where this happens.

For the discussion, we recall that NSF, Grad 13, Burnett, and super-Burnett can all be obtained by reduction of the R13 equations. For both molecule types we observe that NSF deviates from R13 already for relatively small frequencies, while Grad 13 agrees up to larger frequencies. Similarly, the super-Burnett equations agree with R13 for up to higher frequencies than the Burnett equations.

The comparison with experimental data is somewhat surprising. The Burnett equations for Maxwell molecules have a remarkably good agreement with the data for up to rather large frequencies. Considering that the Burnett equations can be obtained by Chapman-Enskog expansion of the R13 and Grad 13 equations, it is not expected that they give a much better agreement than these. Moreover, the super-Burnett equations, which are of third order in the Knudsen number ε, should give a better agreement than the Burnett equations which are only of second order. From this is must be concluded that the good agreement of the Burnett equations for Maxwell molecules is accidental rather than systematic.

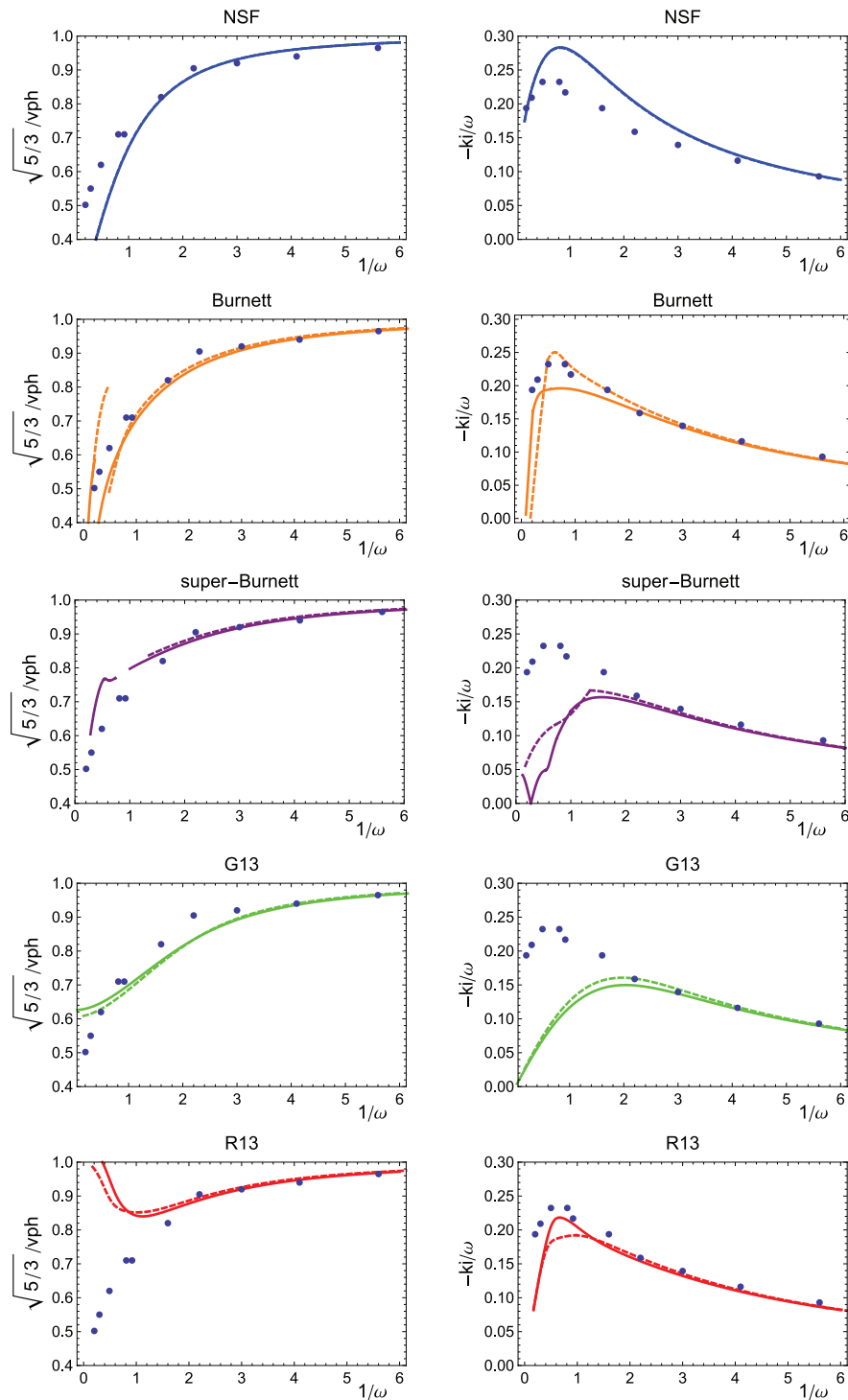FIG. 2. Inverse dimensionless phase velocity $\sqrt{5/3}/v_{ph}$ (left) and reduced damping $(-k_i)/\omega$ (right) as functions of inverse frequency $1/\omega$ for various theories of extended hydrodynamics: Navier-Stokes-Fourier, Burnett, super-Burnett, Grad13, and R13. Dashed lines are for Maxwell molecules, continuous lines are for hard sphere molecules, the dots represent measurements for argon.[39]

Comparison of the curves shows distinct differences between the predictions for Maxwell molecules and hard sphere gas, for which all higher order equations predict lower damping. The differences are of the order of 20% or so, simply a reflection of the difference in transport coefficients, which show similar variation. The experiments are performed with argon, which is neither a Maxwell gas, nor a hard sphere gas, but probably is best described by the Lennard-Jones potential. As of now, we have not computed the corresponding coefficients $a^{(\alpha,\beta)}$ which would be needed for a more detailed discussion of the theories' agreement to experiments.

IV. GRAD'S MOMENT SYSTEMS

Typically, in kinetic theory the gas is described on the microscopic level, through the distribution function $f(x_i, t, c_i)$ which gives the number density of particles at a location with certain microscopic velocities. Thus, the distribution function describes the detailed microscopic state of the gas. The space-time evolution of the distribution function is described by the Boltzmann equation,[1,2]

$$\frac{\partial f}{\partial t} + c_k \frac{\partial f}{\partial x_k} + G_k \frac{\partial f}{\partial c_k} = \int \int_0^{2\pi} \int_0^{\pi/2} \left(f' f^{1\prime} - f f^1 \right) g \, \sigma \sin \Theta \, d\Theta \, d\epsilon \, d\mathbf{c}^1. \tag{8}$$

Here, $f' = f(\mathbf{x}, t, \mathbf{c}')$ and so on, where $\mathbf{c}$ and $\mathbf{c}^1$ are the velocities of two colliding particles before the collision, and $\mathbf{c}'$ and $\mathbf{c}^{1\prime}$ are their velocities after the collision. G_k is the specific body force, e.g., gravity. The right-hand side of the Boltzmann equation is the collision term, it will be denoted with the symbol $\mathcal{S}$. The relative velocity is denoted as $g = |\mathbf{c} - \mathbf{c}^1|$, Θ is the collision angle, and the angle ϵ describes the orientation of the collision plane. The differential cross section σ depends on the particle interaction potential. In the following, we shall consider Maxwell molecules, where the product σg is a function of the collision angle only,[3] $\sigma_{MM} g = F_M(\Theta)$, and hard sphere molecules of diameter d, where $\sigma_{HS} = d^2 \cos \Theta$.

If the full distribution function is known, all its moments are known as well. Inversely, when all moments of the distribution are known, the distribution can be reconstructed. Thus, use of moments offers an alternative description of the gas. In principle, the Boltzmann equation can be replaced by an infinite array of moment equations. Clearly, this has little value, as the Boltzmann equation offers a straightforward and more accessible description of the gas. However, for a wider range of gas flows, in particular those at sufficiently small Knudsen numbers, gas processes are not dominated by individual behavior, but by collective behavior. Then, the local gas state can be described by a small number of moments, and their corresponding equations. The best known example is classical hydrodynamics, which considers only mass density, flow velocity and temperature as variables, and gives highly accurate results for low Knudsen number flows.

Our goal in the following is to start with a linearized, but nominally infinite moment system and use the smallness of the Knudsen number to reduce it to rather compact systems (hydrodynamics, the R13 equations, Burnett equations) which contain all elements of the infinite system that are required for a certain order of accuracy as measured by powers of the Knudsen number. The reduction of the equations with the order of magnitude method will require inversion of the matrices $\mathcal{C}_{ab}^{(n)}$ that appear on the right-hand sides of the equations. For an infinite moment number these matrices are infinite, and, in general, inversion is impossible. Therefore, instead of dealing with an infinite set of moments, we shall consider a finite set of sufficient size N, that will be chosen such that the $\mathcal{C}_{ab}^{(n)}$ are $N \times N$ matrices. With this finite matrices arise that can be inverted. However, the finite systems needs to be closed and we follow Grad's moment method, where the distribution function is constructed from the chosen set of moments, for the closure. Details of the derivation can be found in Ref. 3 or 41, in this section we only present the final moment system, which will be reduced by the order of magnitude method afterwards.

A. Moments

Moments of the distribution function are defined as weighted averages in microscopic velocity; their transport equations are obtained by averaging of the Boltzmann equation. While the distribution function gives a rather individual description of the gas (the number of particles with a certain

velocity), the moments describe the collective behavior of all particles (integration over all velocities). Well-known moments are the mass density ρ, the flow velocity v_i, the density of internal energy ρu, the pressure tensor $p_{ij} = p\delta_{ij} + \sigma_{ij}$, where p is the pressure and σ_{ij} is the anisotropic stress with $\sigma_{kk} = 0$, and the heat flux vector q_i. These moments are defined as

$$\rho = m\int f\,d\mathbf{c}, \quad \rho v_i = m\int c_i f\,d\mathbf{c}, \quad \rho u = \frac{3}{2}\rho\theta = \frac{m}{2}\int C^2 f\,d\mathbf{c},$$

$$p_{ij} = p\delta_{ij} + \sigma_{ij} = m\int C_i C_j f\,d\mathbf{c}, \quad q_i = \frac{m}{2}\int C^2 C_i f\,d\mathbf{c}, \tag{9}$$

where $C_i = c_i - v_i$ is the peculiar velocity and m is the mass of one particle. Above, we introduced the temperature in specific energy units, $\theta = \frac{k}{m}T$, where k is the Boltzmann constant and T is thermodynamic temperature. By taking the trace of the equation for p_{ij} and employing the definition of temperature, we find the equation of state of the ideal gas, $p = \rho\theta$. In what follows we require additional moments and it is convenient to introduce a general notation. We define the trace-free central moments as

$$u^a_{i_1\cdots i_n} = m\int C^{2a} C_{\langle i_1} C_{i_2}\cdots C_{i_n\rangle} f\,d\mathbf{c}. \tag{10}$$

In this notation, indices between angular brackets denote the trace-free and symmetric part of a tensor.[3]

   In this paper we shall only discuss flow conditions where the deviations from an equilibrium rest state at ρ_0, θ_0 are small. Also we switch to dimensionless quantities, which are defined by means of the equilibrium rest state and a characteristic length L of the process. Dimensionless space and time coordinates are introduced as $x = L\hat{x}, t = L\hat{t}/\sqrt{\theta_0}$. The variables for density, velocity and temperature are their dimensionless deviations from the equilibrium rest state,

$$\hat{\rho} = \frac{\rho - \rho_0}{\rho_0}, \quad \hat{v}_i = \frac{v_i}{\sqrt{\theta_0}}, \quad \hat{\theta} = \frac{\theta - \theta_0}{\theta_0}, \tag{11}$$

all other moments are made dimensionless as

$$\hat{u}^a_{i_1\cdots i_n} = \frac{u^a_{i_1\cdots i_n}}{\rho_0\sqrt{\theta_0}^{2a+n}}. \tag{12}$$

Note that the values of the higher scalar moments u^a have equilibrium values while all $u^a_{i_1\cdots i_n}$ with $n \geq 1$ vanish for a Maxwell distribution. In linearized formulation the equilibrium values of the scalar moments are given by

$$\hat{u}^a_{|E} = \left(1 + \hat{\rho} + a\hat{\theta}\right)(2a + 1)!! \tag{13}$$

and these are used to define the scalar non-equilibrium moments

$$\hat{w}^a = \hat{u}^a - \hat{u}^a_{|E} = \hat{u}^a - \left(1 + \hat{\rho} + a\hat{\theta}\right)(2a + 1)!!. \tag{14}$$

In dimensionless formulation the collision terms are scaled by the appropriate Knudsen number,

$$\varepsilon = \frac{\mu_0\sqrt{\theta_0}}{p_0 L}, \tag{15}$$

where μ_0 is the viscosity of the reference state. Typically, the Knudsen number is defined as the ratio between the mean free path of the gas and the characteristic length scale. The mean free path of a hard sphere gas is[1] $\frac{8}{5}\sqrt{\frac{2}{\pi}}\frac{\mu_0\sqrt{\theta_0}}{p_0}$, hence our definition of Knudsen number differs by the factor $\frac{8}{5}\sqrt{\frac{2}{\pi}} = 1.2766$ from that used in the literature on hard sphere gases.

   While the above dimensionless quantities are indicated by a hat on top of the symbol, we shall in the following discard the hats in order to streamline notation.

B. Moment equations

To derive a closed set of moment equations, we chose moments such that there are N non-equilibrium moments at each tensorial degree. Ideally, N would go to infinity, but we will consider finite N and use the Grad distribution for closure. From the transfer equations of Boltzmann's equation,[3] we have besides the conservation laws of mass, momentum and energy, the following equations for higher moments:

$$\frac{\partial w^a}{\partial t} + \frac{\partial u_k^a}{\partial x_k} - (2a+1)!!\frac{2a}{3}\frac{\partial q_k}{\partial x_k} = -\frac{1}{\varepsilon}\sum_{b=2}^{N+1}\mathcal{C}_{ab}^{(0)}w^b \quad (a = 2, \ldots, N+1),$$

$$\frac{\partial u_i^a}{\partial t} + \frac{\partial u_{ik}^a}{\partial x_k} + \frac{1}{3}\frac{\partial w^{a+1}}{\partial x_i} - \frac{(2a+3)!!}{3}\frac{\partial \sigma_{ik}}{\partial x_k} + (2a+3)!!\frac{a}{3}\frac{\partial \theta}{\partial x_i} = -\frac{1}{\varepsilon}\sum_{b=1}^{N}\mathcal{C}_{ab}^{(1)}u_i^b \quad (a = 1, \ldots, N),$$

$$\frac{\partial u_{ij}^a}{\partial t} + \frac{\partial u_{ijk}^a}{\partial x_k} + \frac{2}{5}\frac{\partial u_{\langle i}^{a+1}}{\partial x_{j\rangle}} + \frac{2(2a+5)!!}{15}\frac{\partial v_{\langle i}}{\partial x_{j\rangle}} = -\frac{1}{\varepsilon}\sum_{b=0}^{N-1}\mathcal{C}_{ab}^{(2)}u_{ij}^b \quad (a = 0, \ldots, N-1),$$

$$\frac{\partial u_{i_1\cdots i_n}^a}{\partial t} + \frac{\partial u_{i_1\cdots i_n k}^a}{\partial x_k} + \frac{n}{2n+1}\frac{\partial u_{\langle i_1\cdots i_{n-1}}^{a+1}}{\partial x_{i_n\rangle}} = -\frac{1}{\varepsilon}\sum_{b=0}^{N-1}\mathcal{C}_{ab}^{(n)}u_{i_1\cdots i_n}^b \quad (a = 0, \ldots, N-1).$$

(16)

Closure is required on the right-hand side, to identify the matrices $\mathcal{C}_{ab}^{(n)}$, and on the left-hand side, to identify the moments which are not among the variables, namely, u_k^{N+1}, u_{ik}^N, and $u_{i_1\cdots i_{n-1}}^N$.

