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Consistent, explicit, and accessible Boltzmann collision operator for polyatomic gases

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Based on a continuous internal energy state variable, we propose an explicit, fully nonlinear Boltzmann collision operator for the evolution of the distribution function describing a polyatomic gas with a constant heat capacity. The particle interaction is a polyatomic generalization of the variable hard-sphere model, used in a recent rigorous mathematical analysis, and includes frozen collisions. The model is consistent with the monatomic case and allows easy evaluations for moment equations and the Chapman-Enskog expansion. Using a publicly available computer algebra code we can explicitly compute nonlinear production terms for macroscopic systems of moments. The range of Prandtl number values recovers the Eucken formula for a specific choice of frozen collisions.

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I. INTRODUCTION

Nonequilibrium processes in gas flows are the focus of collisional kinetic theory and the Boltzmann equation [1]. They are relevant as soon as there are not enough gas particle collisions to maintain local equilibrium, and classical fluid dynamic models, such as the laws of Navier-Stokes and Fourier, lose validity. Insufficient collisions may occur either due to a microscopic or rarefied setting, typically characterized by a large Knudsen number, which is given by the ratio between the mean free path and an observation length scale. The Boltzmann equation is known to describe the whole regime of the Knudsen number, but also serves as the starting point to derive improved continuum models [2]. While originally derived and studied for the description of monatomic gas particle collisions, nowadays the proper modeling of collisions of polyatomic particles is a highly active field of research [3–5], especially because it is highly relevant in applications to step out from the monatomic framework.

The aim of this paper is to establish a concrete binary collision model for the Boltzmann equation describing a single polyatomic gas which is explicit and consistent with the monatomic case and to provide an easy evaluation technique of the collision operator based on polynomial expansions. For simplicity, we restrict this paper to polyatomic gases with constant heat capacity, in the literature known also as polytropic or calorically perfect gases [6].

We choose to work in the so-called continuous internal energy approach investigated in Refs. [7–9], which is more accessible mathematically and computationally than the semiclassical approach [3,4,10], yet reproduces physical requirements. The accessibility of the continuous model comes from the Borgnakke-Larsen procedure [11], used to parametrize the collision process. One of the main improvements in this paper is the inclusion of frozen collisions in a consistent way into a complete collision operator. Frozen collisions do not change the internal energies of the particles and, as a consequence, the Borgnakke-Larsen procedure is not applicable. Such a consideration is often the basis for Bhatnagar-Gross-Krook (BGK) relaxation operators [12,13]. For the complete polyatomic collision operator we propose a convex combination of frozen and purely polyatomic (nonfrozen) collisions. We also impose consistency conditions for the collision frequency, which leads to the proper monatomic limit of the model, by extending the approach of Ref. [14] written in the BGK context. Moreover, our approach uses recent mathematical results [15] for the transition probabilities of the collisions which also ensures mathematical well-posedness of the collision operator. We enrich this transition probability with a set of parameters that can successfully model physical properties, as, for instance, they allow us to match the temperature dependence of viscosity and, at the same time, offer a wide range for the Prandtl number that includes the Eucken formula. To facilitate the practical use of this operator, we also provide a computer algebra code [16] for its explicit evaluation.

II. POLYATOMIC COLLISIONS

A. Distribution function

Next to the particle velocity $\boldsymbol{c} \in \mathbb{R}^3$, we use an internal state variable $J \in \mathbb{R}^+$ such that for the internal energy $I \in \mathbb{R}^+$ of a particle we have $I = I_0(J/J_0)^{2/\delta}$ with a constant degeneracy level δ, related to the internal degrees of freedom or the adiabatic coefficient γ through [7,9,12]

$$\gamma = \frac{5+\delta}{3+\delta}, \tag{1}$$

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and a reference internal phase space volume J_0 with energy I_0. We can work with either a distribution function $g \geqslant 0$ defined on the phase space $(\boldsymbol{c}, J)$ or with a distribution $f \geqslant 0$ defined on $(\boldsymbol{c}, I)$ such that

$$g(\boldsymbol{x}, t, \boldsymbol{c}, J) d\boldsymbol{c} dJ = f(\boldsymbol{x}, t, \boldsymbol{c}, I) d\boldsymbol{c} dI \tag{2}$$

is the number density of particles at space point $\boldsymbol{x}$ and time t with velocity $\boldsymbol{c}$ and internal state J, or internal energy I, respectively. Similarly as in Ref. [17], the phase space can be redefined from $(\boldsymbol{c}, J)$ to $(\boldsymbol{c}, I)$ and vice versa, such that

$$d\boldsymbol{c} dJ = \varphi(I) d\boldsymbol{c} dI \quad \text{with} \quad \varphi(I) = \frac{J_0}{I_0^{\delta/2}} \frac{\delta}{2} I^{\frac{\delta}{2}-1}, \tag{3}$$

which together with (2) yields

$$f(\boldsymbol{c}, I) = \varphi(I) g(\boldsymbol{c}, J(I)). \tag{4}$$

Accordingly, we will use I and J in an essentially equivalent manner.

With the peculiar velocity $\boldsymbol{C} = \boldsymbol{c} - \boldsymbol{v}$ based on the fluid velocity $\boldsymbol{v}$, we define temperature θ (in units of specific energy) through the energy density

$$\rho \frac{3+\delta}{2} \theta = \iint_{\mathbb{R}^3 \times \mathbb{R}^+} \left(\frac{m}{2} C^2 + I \right) f d\boldsymbol{c} dI, \tag{5}$$

which gives the adiabatic coefficient (1) and the equilibrium distribution

$$f_{\mathrm{eq}}(\boldsymbol{c}, I) = \frac{\frac{\rho}{m} I^{\frac{\delta}{2}-1} e^{-\frac{\frac{m}{2}C^2 + I}{m\theta}}}{(2\pi\theta)^{3/2} (m\theta)^{\delta/2} \Gamma(\frac{\delta}{2})}. \tag{6}$$

This can be written as $g