In order to streamline the application of the order of magnitude method, it is useful to reassign the numbering of the moments such that all summations in the production terms go from 1 to N. In order to achieve this, we introduce moments $\tilde{w}^a$, $\tilde{u}_{i_1\cdots i_n}^a$ as

$$w^{a+1} = \tilde{w}^a,$$
$$u_k^a = \tilde{u}_k^a, \text{ with } \tilde{u}_i^1 = 2q_i,$$
$$u_{ij}^{a-1} = \tilde{u}_{ij}^a, \text{ with } \tilde{u}_{ij}^1 = \sigma_{ij},$$
$$u_{i_n\cdots i_n}^{a-1} = \tilde{u}_{i_1\cdots i_n}^a,$$

(17)

and we renumber the production matrices as well, as

$$\mathcal{C}_{a+1,b+1}^{(0)} = \tilde{\mathcal{C}}_{ab}^{(0)}, \quad \mathcal{C}_{ab}^{(1)} = \tilde{\mathcal{C}}_{ab}^{(1)}, \quad \mathcal{C}_{a-1,b-1}^{(2)} = \tilde{\mathcal{C}}_{ab}^{(2)}, \quad \mathcal{C}_{a-1,b-1}^{(n)} = \tilde{\mathcal{C}}_{ab}^{(n)}.$$

(18)

With this notation closure relations are required for $\tilde{u}_k^{N+1}$, $\tilde{u}_{ik}^{N+1}$, and $\tilde{u}_{i_1\cdots i_{n-1}}^{N+1}$ which can be obtained through the closure theory of Grad.[3, 10, 11] It turns out that we will not require moment equations with tensorial degree higher than three. The remaining closure relations can then be written

$$\tilde{u}_k^{N+1} = \sum_{b=1}^{N}\tilde{\mathcal{R}}_{ab}^{(1)}\tilde{u}_k^b, \quad \tilde{u}_{ik}^{N+1} = \sum_{b=1}^{N}\tilde{\mathcal{R}}_{ab}^{(2)}\tilde{u}_{ik}^b$$

(19)

with the coefficient matrices

$$\tilde{\mathcal{R}}_{ab}^{(1,2)} = \begin{bmatrix} 0 & 1 & & & & \\ & 0 & 1 & & & \\ & & 0 & 1 & & \\ & & & \ddots & \ddots & \\ & & & & 0 & 1 \\ \lambda_1^{(1,2)} & \lambda_2^{(1,2)} & \cdots & & & \lambda_N^{(1,2)} \end{bmatrix}_{ab} \quad (a, b = 1, \ldots, N),$$

(20)

where the values for $\lambda_b^{(1,2)}$ follow from the Grad distribution function as

$$\lambda_c^{(1)} = \sum_{b=0}^{N} \Lambda_{N+1,b}^{(1)} \left[\hat{\Lambda}^{(1)} \right]_{bc}^{-1}, \quad (c = 1, \ldots, N),$$

$$\lambda_c^{(2)} = \sum_{b=0}^{N-1} \Lambda_{Nb}^{(2)} \left[\hat{\Lambda}^{(2)} \right]_{bc}^{-1}, \quad (c = 0, \ldots, N-1)$$

with the matrices

$$\hat{\Lambda}_{ab}^{(1)} = \frac{1}{3} \left(2(a+b)+3 \right)!! \quad (a, b = 0, 1, \ldots, N),$$

$$\hat{\Lambda}_{ab}^{(2)} = \frac{2}{15} \left(2(a+b)+5 \right)!! \quad (a, b = 0, 1, \ldots, N-1).$$

With all of the above, we can now write the closed set of moment equations as the conservation laws

$$\frac{\partial \rho}{\partial t} + \frac{\partial v_k}{\partial x_k} = 0,$$

$$\frac{\partial v_i}{\partial t} + \frac{\partial \rho}{\partial x_i} + \frac{\partial \theta}{\partial x_i} + \frac{\partial \sigma_{ik}}{\partial x_k} = G_i, \tag{21}$$

$$\frac{3}{2} \frac{\partial \theta}{\partial t} + \frac{\partial v_k}{\partial x_k} + \frac{\partial q_k}{\partial x_k} = 0,$$

together with the equations for higher moments

$$\frac{\partial \tilde{w}^a}{\partial t} + \sum_{b=1}^{N} \tilde{\mathcal{R}}_{ab}^{(1)} \frac{\partial \tilde{u}_k^b}{\partial x_k} - (2a+3)!! \frac{2(a+1)}{3} \frac{\partial q_k}{\partial x_k} = -\frac{1}{\varepsilon} \sum_{b=1}^{N} \tilde{\mathcal{C}}_{ab}^{(0)} \tilde{w}^b,$$

$$\frac{\partial \tilde{u}_i^a}{\partial t} + \sum_{b=1}^{N} \tilde{\mathcal{R}}_{ab}^{(2)} \frac{\partial \tilde{u}_{ik}^b}{\partial x_k} + \frac{1}{3} \frac{\partial \tilde{w}^a}{\partial x_i} - \frac{(2a+3)!!}{3} \frac{\partial \sigma_{ik}}{\partial x_k} + (2a+3)!! \frac{a}{3} \frac{\partial \theta}{\partial x_i} = -\frac{1}{\varepsilon} \sum_{b=1}^{N} \tilde{\mathcal{C}}_{ab}^{(1)} \tilde{u}_i^b,$$

$$\frac{\partial \tilde{u}_{ij}^a}{\partial t} + \frac{\partial \tilde{u}_{ijk}^a}{\partial x_k} + \frac{2}{5} \frac{\partial \tilde{u}_{\langle i}^a}{\partial x_{j\rangle}} + \frac{2(2a+3)!!}{15} \frac{\partial v_{\langle i}}{\partial x_{j\rangle}} = -\frac{1}{\varepsilon} \sum_{b=1}^{N} \tilde{\mathcal{C}}_{ab}^{(2)} \tilde{u}_{ij}^b, \tag{22}$$

$$\frac{\partial \tilde{u}_{ijk}^a}{\partial t} + \frac{\partial \tilde{u}_{ijkl}^a}{\partial x_l} + \frac{3}{7} \sum_{b=1}^{N} \tilde{\mathcal{R}}_{ab}^{(2)} \frac{\partial \tilde{u}_{\langle ij}^b}{\partial x_{k\rangle}} = -\frac{1}{\varepsilon} \sum_{b=1}^{N} \tilde{\mathcal{C}}_{ab}^{(3)} \tilde{u}_{ijk}^b,$$

with $a = 1, \ldots, N$ in all equations. Grad's closure would imply also $\tilde{u}_{ijkl}^a = 0$, but at the level of Knudsen number accuracy we are interested in, we shall need to include this moment formally in the system. For the evolution of the higher moments, see Eq. (16)$_4$.

C. Production matrices

The production terms for Maxwell molecules can be computed without knowledge of the distribution function. Importantly, the resulting matrices are of lower triangular form,[34] so that inversion is possible step by step, and the infinite case can be considered. This special feature of Maxwell molecules made the derivation of the R13 equations for Maxwell molecules possible in a rather straightforward manner (as compared to what is necessary for other molecule types as discussed here), see Refs. 3, 5, and 7. For the BGK model the matrices are simply diagonal, and the derivation of the R13 equations is similarly simple.[3,7]

For hard sphere molecules, the production terms must be computed from the explicit Grad distribution function. The necessary computations are outlined in Ref. 42. Computation with a Mathematica script are rather cumbersome and computational expensive for large N. The final

coefficients of the equations as shown in Tables I and II will change when N is enlarged. However, our computations showed that the step from $N = 2$ to $N = 3$ changed the coefficients by less than 5%, so that fast convergence can be expected. Consequently, the application of the order of magnitude method as outlined in the following will use $N = 3$ for the equations of third order; for this case the relevant matrices read

$$
\mathcal{C}_{ab}^{(0)} = \nu \begin{bmatrix} \frac{1}{24} & \frac{1}{28} & -\frac{1}{3024} \\ -\frac{141}{16} & \frac{37}{56} & \frac{53}{2016} \\ \frac{2639}{16} & -\frac{317}{8} & \frac{727}{288} \end{bmatrix}, \quad \mathcal{C}_{ab}^{(1)} = \nu \begin{bmatrix} \frac{13}{48} & \frac{11}{336} & -\frac{1}{3024} \\ -\frac{197}{48} & \frac{205}{336} & \frac{89}{3024} \\ \frac{4923}{64} & -\frac{11539}{4488} & \frac{9113}{4032} \end{bmatrix},
$$

$$
\mathcal{C}_{ab}^{(2)} = \nu \begin{bmatrix} \frac{23}{32} & \frac{5}{112} & -\frac{1}{2016} \\ -\frac{89}{192} & \frac{541}{672} & \frac{149}{4032} \\ \frac{3689}{128} & -\frac{6005}{448} & \frac{1945}{896} \end{bmatrix}, \quad \mathcal{C}_{ab}^{(3)} = \nu \begin{bmatrix} \frac{423}{448} & \frac{47}{672} & -\frac{1}{1344} \\ -\frac{309}{896} & \frac{4705}{402} & \frac{3859}{88704} \\ \frac{105989}{1792} & -\frac{22111}{1152} & \frac{56293}{19712} \end{bmatrix}.
$$

$$(23)$$

In the above ν denotes the dimensionless collision frequency which must be chosen such that the proper viscosity appears in the Knudsen number ε.

V. MODEL REDUCTION WITH THE ORDER OF MAGNITUDE METHOD

The Grad moment system derived in Sec. IV is still an infinite system, since we have included moments $u_{\langle i_1 \cdots i_n \rangle}^a$ of all tensorial ranks n (with N moments at each rank, plus the hydrodynamic variables). Even if we decide to limit tensorial rank by a value n_{max} we still had to deal with a large number of variables and equations. The order of magnitude method[7,8] employs the Knudsen number ε as scaling parameter to construct reduced sets of equations that are relevant for a certain order of accuracy in terms of powers of the Knudsen number. Specifically, the method uses a sequence of leading order Chapman-Enskog expansions in the Knudsen number to construct the moments such that the number of moments at a given Chapman-Enskog order is minimal. We perform the method up to third order, which results in the regularized 13 moment equations.

The method was used to derive the R13 equations for Maxwell molecules in Ref. 7. In Ref. 8 it was outlined how the method can be used to generalize the Grad 13 moment equations to general molecule interaction; the discussion showed in particular that Grad's original 13 moment equations are suitable only for Maxwell molecules. Here now, we generalize the linear R13 equations to arbitrary molecule type, with coefficients computed for hard sphere molecules.

A. Conservation and order of magnitude

Density, velocity, and temperature are the variables in the conservation laws, and have equilibrium values. Thus, these moments and their equations—the conservation laws for mass, momentum and energy—remain unchanged throughout the application of the method, they are given in (21). The conservation laws contain the additional moments σ_{ij}, the stress, and q_i, the heat flux, thus, they are not a closed system for the hydrodynamic variables $\{\rho, v_i, \theta\}$. For closure additional equations for stress and heat flux must be provided, these will be developed from the moment equations (22) by reduction.

The reduction is based on determining the leading order of all non-equilibrium moments in the sense of the Chapman-Enskog expansion. For its determination we write the Chapman-Enskog expansion of the moments as

$$
\begin{aligned}
\tilde{w}^b &= \tilde{w}_0^b + \varepsilon \tilde{w}_1^b + \varepsilon^2 \tilde{w}_2^b + \cdots, \\
\tilde{u}_i^b &= \tilde{u}_{i,0}^b + \varepsilon \tilde{u}_{i,1}^b + \varepsilon^2 \tilde{u}_{i,2}^b + \cdots, \\
\tilde{u}_{ij}^b &= \tilde{u}_{ij,0}^b + \varepsilon \tilde{u}_{ij,1}^b + \varepsilon^2 \tilde{u}_{ij,2}^b + \cdots, \\
\tilde{u}_{i_1 \cdots i_n}^b &= \tilde{u}_{i_1 \cdots i_n,0}^b + \varepsilon \tilde{u}_{i_1 \cdots i_n,1}^b + \varepsilon^2 \tilde{u}_{i_1 \cdots i_n,2}^b + \cdots.
\end{aligned}
$$

$$(24)$$

By inserting the expansion into the moment equations we can determine the leading term for each moment, which gives the order of magnitude. As an example we consider the expansion of a quantity $\phi = \phi_0 + \varepsilon\phi_1 + \varepsilon^2\phi_2 + \varepsilon^3\phi_3 + \cdots$. If the evaluation of the equations yields that $\phi_\lambda \neq 0$ and $\phi_\alpha = 0$ for all $\alpha < \lambda$, then $\varepsilon^\lambda\phi_\lambda$ is the leading term in the expansion, and we say that ϕ is of order λ.

B. First order: Navier-Stokes-Fourier equations

1. Chapman-Enskog expansion

It is easy to conclude that density ρ, velocity v_i and temperature θ have zeroth order contributions while all other moments $\tilde{w}^b$, $\tilde{u}_i^b$, $\tilde{u}_{ij}^b$, $\tilde{u}_{i_1\cdots i_n}^b$ are at least of first order in ε. We now perform the Chapman-Enskog expansion, asking for the first order contributions. Since the zeroth order terms vanish, we insert the expansion

$$\tilde{w}^b = \varepsilon\tilde{w}_1^b + \varepsilon^2\tilde{w}_2^b + \cdots,$$

$$\tilde{u}_i^b = \varepsilon\tilde{u}_{i,1}^b + \varepsilon^2\tilde{u}_{i,2}^b + \cdots,$$

$$\tilde{u}_{ij}^b = \varepsilon\tilde{u}_{ij,1}^b + \varepsilon^2\tilde{u}_{ij,2}^b + \cdots, \tag{25}$$

$$\tilde{u}_{i_1\cdots i_n}^b = \varepsilon\tilde{u}_{i_1\cdots i_n,1}^b + \varepsilon^2\tilde{u}_{i_1\cdots i_n,2}^b + \cdots,$$

and evaluate the leading terms, which are those with ε^0. The result are explicit equations for the first order contributions,

$$0 = -\sum_{b=1}^N \tilde{\mathcal{C}}_{ab}^{(0)}\tilde{w}_1^b \quad (a = 1, \ldots, N),$$

$$(2a+3)!!\frac{a}{3}\frac{\partial\theta}{\partial x_i} = -\sum_{b=1}^N \tilde{\mathcal{C}}_{ab}^{(1)}\tilde{u}_{i,1}^b \quad (a = 1, \ldots, N),$$

$$(2a+3)!!\frac{2}{15}\frac{\partial v_{\langle i}}{\partial x_{j\rangle}} = -\sum_{b=1}^N \tilde{\mathcal{C}}_{ab}^{(2)}\tilde{u}_{ij,1}^b \quad (a = 1, \ldots, N), \tag{26}$$

$$0 = -\sum_{b=1}^N \tilde{\mathcal{C}}_{ab}^{(n)}\tilde{u}_{i_1\cdots i_n,1}^b \quad (a = 1, \ldots, N).$$

Thus, only the vector and 2-tensor moments have first order contributions, while the scalar moments and the higher tensors are at least of second order. The leading terms for vectors and 2-tensors are obtained from matrix inversion as

$$\tilde{u}_{i,1}^b = -\kappa_b\frac{\partial\theta}{\partial x_i}, \quad \tilde{u}_{ij,1}^b = -\mu_b\frac{\partial v_{\langle i}}{\partial x_{j\rangle}}, \tag{27}$$

with the coefficients

$$\kappa_a = \sum_{b=1}^N \left[\tilde{\mathcal{C}}^{(1)}\right]_{ab}^{-1}(2b+3)!!\frac{b}{3}, \quad \mu_a = \sum_{a=1}^N \left[\tilde{\mathcal{C}}^{(2)}\right]_{ab}^{-1}(2b+3)!!\frac{2}{15}, \tag{28}$$

with $a = 1, \ldots, N$.

If we are interested in heat flux $q_i = \frac{1}{2}\tilde{u}_i^1$ and stress $\sigma_{ij} = \tilde{u}_{ij}^1$ to first order only, we need just the above to find the laws of Fourier and Navier-Stokes,

$$q_i^{NSF} = -\hat{\kappa}\frac{\partial\theta}{\partial x_i}, \quad \sigma_{ij}^{NSF} = -2\hat{\mu}\frac{\partial v_{\langle i}}{\partial x_{j\rangle}} \tag{29}$$

with the dimensionless heat conductivity $\hat{\kappa} = \varepsilon\frac{\kappa_1}{2}$ and the dimensionless viscosity $\hat{\mu} = \varepsilon\frac{\mu_1}{2}$. Equation (28) shows that κ_1 and μ_1 depend on the complete production matrices $\mathcal{C}_{ab}^{(n)}$ for vectors and tensors. Since in (15) we have defined the Knudsen number ε as the dimensionless viscosity, the

value of μ_1 must be adjusted to $\mu_1 = 2$ by proper choice of the dimensionless collision frequency ν in the production matrices $C_{ab}^{(n)}$. The dimensionless ratio of heat conductivity and viscosity is the Prandtl number,

$$\mathrm{Pr} = \frac{5}{2}\frac{\mu}{\kappa} = \frac{5}{2}\frac{\varepsilon\frac{\mu_1}{2}}{\varepsilon\frac{\kappa_1}{2}} = \frac{5}{2}\frac{\mu_1}{\kappa_1} = \frac{5}{\kappa_1}. \tag{30}$$

2. Reconstructing variables (1st and 2nd order)

To first order, all vectorial moments, including heat flux, are proportional to the temperature gradient, and all 2-tensorial moments, including stress, are proportional to the trace-free symmetric part of the velocity gradient. Therefore, to first order the vectorial moments are linearly dependent to each other, and the 2-tensorial moments are linearly dependent to each other. Then, to first order, all vectorial moments can be expressed through the heat flux, and all 2-tensorial moments can be expressed through the stress,

$$\tilde{u}_{i,1}^a = -\kappa_a \frac{\partial \theta}{\partial x_i} = 2\frac{\kappa_a}{\kappa_1}q_{i,1}, \qquad \tilde{u}_{ij,1}^a = -\mu_a \frac{\partial v_{\langle i}}{\partial x_{j\rangle}} = \frac{\mu_a}{\mu_1}\sigma_{ij,1} \tag{31}$$

with $a = 2, \ldots, N$. These equations suggest to define second order variables as

$$\tilde{w}_i^a = \tilde{u}_i^a - 2\frac{\kappa_a}{\kappa_1}q_i, \qquad \tilde{w}_{ij}^a = \tilde{u}_{ij}^a - \frac{\mu_a}{\mu_1}\sigma_{ij} \tag{32}$$

with $a = 2, \ldots, N$. By combining (31) and (32) it is seen that the $\tilde{w}_i^a$, $\tilde{w}_{ij}^a$ have no first order contributions, thus they are at least of second order. With this variable change, heat flux q_i and stress σ_{ij} remain as the only first order variables.

We now rewrite the moment equations in terms of the new variables. The equations for q_i and σ_{ij} become

$$\frac{\partial q_i}{\partial t} + \left[\frac{\mu_2}{2\mu_1} - \frac{5}{2}\right]\frac{\partial \sigma_{ik}}{\partial x_k} + \frac{1}{2}\frac{\partial \tilde{w}_{ik}^2}{\partial x_k} + \frac{1}{6}\frac{\partial \tilde{w}^1}{\partial x_i} = -\frac{1}{\varepsilon}\frac{5}{\kappa_1}\left[q_i + \varepsilon\frac{\kappa_1}{2}\frac{\partial \theta}{\partial x_i}\right] - \frac{1}{\varepsilon}\frac{1}{2}\sum_{b=2}^{N}\tilde{C}_{1b}^{(1)}\tilde{w}_i^b, \tag{33}$$

$$\frac{\partial \sigma_{ij}}{\partial t} + \frac{4}{5}\frac{\partial q_{\langle i}}{\partial x_{j\rangle}} + \frac{\partial \tilde{u}_{ijk}^1}{\partial x_k} = -\frac{1}{\varepsilon}\frac{2}{\mu_1}\left[\sigma_{ij} + \varepsilon\mu_1\frac{\partial v_{\langle i}}{\partial x_{j\rangle}}\right] - \frac{1}{\varepsilon}\sum_{b=2}^{N}\tilde{C}_{1b}^{(2)}\tilde{w}_{ij}^b. \tag{34}$$

After eliminating the time derivatives of q_i and σ_{ij} with the above, the equations for the higher moments are

$$\frac{\partial \tilde{w}^a}{\partial t} + \left[2\sum_{b=1}^{N}\tilde{\mathcal{R}}_{ab}^{(1)}\frac{\kappa_b}{\kappa_1} - (2a+3)!!\frac{2(a+1)}{3}\right]\frac{\partial q_k}{\partial x_k} + \sum_{b=2}^{N}\tilde{\mathcal{R}}_{ab}^{(1)}\frac{\partial \tilde{w}_k^b}{\partial x_k} = -\frac{1}{\varepsilon}\sum_{b=1}^{N}\tilde{C}_{ab}^{(0)}\tilde{w}^b$$

$$(a = 1, \ldots, N), \tag{35}$$

$$\frac{\partial \tilde{w}_i^a}{\partial t} + \left[\sum_{b=1}^{N}\tilde{\mathcal{R}}_{ab}^{(2)}\frac{\mu_b}{\mu_1} - \frac{(2a+3)!!}{3} - 2\frac{\kappa_a}{\kappa_1}\left[\frac{\mu_2}{2\mu_1} - \frac{5}{2}\right]\right]\frac{\partial \sigma_{ik}}{\partial x_k}$$

$$+ \frac{1}{3}\frac{\partial \tilde{w}^a}{\partial x_i} - \frac{\kappa_a}{\kappa_1}\frac{1}{3}\frac{\partial \tilde{w}^1}{\partial x_i} + \sum_{b=2}^{N}\tilde{\mathcal{R}}_{ab}^{(2)}\frac{\partial \tilde{w}_{ik}^b}{\partial x_k} - \frac{\kappa_a}{\kappa_1}\frac{\partial \tilde{w}_{ik}^2}{\partial x_k}$$

$$= -\frac{1}{\varepsilon}\frac{2}{\kappa_1}\left[\frac{a(2a+3)!!}{3} - 5\frac{\kappa_a}{\kappa_1}\right]\left[q_i + \varepsilon\frac{\kappa_1}{2}\frac{\partial \theta}{\partial x_i}\right] - \frac{1}{\varepsilon}\sum_{b=2}^{N}\left[\tilde{C}_{ab}^{(1)} - \frac{\kappa_a}{\kappa_1}\tilde{C}_{1b}^{(1)}\right]\tilde{w}_i^b$$

$$(a = 2, \ldots, N) \tag{36}$$

$$\frac{\partial \tilde{w}_{ij}^a}{\partial t} + \frac{\partial \tilde{u}_{ijk}^a}{\partial x_k} - \frac{\mu_a}{\mu_1}\frac{\partial \tilde{u}_{ijk}^1}{\partial x_k} + \frac{2}{5}\frac{\partial \tilde{w}_{\langle i}^a}{\partial x_{j\rangle}} + \left[\frac{4}{5}\frac{\kappa_a}{\kappa_1} - \frac{4}{5}\frac{\mu_a}{\mu_1}\right]\frac{\partial q_{\langle i}}{\partial x_{j\rangle}}$$

$$= -\frac{1}{\varepsilon}\frac{2}{\mu_1}\left[\frac{(2a+3)!!}{15} - \frac{\mu_a}{\mu_1}\right]\left[\sigma_{ij} + \varepsilon\mu_1\frac{\partial v_{\langle i}}{\partial x_{j\rangle}}\right] - \frac{1}{\varepsilon}\sum_{b=2}^{N}\left[\tilde{\mathcal{C}}_{ab}^{(2)} - \frac{\mu_a}{\mu_1}\tilde{\mathcal{C}}_{1b}^{(2)}\right]\tilde{w}_{ij}^b$$

$$(a = 2, \ldots, N), \qquad (37)$$

$$\frac{\partial \tilde{u}_{ijk}^a}{\partial t} + \frac{\partial \tilde{u}_{ijkl}^a}{\partial x_l} + \frac{3}{7}\sum_{b=2}^{N}\tilde{\mathcal{R}}_{ab}^{(2)}\frac{\partial \tilde{w}_{\langle ij}^b}{\partial x_{k\rangle}} + \frac{3}{7}\sum_{b=1}^{N}\tilde{\mathcal{R}}_{ab}^{(2)}\frac{\mu_b}{\mu_1}\frac{\partial \sigma_{\langle ij}}{\partial x_{k\rangle}} = -\frac{1}{\varepsilon}\sum_{b=1}^{N}\tilde{\mathcal{C}}_{ab}^{(3)}\tilde{u}_{ijk}^b$$

$$(a = 1, \ldots, N). \qquad (38)$$

To obtain these forms of the equations, we have used that

$$\sum_{b=1}^{N}\tilde{\mathcal{C}}_{ab}^{(1)}\kappa_b = \sum_{b=1}^{N}\tilde{\mathcal{C}}_{ab}^{(1)}\left[\sum_{b=1}^{N}\left[\tilde{\mathcal{C}}^{(1)}\right]_{bc}^{-1}(2c+3)!!\frac{c}{3}\right] = (2a+3)!!\frac{a}{3},$$

$$\sum_{b=1}^{N}\tilde{\mathcal{C}}_{ab}^{(2)}\mu_b = \sum_{b=1}^{N}\tilde{\mathcal{C}}_{ab}^{(2)}\left[\sum_{c=1}^{N}\left[\tilde{\mathcal{C}}^{(2)}\right]_{bc}^{-1}(2c+3)!!\frac{2}{15}\right] = (2a+3)!!\frac{2}{15}. \qquad (39)$$

For summation boundaries on the rhs recall that $\tilde{w}_i^1 = \tilde{w}_{ij}^1 = 0$.

C. Establishing the order of moments

At the present point of the proceedings we have established the hydrodynamic variables ρ, v_i, θ as the only zeroth order quantities. The corresponding equations are the conservation laws (21). The latter contain heat flux q_i and stress σ_{ij}, which are the only first order variables; the corresponding equations are the balance laws (33) and (34). These contain the second or higher order moments $\tilde{w}^b$, $\tilde{w}_i^b$, $\tilde{w}_{ij}^b$, $\tilde{u}_{ijk}^1$, which come with their own balance laws (35)–(38). These, in turn, contain even higher order moments, and so on. We shall now again use a leading order Chapman-Enskog expansion to identify the leading terms of the second order moments.

1. Preparation of equations

For the next level, we perform the Chapman-Enskog expansion only of the second or higher order variables, that is we write

$$\tilde{w}^b = \varepsilon^2\tilde{w}_2^b + \varepsilon^3\tilde{w}_3^b + \cdots,$$
$$\tilde{w}_i^b = \varepsilon^2\tilde{w}_{i,2}^b + \varepsilon^3\tilde{w}_{i,3}^b + \cdots,$$
$$\tilde{w}_{ij}^b = \varepsilon^2\tilde{w}_{ij,2}^b + \varepsilon^3\tilde{w}_{ij,3}^b + \cdots, \qquad (40)$$
$$\tilde{u}_{i_1\cdots i_n}^b = \varepsilon^2\tilde{u}_{i_1\cdots i_n,2}^b + \varepsilon^3\tilde{u}_{i_1\cdots i_n,3}^b + \cdots,$$

and insert these into (35)–(38).

For the evaluation we have to keep in mind that q_i and σ_{ij} are first order in the Knudsen number. It is best to make this explicit by writing

$$q_i = \varepsilon\bar{q}_i, \quad \sigma_{ij} = \varepsilon\bar{\sigma}_{ij}, \qquad (41)$$

where $\bar{q}_i$ and $\bar{\sigma}_{ij}$ are zeroth order quantities, and the factor ε makes the order explicit.

A finer point is the occurrence of the terms

$$\Delta q_i = q_i + \varepsilon\frac{\kappa_1}{2}\frac{\partial\theta}{\partial x_i} = q_i - q_i^{NSF} \quad \text{and} \quad \Delta\sigma_{ij} = \sigma_{ij} + \varepsilon\mu_1\frac{\partial v_{\langle i}}{\partial x_{j\rangle}} = \sigma_{ij} - \sigma_{ij}^{NSF}. \qquad (42)$$

As indicated, these are the difference between stress and heat flux and the first order Navier-Stokes-Fourier approximation (29). In a Chapman-Enskog expansion, these combined terms vanish to first order, and thus we conclude that they are of second order. To clearly indicate this for the evaluation, we write

$$q_i + \varepsilon \frac{\kappa_1}{2} \frac{\partial \theta}{\partial x_i} = \varepsilon^2 \overline{\left[q_i + \varepsilon \frac{\kappa_1}{2} \frac{\partial \theta}{\partial x_i} \right]} \quad \text{and} \quad \sigma_{ij} + \varepsilon \mu_1 \frac{\partial v_{\langle i}}{\partial x_{j \rangle}} = \varepsilon^2 \overline{\left[\sigma_{ij} + \varepsilon \mu_1 \frac{\partial v_{\langle i}}{\partial x_{j \rangle}} \right]}. \tag{43}$$

The leading order approximations for the variables $\tilde{w}^b$, $\tilde{w}_i^b$, $\tilde{w}_{ij}^b$, $\tilde{u}_{i_1 \cdots i_n}^b$ are obtained by inversion of the matrices $\tilde{\mathcal{C}}_{ab}^{(n)}$. It turns out that the variables $\tilde{w}^b$, $\tilde{w}_i^b$, $\tilde{w}_{ij}^b$, $\tilde{u}_{ijk}^b$ all have second order contributions. We proceed by reconstructing variables such that we have the minimum number of variables of order 2.

2. Leading order expansion

With the above consideration of the Knudsen order of magnitude of the terms appearing in the equations, we can now perform the Chapman-Enskog expansion, where, again, we are interested only in the leading order terms. We find at first

$$\left(2 \sum_{b=1}^N \tilde{\mathcal{R}}_{ab}^{(1)} \frac{\kappa_b}{\kappa_1} - (2a+3)!! \frac{2(a+1)}{3} \right) \frac{\partial \bar{q}_k}{\partial x_k} = - \sum_{b=1}^N \tilde{\mathcal{C}}_{ab}^{(0)} \tilde{w}_2^b, \tag{44}$$

$$\left(\sum_{b=1}^N \tilde{\mathcal{R}}_{ab}^{(2)} \frac{\mu_b}{\mu_1} - \frac{(2a+3)!!}{3} - 2 \frac{\kappa_a}{\kappa_1} \left[\frac{\mu_2}{2\mu_1} - \frac{5}{2} \right] \right) \frac{\partial \bar{\sigma}_{ik}}{\partial x_k}$$

$$+ \frac{2}{\kappa_1} \left(\frac{a(2a+3)!!}{3} - 5\frac{\kappa_a}{\kappa_1} \right) \overline{\left[q_i + \varepsilon \frac{\kappa_1}{2} \frac{\partial \theta}{\partial x_i} \right]} = - \sum_{b=2}^N \left[\tilde{\mathcal{C}}_{ab}^{(1)} - \frac{\kappa_a}{\kappa_1} \tilde{\mathcal{C}}_{1b}^{(1)} \right] \tilde{w}_{i,2}^b, \tag{45}$$

$$\left(\frac{4}{5} \frac{\kappa_a}{\kappa_1} - \frac{4}{5} \frac{\mu_a}{\mu_1} \right) \frac{\partial \bar{q}_{\langle i}}{\partial x_{j \rangle}} + \frac{2}{\mu_1} \left(\frac{(2a+3)!!}{15} - \frac{\mu_a}{\mu_1} \right) \overline{\left[\sigma_{ij} + \varepsilon \mu_1 \frac{\partial v_{\langle i}}{\partial x_{j \rangle}} \right]} = - \sum_{b=2}^N \left[\tilde{\mathcal{C}}_{ab}^{(2)} - \frac{\mu_a}{\mu_1} \tilde{\mathcal{C}}_{1b}^{(2)} \right] \tilde{w}_{ij,2}^b, \tag{46}$$

$$\frac{3}{7} \sum_{b=1}^N \tilde{\mathcal{R}}_{ab}^{(2)} \frac{\mu_b}{\mu_1} \frac{\partial \bar{\sigma}_{\langle ij}}{\partial x_{k \rangle}} = - \sum_{b=1}^N \tilde{\mathcal{C}}_{ab}^{(3)} \tilde{u}_{ijk,2}^b \quad (a = 1, \dots, N). \tag{47}$$

The leading order approximations for the variables $\tilde{w}^b$, $\tilde{w}_i^b$, $\tilde{w}_{ij}^b$, $\tilde{u}_{i_1 \cdots i_n}^b$ are obtained by inversion of the matrices $\tilde{\mathcal{C}}_{ab}^{(n)}$. We suppress the equations for $\tilde{u}_{i_1 \cdots i_n}^b$ with four or more indices ($n \geq 4$) which show that those moments have no second order contributions, and thus are of third order or higher in the Knudsen number.

The variables $\tilde{w}^b$, $\tilde{w}_i^b$, $\tilde{w}_{ij}^b$, $\tilde{u}_{ijk}^b$ all have second order contributions. We proceed by reconstructing variables such that we have the minimum number of variables of order 2. We treat the moments at different orders separately in Subsections V C 3–V C 7. We also return to non-scaled variable notation at this point.

3. Scalar moments

The second order contribution to the scalar moments $\tilde{w}^c$ one finds as

$$\varepsilon^2 \tilde{w}_2^c = -\varepsilon \zeta_c \frac{\partial q_k}{\partial x_k} \quad (c = 1, \dots, N) \tag{48}$$

with the coefficients

$$\zeta_c = \sum_{a=1}^N \left[\tilde{\mathcal{C}}^{(0)} \right]_{ca}^{-1} \left[2 \sum_{b=1}^N \tilde{\mathcal{R}}_{ab}^{(1)} \frac{\kappa_b}{\kappa_1} - (2a+3)!! \frac{2(a+1)}{3} \right] \quad (c = 1, \dots, N). \tag{49}$$

Within second order, all scalar moments are linearly dependent,

$$\tilde{w}_2^c = \frac{\zeta_c}{\zeta_1} \tilde{w}_2^1. \tag{50}$$

We choose $\tilde{w}^1$ as the only scalar moment at second order, and introduce third order moments $\tilde{z}^c$ defined as

$$\tilde{z}^c = \tilde{w}^c - \frac{\zeta_c}{\zeta_1} \tilde{w}^1 \qquad (c = 2, \ldots, N). \tag{51}$$

Then, the scalar variables are density ρ and temperature θ at zeroth order, the second order variable $\tilde{w}^1$, and the third order variables $\tilde{z}^c$ ($c \geq 2$).

4. Vectors

For the second order contribution to the vectors one finds

$$\varepsilon^2 \tilde{w}_{i,2}^b = -\varepsilon \vartheta_b \frac{\partial \sigma_{ik}}{\partial x_k} - \eta_b \left[q_i + \varepsilon \frac{\kappa_1}{2} \frac{\partial \theta}{\partial x_i} \right] \qquad (b = 2, \ldots, N), \tag{52}$$

where we have introduced the abbreviations

$$\tilde{\mathcal{D}}_{ab}^{(1)} = \tilde{\mathcal{C}}_{ab}^{(1)} - \frac{\kappa_a}{\kappa_1} \tilde{\mathcal{C}}_{1b}^{(1)} \qquad (a, b = 2, \ldots, N),$$

$$\vartheta_b = \sum_{a=2}^{N} [\tilde{\mathcal{D}}^{(1)}]_{ba}^{-1} \left[\sum_{c=1}^{N} \tilde{\mathcal{R}}_{ac}^{(2)} \frac{\mu_c}{\mu_1} - \frac{(2a+3)!!}{3} - \frac{\kappa_a}{\kappa_1} \left[\frac{\mu_2}{\mu_1} - 5 \right] \right] \qquad (b = 2, \ldots, N), \tag{53}$$

$$\eta_b = \frac{2}{\kappa_1} \sum_{a=2}^{N} [\tilde{\mathcal{D}}^{(1)}]_{ba}^{-1} \left[(2a+3)!! \frac{a}{3} - 5 \frac{\kappa_a}{\kappa_1} \right] \qquad (b = 2, \ldots, N).$$

Within the leading order the $\tilde{w}_i^b$ are linearly dependent. Indeed, choosing $\tilde{w}_i^2$ and $\tilde{w}_i^3$ as the base variables, we have

$$\tilde{w}_{i,2}^b = \frac{\eta_b \vartheta_3 - \eta_3 \vartheta_b}{\eta_2 \vartheta_3 - \eta_3 \vartheta_2} \tilde{w}_{i,2}^2 + \frac{\eta_2 \vartheta_b - \eta_b \vartheta_2}{\eta_2 \vartheta_3 - \eta_3 \vartheta_2} \tilde{w}_{i,2}^3 \qquad (b = 4, \ldots, N). \tag{54}$$

Accordingly, we can define the third order vectors as

$$\tilde{z}_i^b = \tilde{w}_i^b - \frac{\eta_b \vartheta_3 - \eta_3 \vartheta_b}{\eta_2 \vartheta_3 - \eta_3 \vartheta_2} \tilde{w}_i^2 - \frac{\eta_2 \vartheta_b - \eta_b \vartheta_2}{\eta_2 \vartheta_3 - \eta_3 \vartheta_2} \tilde{w}_i^3 \qquad (b = 4, \ldots, N). \tag{55}$$

With this, the vector variables are velocity v_i at zeroth order, heat flux q_i at first order, the second order variables $\tilde{w}_i^2$, $\tilde{w}_i^3$, and the third order variables $\tilde{z}_i^c$ ($c \geq 4$).

5. 2-tensors

For the second order contribution to the 2-tensors one finds

$$\varepsilon^2 \tilde{w}_{ij,2}^b = -\varphi_b \varepsilon \frac{\partial q_{\langle i}}{\partial x_{j \rangle}} - \phi_b \left[\sigma_{ij} + \varepsilon \mu_1 \frac{\partial v_{\langle i}}{\partial x_{j \rangle}} \right] \qquad (b = 2, \ldots, N) \tag{56}$$

with the abbreviations

$$\tilde{\mathcal{D}}_{ab}^{(2)} = \tilde{\mathcal{C}}_{ab}^{(2)} - \frac{\mu_a}{\mu_1} \tilde{\mathcal{C}}_{1b}^{(2)}, \qquad (a, b = 2, \ldots, N),$$

$$\varphi_b = \frac{4}{5} \sum_{a=2}^{N} [\tilde{\mathcal{D}}^{(2)}]_{ba}^{-1} \left[\frac{\kappa_a}{\kappa_1} - \frac{\mu_a}{\mu_1} \right], \qquad (b = 2, \ldots, N) \tag{57}$$

$$\phi_b = \frac{2}{\mu_1} \sum_{a=2}^{N} [\tilde{\mathcal{D}}^{(2)}]_{ba}^{-1} \left[\frac{(2a+3)!!}{15} - \frac{\mu_a}{\mu_1} \right], \qquad (b = 2, \ldots, N).$$

Hence, to second order, the 2-tensor variables are linearly dependent. We chose $\tilde{w}_{ij}^2$ and $\tilde{w}_{ij}^3$ as the 2-tensor variables at second order, and have

$$\tilde{w}_{ij,2}^b = \frac{\phi_b\varphi_3 - \phi_3\varphi_b}{\phi_2\varphi_3 - \phi_3\varphi_2}\tilde{w}_{ij,2}^2 + \frac{\phi_2\varphi_b - \phi_b\varphi_2}{\phi_2\varphi_3 - \phi_3\varphi_2}\tilde{w}_{ij,2}^3 \quad (b = 4, \ldots, N). \tag{58}$$

Accordingly, we define the third order variables as

$$\tilde{z}_{ij}^b = \tilde{w}_{ij}^b - \frac{\phi_b\varphi_3 - \phi_3\varphi_b}{\phi_2\varphi_3 - \phi_3\varphi_2}\tilde{w}_{ij}^2 - \frac{\phi_2\varphi_b - \phi_b\varphi_2}{\phi_2\varphi_3 - \phi_3\varphi_2}\tilde{w}_{ij}^3 \quad (b = 4, \ldots, N). \tag{59}$$

With this, the 2-tensor variables are the stress σ_{ij} at first order, the second order variables $\tilde{w}_{ij}^2$, $\tilde{w}_{ij}^3$, and the third order variables $\tilde{z}_{ij}^c$ ($c \geq 4$).

6. 3-tensors

For the second order contribution to the 3-tensors one finds

$$\varepsilon^2 \tilde{u}_{ijk,2}^b = -\varepsilon\xi_b \frac{\partial\sigma_{\langle ij}}{\partial x_{k\rangle}} \quad (b = 1, \ldots, N) \tag{60}$$

with the coefficients

$$\xi_b = \frac{3}{7}\sum_{a=1}^N \left[\tilde{\mathcal{C}}^{(3)}\right]_{ba}^{-1}\sum_{c=1}^N \tilde{\mathcal{R}}_{ac}^{(2)}\frac{\mu_c}{\mu_1}, \quad (b = 1, \ldots, N). \tag{61}$$

To second order, the 3-tensor variables are linearly dependent,

$$\tilde{u}_{ijk,2}^b = \frac{\xi_b}{\xi_1}\tilde{u}_{ijk,2}^1 \quad (b = 2, \ldots, N) \tag{62}$$

which suggest the definition of third order variables

$$\tilde{z}_{ijk}^b = \tilde{u}_{ijk}^b - \frac{\xi_b}{\xi_1}\tilde{u}_{ijk}^1 \quad (b = 2, \ldots, N). \tag{63}$$

With this, the 3-tensor variables are the second order moment $\tilde{u}_{ijk}^1$, and the third order variables $\tilde{z}_{ijk}^c$ ($c \geq 2$).

7. Higher moments

For moments $\tilde{u}_{i_1\cdots i_n}^b$ with four or more indices ($n \geq 4$) one finds

$$0 = -\sum_{b=1}^N \tilde{\mathcal{C}}_{ab}^{(n)}\tilde{u}_{i_1\cdots i_n,2}^b \quad (n \geq 4, \ a = 1, \ldots, N). \tag{64}$$

Accordingly, these moments have no second order contributions, and thus are of third order or higher in the Knudsen number.

8. Equations for q_i and σ_{ij}

We have now identified the following variables and orders:

$$
\begin{array}{ll}
\rho, v_i, \theta & \text{zeroth order,} \\
\sigma_{ij}, q_i & \text{first order,} \\
\tilde{w}^1, \tilde{w}_i^2, \tilde{w}_i^3, \tilde{w}_{ij}^2, \tilde{w}_{ij}^3, \tilde{u}_{ijk}^1 & \text{second order,} \\
\tilde{z}^b, \tilde{z}_i^b, \tilde{z}_{ij}^b, \tilde{z}_{ijk}^b, & \text{at least third order.}
\end{array}
\tag{65}
$$

We have to rewrite the equations for these variables. The equations for heat flux q_i and stress σ_{ij} read after reformulation,

$$\frac{\partial q_i}{\partial t} + \left[\frac{\mu_2}{2\mu_1} - \frac{5}{2}\right]\frac{\partial \sigma_{ik}}{\partial x_k} + \frac{1}{2}\frac{\partial \tilde{w}_{ik}^2}{\partial x_k} + \frac{1}{6}\frac{\partial \tilde{w}^1}{\partial x_i} = -\frac{1}{\varepsilon}\frac{5}{\kappa_1}\left[q_i + \varepsilon\frac{\kappa_1}{2}\frac{\partial \theta}{\partial x_i}\right] - \frac{1}{\varepsilon}\frac{1}{2}\sum_{b=2}^{3}\tilde{\mathcal{C}}_{1b}^{(1)}\tilde{w}_i^b$$

$$-\frac{1}{\varepsilon}\frac{1}{2}\sum_{b=4}^{N}\tilde{\mathcal{C}}_{1b}^{(1)}\left(\frac{\eta_b\vartheta_3 - \eta_3\vartheta_b}{\eta_2\vartheta_3 - \eta_3\vartheta_2}\tilde{w}_i^2 + \frac{\eta_2\vartheta_b - \eta_b\vartheta_2}{\eta_2\vartheta_3 - \eta_3\vartheta_2}\tilde{w}_i^3\right) - \frac{1}{\varepsilon}\frac{1}{2}\sum_{b=4}^{N}\tilde{\mathcal{C}}_{1b}^{(1)}\tilde{z}_i^b, \tag{66}$$

$$\frac{\partial \sigma_{ij}}{\partial t} + \frac{4}{5}\frac{\partial q_{\langle i}}{\partial x_{j\rangle}} + \frac{\partial \tilde{u}_{ijk}^1}{\partial x_k} = -\frac{1}{\varepsilon}\frac{2}{\mu_1}\left[\sigma_{ij} + \varepsilon\mu_1\frac{\partial v_{\langle i}}{\partial x_{j\rangle}}\right] - \frac{1}{\varepsilon}\sum_{b=2}^{3}\tilde{\mathcal{C}}_{1b}^{(2)}\tilde{w}_{ij}^b$$

$$-\frac{1}{\varepsilon}\sum_{b=4}^{N}\tilde{\mathcal{C}}_{1b}^{(2)}\left(\frac{\phi_b\varphi_3 - \phi_3\varphi_b}{\phi_2\varphi_3 - \phi_3\varphi_2}\tilde{w}_{ij}^2 + \frac{\phi_2\varphi_b - \phi_b\varphi_2}{\phi_2\varphi_3 - \phi_3\varphi_2}\tilde{w}_{ij}^3\right) - \frac{1}{\varepsilon}\sum_{b=4}^{N}\tilde{\mathcal{C}}_{1b}^{(2)}\tilde{z}_{ij}^b. \tag{67}$$

The second rows of both equations contain the contributions of higher moments $\tilde{w}_i^b$, $\tilde{w}_{ij}^b$ for $b \geq 4$. The evaluation of the terms requires the matrix elements $\tilde{\mathcal{C}}_{1b}^{(n)}$ for $b \geq 4$, which, at present, we do not have. The discussion of the order of variables suggests that for proper consideration at second order we should include all second order variables, that is consider at least the case $N = 3$. From now on we will continue under this limitation. Then, the terms in the second row drop out, and the equations for heat flux and stress reduce to

$$\frac{\partial q_i}{\partial t} + \left[\frac{\mu_2}{2\mu_1} - \frac{5}{2}\right]\frac{\partial \sigma_{ik}}{\partial x_k} + \frac{1}{2}\frac{\partial \tilde{w}_{ik}^2}{\partial x_k} + \frac{1}{6}\frac{\partial \tilde{w}^1}{\partial x_i} = -\frac{1}{\varepsilon}\frac{5}{\kappa_1}\left[q_i + \varepsilon\frac{\kappa_1}{2}\frac{\partial \theta}{\partial x_i}\right] - \frac{1}{\varepsilon}\frac{1}{2}\sum_{b=2}^{3}\tilde{\mathcal{C}}_{1b}^{(1)}\tilde{w}_i^b,$$

$$\frac{\partial \sigma_{ij}}{\partial t} + \frac{4}{5}\frac{\partial q_{\langle i}}{\partial x_{j\rangle}} + \frac{\partial \tilde{u}_{ijk}^1}{\partial x_k} = -\frac{1}{\varepsilon}\frac{2}{\mu_1}\left[\sigma_{ij} + \varepsilon\mu_1\frac{\partial v_{\langle i}}{\partial x_{j\rangle}}\right] - \frac{1}{\varepsilon}\sum_{b=2}^{3}\tilde{\mathcal{C}}_{1b}^{(2)}\tilde{w}_{ij}^b. \tag{68}$$

D. Model reduction by orders

We have now established the leading order of moments, and introduced new moments such that at zeroth to second order in ϵ we have the minimum number of variables possible. With this, we have the necessary foundation for the application of the order of magnitude method to reduce the equations. We first rewrite them in the most convenient way, which includes to make the ε-order of all terms explicit. The model reduction follows then step by step.

1. Rescaled equations

As long as we consider only the case with 3×3 production matrices, and ask only for equations up to 3rd order, we shall not need the 3rd order variables $\tilde{z}_{i_1\cdots i_n}^a$. For the scaling arguments considered next, it is useful to rewrite the moment equations (33)–(38) such that the production terms on the right-hand side are written as the difference between the moments and their leading contributions (29), (48), (52), (56), and (60). This introduces the coefficients Pr, ϑ_b, η_b, φ_b, ϕ_b, ζ_c, ξ_b into the equations, as well as new coefficients $a^{(\alpha, \beta)}$ whose definitions are given further below.

The order of magnitude method relies on the leading orders for the moments (in the Chapman-Enskog sense), as established above. To clearly have the orders of all variables visible in the equations, we make the scaling of all quantities explicit, by writing

$$\sigma_{ij} = \varepsilon\bar{\sigma}_{ij}, \quad q_i = \varepsilon\bar{q}_i,$$

$$\tilde{w}^a = \varepsilon^2\bar{w}^a, \quad \tilde{w}_i^a = \varepsilon^2\bar{w}_i^a, \quad \tilde{w}_{ij}^a = \varepsilon^2\bar{w}_{ij}^a, \quad \tilde{u}_{ijk}^a = \varepsilon^2\bar{u}_{ijk}^a, \tag{69}$$

$$\tilde{u}_{ijkl}^a = \varepsilon^3\bar{u}_{ijkl}^a.$$

Here, the quantities with an overbar ($\bar{\sigma}_{ij}$, $\bar{q}_i$, etc.) are considered to be of order unity while the ϵ-order is made explicit by the factors ε^n.

With all this, and some reordering of terms, our moment equations assume the form

$$\varepsilon\left[\frac{\partial\bar{q}_i}{\partial t}+a^{(1,1)}\frac{\partial\bar{\sigma}_{ik}}{\partial x_k}\right]+\varepsilon^2\left[\frac{1}{2}\frac{\partial\bar{w}_{ik}^2}{\partial x_k}+\frac{1}{6}\frac{\partial\bar{w}^1}{\partial x_i}\right]=-a^{(1,0)}\left[\bar{q}_i+\frac{5}{2\Pr}\frac{\partial\theta}{\partial x_i}\right]$$
$$-\varepsilon\frac{1}{2}\sum_{b=2}^3\tilde{\mathcal{C}}_{1b}^{(1)}\left[\bar{w}_i^b+\vartheta_b\frac{\partial\bar{\sigma}_{ik}}{\partial x_k}+\eta_b\left[\bar{q}_i+\frac{5}{2\Pr}\frac{\partial\theta}{\partial x_i}\right]\right],$$

(70)

$$\varepsilon\left[\frac{\partial\bar{\sigma}_{ij}}{\partial t}+a^{(2,1)}\frac{\partial\bar{q}_{\langle i}}{\partial x_{j\rangle}}\right]+\varepsilon^2\frac{\partial\bar{u}_{ijk}^1}{\partial x_k}=-a^{(2,0)}\left[\bar{\sigma}_{ij}+2\frac{\partial v_{\langle i}}{\partial x_{j\rangle}}\right]$$
$$-\varepsilon\sum_{b=2}^3\tilde{\mathcal{C}}_{1b}^{(2)}\left[\bar{w}_{ij}^b+\varphi_b\frac{\partial\bar{q}_{\langle i}}{\partial x_{j\rangle}}+\phi_b\left[\bar{\sigma}_{ij}+2\frac{\partial v_{\langle i}}{\partial x_{j\rangle}}\right]\right],$$

(71)

$$\varepsilon^2\left[\frac{\partial\bar{w}^a}{\partial t}+\sum_{b=2}^3\tilde{\mathcal{R}}_{ab}^{(1)}\frac{\partial\bar{w}_k^b}{\partial x_k}\right]=-\varepsilon\sum_{b=1}^3\tilde{\mathcal{C}}_{ab}^{(0)}\left[\bar{w}^b+\zeta_b\frac{\partial\bar{q}_k}{\partial x_k}\right]\quad(a=1,2,3),$$

(72)

$$\varepsilon^2\left[\frac{\partial\bar{w}_i^a}{\partial t}+\frac{1}{3}\frac{\partial\bar{w}^a}{\partial x_i}-\frac{\kappa_a}{\kappa_1}\frac{1}{3}\frac{\partial\bar{w}^1}{\partial x_i}+\sum_{b=2}^3\tilde{\mathcal{R}}_{ab}^{(2)}\frac{\partial\bar{w}_{ik}^b}{\partial x_k}-\frac{\kappa_a}{\kappa_1}\frac{\partial\bar{w}_{ik}^2}{\partial x_k}\right]$$
$$=-\varepsilon\sum_{b=2}^3\tilde{\mathcal{D}}_{ab}^{(1)}\left[\bar{w}_i^b+\vartheta_b^{(1)}\frac{\partial\bar{\sigma}_{ik}}{\partial x_k}+\eta_b\left[\bar{q}_i+\frac{5}{2\Pr}\frac{\partial\theta}{\partial x_i}\right]\right]\quad(a=2,3),$$

(73)

$$\varepsilon^2\left[\frac{\partial\bar{w}_{ij}^a}{\partial t}+\frac{\partial\bar{u}_{ijk}^a}{\partial x_k}-\frac{\mu_a}{\mu_1}\frac{\partial\bar{u}_{ijk}^1}{\partial x_k}+\frac{2}{5}\frac{\partial\bar{w}_{\langle i}^a}{\partial x_{j\rangle}}\right]$$
$$=-\varepsilon\sum_{b=2}^3\tilde{\mathcal{D}}_{ab}^{(2)}\left[\bar{w}_{ij}^b+\varphi_b\frac{\partial\bar{q}_{\langle i}}{\partial x_{j\rangle}}+\phi_b\left[\bar{\sigma}_{ij}+2\frac{\partial v_{\langle i}}{\partial x_{j\rangle}}\right]\right]\quad(a=2,3),$$

(74)

$$\varepsilon^2\left[\frac{\partial\bar{u}_{ijk}^a}{\partial t}+\frac{3}{7}\sum_{b=2}^3\tilde{\mathcal{R}}_{ab}^{(2)}\frac{\partial\bar{w}_{\langle ij}^b}{\partial x_{k\rangle}}\right]+\varepsilon^3\frac{\partial\bar{u}_{ijkl}^a}{\partial x_l}=-\varepsilon\sum_{b=1}^N\tilde{\mathcal{C}}_{ab}^{(3)}\left[\bar{u}_{ijk}^b+\xi_b\frac{\partial\bar{\sigma}_{\langle ij}}{\partial x_{k\rangle}}\right]\quad(a=1,2,3).$$

(75)

The coefficients in the equations for σ_{ij} and q_i are defined as

$$a^{(1,0)}=\frac{5}{\kappa_1}-\frac{1}{2}\sum_{b=2}^3\tilde{\mathcal{C}}_{1b}^{(1)}\eta_b,\quad a^{(1,1)}=\frac{\mu_2}{2\mu_1}-\frac{5}{2}-\frac{1}{2}\sum_{b=2}^3\tilde{\mathcal{C}}_{1b}^{(1)}\vartheta_b,$$

$$a^{(2,0)}=\frac{2}{\mu_1}-\sum_{b=2}^3\tilde{\mathcal{C}}_{1b}^{(2)}\phi_b,\quad a^{(2,1)}=\frac{4}{5}-\sum_{b=2}^3\tilde{\mathcal{C}}_{1b}^{(2)}\varphi_b.$$

(76)

2. First order: Navier-Stokes-Fourier (again)

The ε-orders can now be used for model reduction in a quite straightforward manner: For increasing order, terms with increasing ε−powers must be considered. Since the goal is to have stress σ_{ij} and heat flux q_i exact up to a given order, we look at Eqs. (70) and (71) first, and then consider the other equations as required.

For the first approximation, only the leading terms in (70) and (71) are needed, these are the zeroth order terms (factor $\varepsilon^0=1$). This gives, once more, the laws of Navier-Stokes and

Fourier (29):

$$q_i = \varepsilon \bar{q}_i = -\frac{5\varepsilon}{2\,\mathrm{Pr}} \frac{\partial \theta}{\partial x_i}, \quad \sigma_{ij} = \varepsilon \bar{\sigma}_{ij} = -2\varepsilon \frac{\partial v_{\langle i}}{\partial x_{j\rangle}} . \tag{77}$$

3. Second order: Generalized Grad 13 moments

For the second order equations, we have to consider the two leading terms in Eqs. (70) and (71) for σ_{ij} and q_i, which are those of zeroth and first order in ε,

$$\varepsilon \left[\frac{\partial \bar{q}_i}{\partial t} + a^{(1,1)} \frac{\partial \bar{\sigma}_{ik}}{\partial x_k} \right] = -a^{(1,0)} \left[\bar{q}_i + \frac{5}{2\,\mathrm{Pr}} \frac{\partial \theta}{\partial x_i} \right]$$
$$- \varepsilon \frac{1}{2} \sum_{b=2}^{3} \tilde{\mathcal{C}}_{1b}^{(1)} \left[\bar{w}_i^b + \vartheta_b \frac{\partial \bar{\sigma}_{ik}}{\partial x_k} + \eta_b \left[\bar{q}_i + \frac{5}{2\,\mathrm{Pr}} \frac{\partial \theta}{\partial x_i} \right] \right], \tag{78}$$

$$\varepsilon \left[\frac{\partial \bar{\sigma}_{ij}}{\partial t} + a^{(2,1)} \frac{\partial \bar{q}_{\langle i}}{\partial x_{j\rangle}} \right] = -a^{(2,0)} \left[\bar{\sigma}_{ij} + 2\frac{\partial v_{\langle i}}{\partial x_{j\rangle}} \right] - \varepsilon \sum_{b=2}^{3} \tilde{\mathcal{C}}_{1b}^{(2)} \left[\bar{w}_{ij}^b + \varphi_b \frac{\partial \bar{q}_{\langle i}}{\partial x_{j\rangle}} + \phi_b \left[\bar{\sigma}_{ij} + 2\frac{\partial v_{\langle i}}{\partial x_{j\rangle}} \right] \right]. \tag{79}$$

In the production terms on the right, we find the higher moments $\bar{w}_i^b$ and $\bar{w}_{ij}^b$, both with the factor ε. Their appropriate equations for the given order follows from considering the leading order terms of (73) and (74), which give, once more, the relations (52) and (56),

$$\bar{w}_i^b = -\vartheta_b \frac{\partial \bar{\sigma}_{ik}}{\partial x_k} - \eta_b \left[\bar{q}_i + \frac{5}{2\,\mathrm{Pr}} \frac{\partial \theta}{\partial x_i} \right] \quad (a = 2, 3), \tag{80}$$

$$\bar{w}_{ij}^b = -\varphi_b \frac{\partial \bar{q}_{\langle i}}{\partial x_{j\rangle}} - \phi_b \left[\bar{\sigma}_{ij} + 2\frac{\partial v_{\langle i}}{\partial x_{j\rangle}} \right] \quad (a = 2, 3).$$

With this, the terms on the right-hand sides just vanish, and the appropriate equations at second order are the generalized Grad-type moment equations (linearized), which read when the scaled variables are replaced by the original ones,

$$\frac{\partial \sigma_{ij}}{\partial t} + a^{(2,1)} \frac{\partial q_{\langle i}}{\partial x_{j\rangle}} = -\frac{a^{(2,0)}}{\varepsilon} \left[\sigma_{ij} + 2\varepsilon \frac{\partial v_{\langle i}}{\partial x_{j\rangle}} \right], \tag{81}$$

$$\frac{\partial q_i}{\partial t} + a^{(1,1)} \frac{\partial \sigma_{ik}}{\partial x_k} = -\frac{a^{(1,0)}}{\varepsilon} \left[q_i + \frac{5}{2\,\mathrm{Pr}} \varepsilon \frac{\partial \theta}{\partial x_i} \right].$$

It was already shown in Ref. 8 that for non-Maxwellian molecules the Grad 13 moments equations must be generalized. Here, this finding is confirmed (for the linear case), and it is shown how the coefficients must be computed within the moment theory, see (76). The values of the coefficients were already given in Table I. The coefficients for the case of Maxwell molecules and hard spheres differ by up to 21%.

4. Second order: Burnett equations

The classical approach to determine stress and heat flux to higher orders is the Chapman-Enskog expansion. Its classical route is to find an approximation to the phase density f by inserting the expansion $f = f^{(0)} + \varepsilon f^{(1)} + \varepsilon^2 f^{(2)} + \cdots$ into the Boltzmann equation and determine the expansion coefficients $f^{(\alpha)}$ successively.[1,3] The alternative is to perform the expansion on the moment equations. This approach was pioneered by Reinecke and Kremer,[22,23] who used large moment systems, closed by the Grad method, to compute the Navier-Stokes-Fourier and Burnett coefficients.

Our original moment system (21) and (22) corresponds to the one used by Reinecke and Kremer[22,23] (who considered the non-linear case), only that we included higher tensorial orders. However, instead of the Chapman-Enskog expansion we used the order of magnitude method to condense the large moment set into the compact 13 moment equations, where to second order (22) is replaced by (81). The order of magnitude method uses the Chapman-Enskog expansion only as a tool to determine the order of magnitude of moments, and for this it uses only the leading term in the expansion while higher contributions are not required. The Chapman-Enskog method itself aims at determining all expansion coefficients.

For Maxwell molecules we have shown in Refs. 5 and 6 that the Chapman-Enskog expansion of the R13 equations yields the Burnett and super-Burnett equations with the same coefficients as obtained from expansion of the phase density. In Ref. 3 we used matching to Burnett coefficients to determine the coefficients in the generalized nonlinear 13 moment equations. We shall now perform the expansion on the generalized Grad 13 equations (81) to compute the Burnett coefficients for hard sphere molecules.

For the expansion we insert

$$\sigma_{ij} = \varepsilon \sigma_{ij}^{(1)} + \varepsilon^2 \sigma_{ij}^{(2)}, \quad q_i = \varepsilon q_i^{(1)} + \varepsilon^2 q_i^{(2)} \tag{82}$$

into Eq. (81) for σ_{ij} and q_i, and determine the expansion coefficients $\sigma_{ij}^{(\alpha)}, q_i^{(\alpha)}$ successively. We shall not give further details for this standard procedure, which was explained in more detail in Refs. 3, 5, and 6. A finer point that must be considered is that time derivatives of ρ, θ, v_i must be replaced by means of the conservation laws (21), which, in turn, contain the expanded quantities. The expansion gives, once more, the laws of Navier-Stokes and Fourier for $\sigma_{ij}^{(1)}$ and $q_i^{(1)}$ and the Burnett corrections,

$$q_i^{(2)} = \frac{\theta_4^B}{2} \frac{\partial^2 v_i}{\partial x_k \partial x_k} + \frac{2}{3} \left(\frac{\theta_4^B}{4} - \theta_2^B \right) \frac{\partial^2 v_k}{\partial x_k \partial x_i},$$

$$\tag{83}$$

$$\sigma_{ij}^{(2)} = -\varpi_2^B \frac{\partial^2 \rho}{\partial x_{\langle i} \partial x_{j \rangle}} - \left(\varpi_2^B - \varpi_3^B \right) \frac{\partial^2 \theta}{\partial x_{\langle i} \partial x_{j \rangle}}.$$

Here we have used the usual notation for Burnett coefficients, which are related to the coefficients in the Grad 13 equations as

$$\theta_2^B = \frac{5}{2 \operatorname{Pr} a^{(1,0)}}, \quad \theta_4^B = 2 \frac{a^{(1,1)}}{a^{(1,0)}}, \quad \varpi_2^B = \frac{2}{a^{(2,0)}}, \quad \varpi_3^B = \frac{5 a^{(2,1)}}{2 a^{(2,0)} \operatorname{Pr}}. \tag{84}$$

Numerical values of the coefficients were already given in Table II. The values depend on the size of the underlying Grad system, N, which in our treatment is $N = 3$. Reinecke and Kremer[23] have computed the coefficients from a bigger system with $N = 5$, their values differ from ours by less than 0.2%.

E. Third order equations for hard spheres

Next, and finally, we are interested in the equations for stress and heat flux up to third order in the Knudsen number ε. As will be seen, the required equations are more complex than for Maxwellian molecules, and additional effort is needed to further reduce the equations.

1. Intermediate result: 29 moments

Our goal is to have third order accuracy for σ_{ij} and q_i, which requires proper terms up to ε^2 in the equations for σ_{ij} and q_i, that is the complete equations (70) and (71). Also, for now, the equations for w_i^a and w_{ij}^a (73) and (74) must be considered with first and second order terms, that is in full. However, the moments $\tilde{w}^a$ and $\tilde{u}_{ijk}^a$ appear only in second order contributions; thus for these it suffices to consider the leading terms in Eqs. (72) and (75), which are, see (48) and (60),

$$\bar{w}^b = -\zeta_b \frac{\partial \bar{q}_k}{\partial x_k} \ , \quad \bar{u}_{ijk}^b = -\xi_b \frac{\partial \bar{\sigma}_{\langle ij}}{\partial x_{k \rangle}} \quad (a = 1, 2, 3) \,. \tag{85}$$

Replacing $\tilde{w}^a$ and $\tilde{u}^a_{ijk}$ with the above, and re-introducing the unscaled variables, we find the relevant third order set of equations as the conservations laws (21) plus the moment equations

$$\frac{\partial q_i}{\partial t} + a^{(1,1)}\frac{\partial \sigma_{ik}}{\partial x_k} + \frac{1}{2}\frac{\partial \tilde{w}^2_{ik}}{\partial x_k} - \frac{\zeta_1}{6}\varepsilon\frac{\partial}{\partial x_i}\frac{\partial q_k}{\partial x_k} = -\frac{1}{\varepsilon}a^{(1,0)}\left[q_i + \frac{5}{2\,\mathrm{Pr}}\varepsilon\frac{\partial \theta}{\partial x_i}\right]$$

$$-\frac{1}{\varepsilon}\frac{1}{2}\sum_{b=2}^{N}\tilde{\mathcal{C}}^{(1)}_{1b}\left[\tilde{w}^b_i + \vartheta_b\varepsilon\frac{\partial \sigma_{ik}}{\partial x_k} + \eta_b\left[q_i + \frac{5}{2\,\mathrm{Pr}}\varepsilon\frac{\partial \theta}{\partial x_i}\right]\right],\tag{86}$$

$$\frac{\partial \sigma_{ij}}{\partial t} + a^{(2,1)}\frac{\partial q_{\langle i}}{\partial x_{j\rangle}} - \xi_1\varepsilon\frac{\partial}{\partial x_k}\frac{\partial \sigma_{\langle ij}}{\partial x_{k\rangle}} = -\frac{1}{\varepsilon}a^{(2,0)}\left[\sigma_{ij} + 2\varepsilon\frac{\partial v_{\langle i}}{\partial x_{j\rangle}}\right]$$

$$-\frac{1}{\varepsilon}\sum_{b=2}^{3}\tilde{\mathcal{C}}^{(2)}_{1b}\left[\tilde{w}^b_{ij} + \varphi_b\varepsilon\frac{\partial q_{\langle i}}{\partial x_{j\rangle}} + \phi_b\left[\sigma_{ij} + 2\varepsilon\frac{\partial v_{\langle i}}{\partial x_{j\rangle}}\right]\right],\tag{87}$$

$$\frac{\partial \tilde{w}^a_i}{\partial t} - \left[\frac{\zeta_a}{3} - \frac{\zeta_1}{3}\frac{\kappa_a}{\kappa_1}\right]\varepsilon\frac{\partial}{\partial x_i}\frac{\partial q_k}{\partial x_k} + \sum_{b=2}^{3}\tilde{\mathcal{R}}^{(2)}_{ab}\frac{\partial \tilde{w}^b_{ik}}{\partial x_k} - \frac{\kappa_a}{\kappa_1}\frac{\partial \tilde{w}^2_{ik}}{\partial x_k}$$

$$= -\frac{1}{\varepsilon}\sum_{b=2}^{3}\tilde{\mathcal{D}}^{(1)}_{ab}\left[\tilde{w}^b_i + \vartheta_b\varepsilon\frac{\partial \sigma_{ik}}{\partial x_k} + \eta_b\left[q_i + \frac{5}{2\,\mathrm{Pr}}\varepsilon\frac{\partial \theta}{\partial x_i}\right]\right]\quad (a = 2, 3),\tag{88}$$

$$\frac{\partial \tilde{w}^a_{ij}}{\partial t} - \left[\xi_a - \xi_1\frac{\mu_a}{\mu_1}\right]\varepsilon\frac{\partial}{\partial x_k}\frac{\partial \sigma_{\langle ij}}{\partial x_{k\rangle}} + \frac{2}{5}\frac{\partial \tilde{w}^a_{\langle i}}{\partial x_{j\rangle}}$$

$$= -\frac{1}{\varepsilon}\sum_{b=2}^{3}\tilde{\mathcal{D}}^{(2)}_{ab}\left[\tilde{w}^b_{ij} + \varphi_b\varepsilon\frac{\partial q_{\langle i}}{\partial x_{j\rangle}} + \phi_b\left[\sigma_{ij} + 2\varepsilon\frac{\partial v_{\langle i}}{\partial x_{j\rangle}}\right]\right]\quad (a = 2, 3).\tag{89}$$

Together with the conservation laws (21), the above form a closed set of moment equations for the 29 variables ρ, v_i, θ, σ_{ij}, q_i, $\tilde{w}^2_i$, $\tilde{w}^3_i$, $\tilde{w}^2_{ij}$, $\tilde{w}^3_{ij}$. We shall proceed shortly with further reducing the equations.

The number of 29 variables required for the third order moment system for hard spheres stands in contrast to the number of only 13 variables that are required for Maxwell molecules. The difference lies in the structure of the matrices $\tilde{\mathcal{C}}^{(1)}_{ab}$ and $\tilde{\mathcal{C}}^{(2)}_{ab}$ which appear on the right-hand sides of the equations for q_i and σ_{ij}. For hard sphere molecules the matrices are fully occupied, see (23), and thus the equations are strongly coupled through the right-hand sides. For Maxwell molecules, however, the matrices are lower triangular matrices,[34] so that $\tilde{\mathcal{C}}^{(1)}_{1b} = \tilde{\mathcal{C}}^{(2)}_{1b} = 0$ for $b \geq 2$. Then, the coupling terms to $\tilde{w}^b_i$, $\tilde{w}^b_{ij}$ on the right-hand sides of (86) and (87) vanish, and only $\tilde{w}^2_{ik}$ remains on the left-hand side of (86). For third order accuracy, it suffices to have $\tilde{w}^2_{ik}$ to second order, that is it can be replaced by the leading order expression $(80)_2$, $\tilde{w}^2_{ij} = -\varphi_2\varepsilon\frac{\partial q_{\langle i}}{\partial x_{j\rangle}} - \phi_2\left[\sigma_{ij} + 2\varepsilon\frac{\partial v_{\langle i}}{\partial x_{j\rangle}}\right]$. With this, only the 13 variables ρ, v_i, θ, σ_{ij}, q_i are required to describe Maxwell molecules to 3rd order: these are the R13 equations.[5,7]

For BGK-like models, the matrices $\tilde{\mathcal{C}}^{(n)}_{ab}$ are diagonal, and the order of magnitude method yields essentially the same equations as for Maxwell molecules, albeit with slightly changed coefficients.[3] For other non-Maxwellian molecular interaction potentials, the production matrices $\tilde{\mathcal{C}}^{(n)}_{ab}$ will be fully occupied, and the equations will be the same as for hard sphere molecules, only with different values for the coefficients, due to different entries in the production matrices.

2. Reducing the moment number

We shall now aim for a reduced set of equations at third order, by repeatedly using scaling arguments.

As a first step we replace the $\tilde{w}_i^a$, $\tilde{w}_{ij}^a$ in the production terms on the right-hand sides of (86) and (87) by means of (88) and (89). This introduces the time derivatives of $\tilde{w}_i^a$, $\tilde{w}_i^a$. The order of the equations remains unchanged when in (86)–(89) $\tilde{w}_{ik}^a$, $\tilde{w}_i^a$ on the left are replaced by their leading order expressions (80). After some algebra, the resulting equations for σ_{ij} and q_i can be written as

$$\frac{\partial q_i}{\partial t} + a^{(1,1)}\frac{\partial \sigma_{ik}}{\partial x_k} - \hat{a}^{(1,2)}\frac{\partial}{\partial x_k}\left[\sigma_{ik} + 2\varepsilon\frac{\partial v_{\langle i}}{\partial x_{k\rangle}}\right] - \hat{a}^{(1,3)}\varepsilon\frac{\partial}{\partial x_k}\frac{\partial q_{\langle i}}{\partial x_{k\rangle}} - \hat{a}^{(1,4)}\varepsilon\frac{\partial}{\partial x_i}\frac{\partial q_k}{\partial x_k}$$

$$= -\frac{1}{\varepsilon}a^{(1,0)}\left[q_i + \frac{5}{2\,\mathrm{Pr}}\varepsilon\frac{\partial \theta}{\partial x_i}\right] + \frac{1}{2}\sum_{a,b=2}^{3}\tilde{\mathcal{C}}_{1b}^{(1)}\left[\tilde{\mathcal{D}}_{ba}^{(1)}\right]^{-1}\frac{\partial \tilde{w}_i^a}{\partial t}, \tag{90}$$

$$\frac{\partial \sigma_{ij}}{\partial t} + a^{(2,1)}\frac{\partial q_{\langle i}}{\partial x_{j\rangle}} - \hat{a}^{(2,2)}\frac{\partial}{\partial x_{\langle i}}\left[q_{j\rangle} + \frac{5}{2\,\mathrm{Pr}}\varepsilon\frac{\partial \theta}{\partial x_{j\rangle}}\right] - \hat{a}^{(2,3)}\varepsilon\frac{\partial}{\partial x_k}\frac{\partial \sigma_{\langle ij}}{\partial x_{k\rangle}} - \hat{a}^{(2,4)}\varepsilon\frac{\partial^2 \sigma_{ij}}{\partial x_k \partial x_k}$$

$$= -\frac{1}{\varepsilon}a^{(2,0)}\left[\sigma_{ij} + 2\varepsilon\frac{\partial v_{\langle i}}{\partial x_{j\rangle}}\right] + \sum_{a,b=2}^{3}\tilde{\mathcal{C}}_{1b}^{(2)}\left[\tilde{\mathcal{D}}_{ba}^{(2)}\right]^{-1}\frac{\partial \tilde{w}_{ij}^a}{\partial t}. \tag{91}$$

The coefficients appearing in these equations, and their values for hard sphere molecules, are

$$\hat{a}^{(1,2)} = \frac{\phi_2}{2} - \frac{1}{2}\sum_{a,b=2}^{N}\tilde{\mathcal{C}}_{1b}^{(1)}\left[\tilde{\mathcal{D}}_{ba}^{(1)}\right]^{-1}\left[\sum_{c=2}^{3}\tilde{\mathcal{R}}_{ac}^{(2)}\phi_c - \frac{\kappa_a}{\kappa_1}\phi_2\right] = 0.170227,$$

$$\hat{a}^{(1,3)} = \frac{\varphi_2}{2} - \frac{1}{2}\sum_{a,b=2}^{N}\tilde{\mathcal{C}}_{1b}^{(1)}\left[\tilde{\mathcal{D}}_{ba}^{(1)}\right]^{-1}\left[\sum_{c=2}^{3}\tilde{\mathcal{R}}_{ac}^{(2)}\varphi_c - \frac{\kappa_a}{\kappa_1}\varphi_2\right] = 2.09368,$$

$$\hat{a}^{(1,4)} = \frac{\zeta_1}{6} - \frac{1}{2}\sum_{a,b=2}^{N}\tilde{\mathcal{C}}_{1b}^{(1)}\left[\tilde{\mathcal{D}}_{ba}^{(1)}\right]^{-1}\left[\frac{\zeta_a}{3} - \frac{\kappa_a}{\kappa_1}\frac{\zeta_1}{3}\right] = 1.47742,$$

$$\hat{a}^{(2,2)} = -\frac{2}{5}\sum_{a,b=2}^{3}\tilde{\mathcal{C}}_{1b}^{(2)}\left[\tilde{\mathcal{D}}^{(2)}\right]_{ba}^{-1}\eta_a = -0.00786213, \tag{92}$$

$$\hat{a}^{(2,3)} = \xi_1 - \sum_{a,b=2}^{3}\tilde{\mathcal{C}}_{1b}^{(2)}\left[\tilde{\mathcal{D}}_{ba}^{(2)}\right]^{-1}\left[\xi_a + \vartheta_a - \xi_1\frac{\mu_a}{\mu_1}\right] = 1.84642,$$

$$\hat{a}^{(2,4)} = \frac{1}{3}\sum_{a,b=2}^{3}\tilde{\mathcal{C}}_{1b}^{(2)}\left[\tilde{\mathcal{D}}_{ba}^{(2)}\right]^{-1}\vartheta_a = -0.00128535.$$

3. Chapman-Enskog reduction of $\frac{\partial \tilde{\omega}_i^a}{\partial t}$, $\frac{\partial \tilde{\omega}_{ij}^a}{\partial t}$

The above equations for σ_{ij} and q_i still contain the time derivatives of the higher moments $\tilde{w}_{ik}^a$, $\tilde{w}_i^a$ on the right-hand sides. In steady state processes these vanish, but for transient processes their computation requires the equations for $\tilde{w}_{ik}^a$, $\tilde{w}_i^a$. The Chapman-Enskog expansion allows us to approximate these terms by means of derivatives of the lower 13 moments. This requires a series of steps that is detailed in the following.

The first step is to approximate $\tilde{w}_{ik}^a$, $\tilde{w}_i^a$ to second order by means of (52) and (56), which results in

$$\frac{\partial \tilde{w}_i^a}{\partial t} = -\vartheta_a\varepsilon\frac{\partial}{\partial x_k}\frac{\partial \sigma_{ik}}{\partial t} - \eta_a\frac{\partial}{\partial t}\left[q_i + \frac{5}{2\,\mathrm{Pr}}\varepsilon\frac{\partial \theta}{\partial x_i}\right],$$

$$\tag{93}$$

$$\frac{\partial \tilde{w}_{ij}^a}{\partial t} = -\varphi_a\varepsilon\frac{\partial}{\partial x_{\langle i}}\frac{\partial q_{j\rangle}}{\partial t} - \phi_a\frac{\partial}{\partial t}\left[\sigma_{ij} + 2\varepsilon\frac{\partial v_{j\rangle}}{\partial x_{\langle i}}\right].$$

Within the order we are interested in, we can replace the first time derivatives (that are multiplied by ε) with the Grad equations (81),

$$\varepsilon\frac{\partial\sigma_{ik}}{\partial t} = -a^{(2,1)}\varepsilon\frac{\partial q_{\langle i}}{\partial x_{k\rangle}} - a^{(2,0)}\left[\sigma_{ik} + 2\varepsilon\frac{\partial v_{\langle i}}{\partial x_{k\rangle}}\right],$$

(94)

$$\varepsilon\frac{\partial q_j}{\partial t} = -a^{(1,1)}\varepsilon\frac{\partial\sigma_{jk}}{\partial x_k} - a^{(1,0)}\left[q_j + \frac{5}{2\,\mathrm{Pr}}\varepsilon\frac{\partial\theta}{\partial x_j}\right].$$

The second terms in each equation are time derivatives of the higher order contributions to heat flux and stress. Here, we use the Burnett expressions (83) for approximation (with $2\frac{\partial}{\partial x_k}\left(\frac{\partial v_{\langle i}}{\partial x_{j\rangle}}\right) = \frac{\partial^2 v_i}{\partial x_k\partial x_k} + \frac{1}{3}\frac{\partial v_k}{\partial x_k\partial x_i}$),

$$\Delta q_i = \varepsilon^2 q_i^{(2)} = \frac{\varepsilon^2}{a^{(1,0)}}\left[2a^{(1,1)}\frac{\partial}{\partial x_k}\frac{\partial v_{\langle i}}{\partial x_{k\rangle}} - \frac{5}{3\,\mathrm{Pr}}\frac{\partial^2 v_k}{\partial x_k\partial x_i}\right],$$

(95)

$$\Delta\sigma_{ij} = \varepsilon^2\sigma_{ij}^{(2)} = \frac{\varepsilon^2}{a^{(2,0)}}\left[-2\frac{\partial^2\rho}{\partial x_{\langle i}\partial x_{j\rangle}} - \left(2 - \frac{5a^{(2,1)}}{2\,\mathrm{Pr}}\right)\frac{\partial^2\theta}{\partial x_{\langle i}\partial x_{j\rangle}}\right],$$

where we can replace velocity and temperature gradients with $\sigma_{jk} \approx -2\varepsilon\frac{\partial v_{\langle j}}{\partial x_{k\rangle}}$ and $q_k \approx -\frac{5}{2\,\mathrm{Pr}}\varepsilon\frac{\partial\theta}{\partial x_k}$ to find

$$a^{(1,0)}\Delta q_i = -a^{(1,1)}\varepsilon\frac{\partial\sigma_{ik}}{\partial x_k} - \frac{5}{3\,\mathrm{Pr}}\varepsilon^2\frac{\partial^2 v_j}{\partial x_i\partial x_j},$$

(96)

$$a^{(2,0)}\Delta\sigma_{ij} = -2\varepsilon^2\frac{\partial^2\rho}{\partial x_{\langle i}\partial x_{j\rangle}} + \left(\frac{4\,\mathrm{Pr}}{5} - a^{(2,1)}\right)\varepsilon\frac{\partial q_{\langle i}}{\partial x_{j\rangle}}.$$

We now apply the time derivative and immediately replace the time derivative of stress and heat flux by the Grad equations (94) and the time derivative of velocity and density using the conservation laws of mass and momentum with $q_i \equiv 0$ and $\sigma_{ij} \equiv 0$ (Euler equations)

$$a^{(1,0)}\frac{\partial}{\partial t}\Delta q_i = a^{(1,1)}\frac{\partial}{\partial x_k}\left[a^{(2,1)}\varepsilon\frac{\partial q_{\langle i}}{\partial x_{k\rangle}} + a^{(2,0)}\Delta\sigma_{ik}\right] + \frac{5}{3\,\mathrm{Pr}}\varepsilon^2\frac{\partial^2}{\partial x_i\partial x_j}\frac{\partial\rho}{\partial x_j} + \frac{5}{3\,\mathrm{Pr}}\varepsilon^2\frac{\partial^2}{\partial x_i\partial x_j}\frac{\partial\theta}{\partial x_j},$$

(97)

$$a^{(2,0)}\frac{\partial}{\partial t}\Delta\sigma_{ij} = 2\varepsilon^2\frac{\partial^2}{\partial x_{\langle i}\partial x_{j\rangle}}\frac{\partial v_k}{\partial x_k} - \left(\frac{4\,\mathrm{Pr}}{5} - a^{(2,1)}\right)\varepsilon\frac{\partial}{\partial x_{\langle i}}\left[a^{(1,1)}\varepsilon\frac{\partial\sigma_{j\rangle k}}{\partial x_k} + a^{(1,0)}\Delta q_{j\rangle}\right].$$

After using the relation

$$\frac{\partial^2}{\partial x_i\partial x_j}\frac{\partial}{\partial x_j} = \frac{3}{2}\frac{\partial}{\partial x_j}\frac{\partial^2}{\partial x_{\langle i}\partial x_{j\rangle}}$$

(98)

in the last two terms of (97) we replace the temperature gradient by the heat flux as before and also realize that the density term can be eliminated by using the divergence of $(96)_2$. Similarly, the deviatoric gradient of $(96)_1$ yields an expression to eliminate the velocity term in (97). We finally find

$$a^{(1,0)}\frac{\partial}{\partial t}\Delta q_i = a^{(2,1)}\left(a^{(1,1)} - \frac{5}{4\,\mathrm{Pr}}\right)\varepsilon\frac{\partial}{\partial x_k}\frac{\partial q_{\langle i}}{\partial x_{k\rangle}} + a^{(2,0)}\left(a^{(1,1)} - \frac{5}{4\,\mathrm{Pr}}\right)\frac{\partial}{\partial x_k}\Delta\sigma_{ik},$$

(99)

$$a^{(2,0)}\frac{\partial}{\partial t}\Delta\sigma_{ij} = a^{(1,1)}\left(a^{(2,1)} - 2\,\mathrm{Pr}\right)\varepsilon\frac{\partial}{\partial x_{\langle i}}\frac{\partial\sigma_{j\rangle k}}{\partial x_k} + a^{(1,0)}\left(a^{(2,1)} - 2\,\mathrm{Pr}\right)\frac{\partial}{\partial x_{\langle i}}\Delta q_{j\rangle}.$$

Now we collect it all, and insert (94) and (99) into (93) to find

$$
\frac{\partial \tilde{w}_i^a}{\partial t} = \left[\vartheta_a - \eta_a \left[\frac{a^{(1,1)}}{a^{(1,0)}} - \frac{5}{4\,\mathrm{Pr}\,a^{(1,0)}} \right] \right] \left\{ a^{(2,1)} \varepsilon \frac{\partial}{\partial x_k} \frac{\partial q_{\langle i}}{\partial x_{k\rangle}} + a^{(2,0)} \frac{\partial}{\partial x_k} \left[\sigma_{ik} + 2\varepsilon \frac{\partial v_{\langle i}}{\partial x_{k\rangle}} \right] \right\},
$$

(100)

$$
\frac{\partial \tilde{w}_{ij}^a}{\partial t} = \left[\varphi_a + \phi_a \left[\frac{2\,\mathrm{Pr}}{a^{(2,0)}} - \frac{a^{(2,1)}}{a^{(2,0)}} \right] \right] \left\{ a^{(1,1)} \varepsilon \frac{\partial}{\partial x_{\langle i}} \frac{\partial \sigma_{j\rangle k}}{\partial x_k} + a^{(1,0)} \frac{\partial}{\partial x_{\langle i}} \left[q_{j\rangle} + \frac{5}{2\,\mathrm{Pr}} \varepsilon \frac{\partial \theta}{\partial x_{j\rangle}} \right] \right\}.
$$

These expressions will be used in (90) and (91) next.

4. The generalized R13 equations (linearized)

Combining the equations for σ_{ij} and q_i (90) and (91) with the just found expressions for the time derivatives (100), we finally find the generalized R13 equations (linearized) as (with $\frac{\partial}{\partial x_{\langle i}} \frac{\partial \sigma_{j\rangle k}}{\partial x_k} = \frac{5}{2} \frac{\partial}{\partial x_k} \frac{\partial \sigma_{\langle ij}}{\partial x_{k\rangle}} - \frac{5}{6} \frac{\partial^2 \sigma_{ij}}{\partial x_k \partial x_k}$)

$$
\frac{\partial q_i}{\partial t} + a^{(1,1)} \frac{\partial \sigma_{ik}}{\partial x_k} - a^{(1,2)} \frac{\partial}{\partial x_k} \left[\sigma_{ik} + 2\varepsilon \frac{\partial v_{\langle i}}{\partial x_{k\rangle}} \right] - a^{(1,3)} \varepsilon \frac{\partial}{\partial x_k} \frac{\partial q_{\langle i}}{\partial x_{k\rangle}} - a^{(1,4)} \varepsilon \frac{\partial}{\partial x_i} \frac{\partial q_k}{\partial x_k}
$$
$$
= -\frac{1}{\varepsilon} a^{(1,0)} \left[q_i + \frac{5}{2\,\mathrm{Pr}} \varepsilon \frac{\partial \theta}{\partial x_i} \right],
$$

(101)

$$
\frac{\partial \sigma_{ij}}{\partial t} + a^{(2,1)} \frac{\partial q_{\langle i}}{\partial x_{j\rangle}} - a^{(2,2)} \frac{\partial}{\partial x_{\langle i}} \left[q_{j\rangle} + \frac{5}{2\,\mathrm{Pr}} \varepsilon \frac{\partial \theta}{\partial x_{j\rangle}} \right] - a^{(2,3)} \varepsilon \frac{\partial}{\partial x_k} \frac{\partial \sigma_{\langle ij}}{\partial x_{k\rangle}} - a^{(2,4)} \varepsilon \frac{\partial^2 \sigma_{ij}}{\partial x_k \partial x_k}
$$
$$
= -\frac{1}{\varepsilon} a^{(2,0)} \left[\sigma_{ij} + 2\varepsilon \frac{\partial v_{\langle i}}{\partial x_{j\rangle}} \right].
$$

(102)

The coefficients in these equations must be computed from those defined earlier as

$$
a^{(1,2)} = \hat{a}^{(1,2)} + \frac{a^{(2,0)}}{2} \sum_{a,b=2}^{3} \tilde{\mathcal{C}}_{1b}^{(1)} \left[\tilde{\mathcal{D}}_{ba}^{(1)} \right]^{-1} \left[\vartheta_a - \eta_a \left[\frac{a^{(1,1)}}{a^{(1,0)}} - \frac{5}{4\,\mathrm{Pr}\,a^{(1,0)}} \right] \right],
$$

$$
a^{(1,3)} = \hat{a}^{(1,3)} + \frac{a^{(2,1)}}{2} \sum_{a,b=2}^{3} \tilde{\mathcal{C}}_{1b}^{(1)} \left[\tilde{\mathcal{D}}_{ba}^{(1)} \right]^{-1} \left[\vartheta_a - \eta_a \left[\frac{a^{(1,1)}}{a^{(1,0)}} - \frac{5}{4\,\mathrm{Pr}\,a^{(1,0)}} \right] \right],
$$

$$
a^{(1,4)} = \hat{a}^{(1,4)}
$$

$$
a^{(2,2)} = \hat{a}^{(2,2)} + a^{(1,0)} \sum_{a,b=2}^{3} \tilde{\mathcal{C}}_{1b}^{(2)} \left[\tilde{\mathcal{D}}_{ba}^{(2)} \right]^{-1} \left[\varphi_a + \phi_a \left[\frac{2\,\mathrm{Pr}}{a^{(2,0)}} - \frac{a^{(2,1)}}{a^{(2,0)}} \right] \right],
$$

$$
a^{(2,3)} = \hat{a}^{(2,3)} + \frac{5}{2} a^{(1,1)} \sum_{a,b=2}^{3} \tilde{\mathcal{C}}_{1b}^{(2)} \left[\tilde{\mathcal{D}}_{ba}^{(2)} \right]^{-1} \left[\varphi_a + \phi_a \left[\frac{2\,\mathrm{Pr}}{a^{(2,0)}} - \frac{a^{(2,1)}}{a^{(2,0)}} \right] \right],
$$

$$
a^{(2,4)} = \hat{a}^{(2,4)} - \frac{5}{6} a^{(1,1)} \sum_{a,b=2}^{3} \tilde{\mathcal{C}}_{1b}^{(2)} \left[\tilde{\mathcal{D}}_{ba}^{(2)} \right]^{-1} \left[\varphi_a + \phi_a \left[\frac{2\,\mathrm{Pr}}{a^{(2,0)}} - \frac{a^{(2,1)}}{a^{(2,0)}} \right] \right].
$$

The coefficients depend in particular on the molecular interaction potential through the production matrices $\mathcal{C}_{ab}^{(n)}$. The values for Maxwell molecules and hard sphere molecules were given in Table I.

5. Super-Burnett equations

The super-Burnett equations follow from the third order moment equations (101) and (102) just as the Burnett equations (83) follow from the second order moment equations (81). For this, we

insert the expansion,

$$\sigma_{ij} = \varepsilon\sigma_{ij}^{(1)} + \varepsilon^2\sigma_{ij}^{(2)} + \varepsilon^3\sigma_{ij}^{(3)}, \quad q_i = \varepsilon q_i^{(1)} + \varepsilon^2 q_i^{(2)} + \varepsilon^3 q_i^{(3)}, \tag{103}$$

and determine the expansion coefficients $\sigma_{ij}^{(\alpha)}$, $q_i^{(\alpha)}$ successively. Again, time derivatives must be replaced by means of the relevant equations.

To first and second order we obtain the already known Navier-Stokes-Fourier and Burnett expressions (29) and (83). The third order contributions are the (linear) super-Burnett contributions

$$q_i^{(3)} = -\theta_1^{sB}\frac{\partial^3\rho}{\partial x_i\partial x_k\partial x_k} - \theta_2^{sB}\frac{\partial^3\theta}{\partial x_k\partial x_k\partial x_i},$$

$$\tag{104}$$

$$\sigma_{ij}^{(3)} = \varpi_1^{sB}\frac{\partial^2}{\partial x_{\langle i}\partial x_{j\rangle}}\frac{\partial v_k}{\partial x_k} - \varpi_2^{sB}\frac{\partial^2}{\partial x_k\partial x_k}\frac{\partial v_{\langle i}}{\partial x_{j\rangle}}.$$

The super-Burnett coefficients depend on all coefficients appearing in the (3rd order) regularized 13 moment equations:

$$\theta_1^{sB} = \frac{1}{a^{(1,0)}}\left[\frac{5}{3\,\mathrm{Pr}}\frac{1}{a^{(1,0)}} - \frac{4}{3}\frac{a^{(1,1)}}{a^{(1,0)}} - \frac{4}{3}\frac{\left(a^{(1,1)} - a^{(1,2)}\right)}{a^{(2,0)}}\right],$$

$$\theta_2^{sB} = \frac{1}{a^{(1,0)}}\left[\frac{5}{3\,\mathrm{Pr}}\frac{1}{a^{(1,0)}} + \frac{5a^{(1,3)}}{3\,\mathrm{Pr}} + \frac{5}{2\,\mathrm{Pr}}a^{(1,4)} - \frac{4}{3}\frac{a^{(1,1)}}{a^{(1,0)}}\right.$$

$$\left. - \frac{25}{6\,\mathrm{Pr}^2} - \frac{2}{3}\frac{\left(a^{(1,1)} - a^{(1,2)}\right)}{a^{(2,0)}}\left(2 - \frac{5}{2\,\mathrm{Pr}}a^{(2,1)}\right)\right],$$

$$\tag{105}$$

$$\varpi_1^{sB} = \frac{1}{a^{(2,0)}}\left[\frac{2}{3} + \frac{5}{3\,\mathrm{Pr}}\frac{a^{(2,1)}}{a^{(2,0)}} + \left(\frac{5}{3\,\mathrm{Pr}} - \frac{a^{(1,1)}}{3}\right)\frac{\left(a^{(2,1)} - a^{(2,2)}\right)}{a^{(1,0)}} - \frac{10}{3}\frac{1}{a^{(2,0)}} - \frac{2}{15}a^{(2,3)}\right],$$

$$\varpi_2^{sB} = \frac{1}{a^{(2,0)}}\left[\frac{16}{15}a^{(2,3)} + \left(a^{(2,1)} - a^{(2,2)}\right)\frac{a^{(1,1)}}{a^{(1,0)}} - 2 - 2a^{(2,4)}\right].$$

The numerical values of the coefficients for hard spheres and Maxwell molecules were given in Table II.

VI. CONCLUSIONS

By means of the order of magnitude method we have derived the regularized 13 moment equations (R13 equations) for arbitrary molecular interaction potential, in the linear case. Specifically, we have used the Grad moment method to derive a large set of closed moment equations which we then combined and reduced based on the Knudsen number order of moments. The coefficients in the final R13 equations depend on the interaction potential. Their values for Maxwell molecules and the hard sphere gas show variation of up to ∼20% between the two models.

The linearized Burnett and super-Burnett equations are obtained by Chapman-Enskog expansion of the R13 equations. The Burnett and super-Burnett coefficients for Maxwell molecules, and the Burnett coefficients for hard spheres agree with established literature values. Super-Burnett coefficients for hard spheres were not reported before, due to the complexity of the derivation, which usually is based on the expansion of the Boltzmann equation. The present computation replaces the Boltzmann equation by a sufficiently large moment set which is reduced to the R13 equations before the expansion is performed. This method, a variant of the Reinecke-Kremer method, while still cumbersome, is far more accessible than the direct expansion of the kinetic equation. Also the Burnett and super-Burnett coefficients depend on interaction potential with variation of up to ∼20% between hard spheres and Maxwell molecules.

The emphasis of the paper is on the derivation of the equations by means of the order of magnitude method. Nevertheless, as an application we used moment equations and the Burnett-type

models to determine phase speed and damping for high frequency sound waves. In response to the variation of transport coefficients in the equations, the predictions of the models differ visibly for higher frequencies.

In future work we will derive boundary conditions for the regularized 13-moment equations specifically for hard sphere interactions. Solutions of a variety of boundary value problems, e.g., heat transfer, Couette, and Poiseuille flows, thermal transpiration flows will be possible and allow to study the influence of the interaction potential in detail.

[1] S. Chapman and T. G. Cowling, *The Mathematical Theory of Non-Uniform Gases* (Cambridge University Press, 1970).

[2] C. Cercignani, *Theory and Application of the Boltzmann Equation* (Scottish Academic Press, Edinburgh, 1975).

[3] H. Struchtrup, *Macroscopic Transport Equations for Rarefied Gas Flows—Approximation Methods in Kinetic Theory*, Interaction of Mechanics and Mathematics Series (Springer, Heidelberg, 2005).

[4] I. Müller and T. Ruggeri, *Rational Extended Thermodynamics*, Springer Tracts in Natural Philosophy Vol. 37 (Springer, New York, 1998).

[5] H. Struchtrup and M. Torrilhon, "Regularization of Grad's 13 moment equations: Derivation and linear analysis," Phys. Fluids **15**(9), 2668–2680 (2003).

[6] M. Torrilhon and H. Struchtrup, "Regularized 13-moment equations: Shock structure calculations and comparison to Burnett models," J. Fluid Mech. **513**, 171–198 (2004).

[7] H. Struchtrup, "Stable transport equations for rarefied gases at high orders in the Knudsen number," Phys. Fluids **16**(11), 3921–3934 (2004).

[8] H. Struchtrup, "Derivation of 13 moment equations for rarefied gas flow to second order accuracy for arbitrary interaction potentials," Multiscale Model. Simul. **3**(1), 221–243 (2005).

[9] M. Torrilhon and H. Struchtrup, "Boundary conditions for regularized 13-moment-equations for micro-channel-flows," J. Comput. Phys. **227**, 1982–2011 (2008).

[10] H. Grad, "On the kinetic theory of rarefied gases," Commun. Pure Appl. Math. **2**, 331–407 (1949).

[11] H. Grad, "Principles of the Kinetic Theory of Gases," in *Handbuch der Physik XII: Thermodynamik der Gase*, edited by S. Flügge (Springer, Berlin, 1958).

[12] X. J. Gu and D. R. Emerson, "A high-order moment approach for capturing non-equilibrium phenomena in the transition regime," J. Fluid Mech. **636**, 177–216 (2009).

[13] X. Gu and D. Emerson, "A computational strategy for the regularized 13 moment equations with enhanced wall-boundary conditions," J. Comput. Phys. **225**, 263–283 (2007).

[14] H. Struchtrup and M. Torrilhon, "Higher-order effects in rarefied channel flows," Phys. Rev. E **78**, 046301 (2008); Erratum: **78**, 069903 (2008).

[15] P. Taheri, M. Torrilhon, and H. Struchtrup, "Couette and Poiseuille flows in microchannels: Analytical solutions for regularized 13-moment equations," Phys. Fluids **21**, 017102 (2009).

[16] P. Taheri and H. Struchtrup, "Rarefaction effects in thermally-driven microflows," Physica A **389**, 3069–3080 (2010).

[17] P. Taheri and H. Struchtrup, "An extended macroscopic transport model for rarefied gas flows in long capillaries with circular cross section," Phys. Fluids **22**, 112004 (2010).

[18] H. Struchtrup and P. Taheri, "Macroscopic transport models for rarefied gas flows: A brief review," IMA J. Appl. Math. **76**(5), 672–697 (2011).

[19] H. Struchtrup, "Resonance in rarefied gases," Continuum Mech. Thermodyn. **24**, 361–376 (2012).

[20] D. Burnett, "The distribution of molecular velocities and the mean motion in a non-uniform gas," Proc. London Math. Soc. **s2-40**, 382–435 (1936).

[21] M. Sh. Shavaliyev, "Super-Burnett corrections to the stress tensor and the heat flux in a gas of Maxwellian molecules," J. Appl. Math. Mech. **57**(3), 573–576 (1993).

[22] S. Reinecke and G. M. Kremer, "A generalization of the Chapman-Enskog and Grad methods," Continuum Mech. Thermodyn. **3**, 155–167 (1991).

[23] S. Reinecke and G. M. Kremer, "Burnett's equations from a (13+9N)-field theory," Continuum Mech. Thermodyn. **8**, 121–130 (1996).

[24] A. V. Bobylev, "The Chapman-Enskog and Grad methods for solving the Boltzmann equation," Sov. Phys. Dokl. **27**, 29–31 (1982).

[25] P. Rosenau, "Extending hydrodynamics via the regularization of the Chapman-Enskog solution," Phys. Rev. A **40**, 7193–7196 (1989).

[26] A. V. Bobylev, "Instabilities in the Chapman-Enskog expansion and hyperbolic Burnett equations," J. Stat. Phys. **124**(2–4), 371–399 (2006).

[27] L. H. Söderholm, "Hybrid Burnett equations: A new method of stabilizing," Transp. Theory Stat. Phys. **36**, 495–512 (2007).

[28] A. V. Bobylev, "Boltzmann equation and hydrodynamics beyond the Navier Stokes level (Harold Grad Lecture)," in *Proceedings of 25th International RGD Symposium, St. Petersburg, Russia*, edited by M. S. Ivanov and A. K. Rebrov (Publishing House of the Siberian Branch of the Russian Academy of Science, Novosibirsk, 2007), pp. 3–12.

[29] A. V. Bobylev, "Generalized Burnett hydrodynamics," J. Stat. Phys. **132**, 569 (2008).

[30] M. Bisi, M. P. Cassinari, and M. Groppi, "Qualitative analysis of the generalized Burnett equations and applications to half space problems," Kinet. Relat. Models **1**, 295 (2008).

[31] A. V. Bobylev, M. Bisi, M. P. Cassinari, and G. Spiga, "Shock wave structure for generalized Burnett equations," Phys. Fluids **23**, 030607 (2011).

[32] A. V. Bobylev and A. Windfall, "Boltzmann equation and hydrodynamics at the Burnett level," Kinet. Relat. Models **5**, 237 (2012).

[33] H. Struchtrup and M. Torrilhon, "Regularized 13 moment equations for hard sphere molecules," AIP Conf. Proc. **1501**, 199–206 (2012).

[34] C. Truesdell and R. G. Muncaster, *Fundamentals of Maxwell's Kinetic Theory of a Simple Monatomic Gas* (Academic Press, New York, 1980).

[35] 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 systems," Phys. Rev. **94**, 511–525 (1954).

[36] L. H. Holway, "New statistical models for kinetic theory: Methods of construction," Phys. Fluids **9**, 1658–1673 (1966).

[37] E. M. Shakhov, "Generalization of the Krook kinetic relaxation equation," Fluid Dyn. (English translation of Izvestiya Akademii Nauk SSSR, Mekhanika Zhidkosti i Gaza) **3**, 95–96 (1968).

[38] H. Struchtrup, "Unique moment set from the order of magnitude method," Kinet. Relat. Models **5**, 417–440 (2012).

[39] E. Meyer and G. Sessler, "Schallausbreitung in Gasen bei hohen Frequenzen und sehr niedrigen Druecken," Z. Phys. **149**, 15–39 (1957).

[40] R. Schotter, "Rarefied acoustics in the noble gases," Phys. Fluids **17**, 1163–1168 (1974).

[41] M. Torrilhon, J. D. Au, and H. Struchtrup, "Explicit fluxes and productions for large systems of the moment method based on extended thermodynamics," Continuum Mech. Thermodyn. **15**(1), 97–111 (2003).

[42] V. Gupta and M. Torrilhon, "Automated Boltzmann collision integrals for moment equations," AIP Conf. Proc. **1501**, 67–74 (2012).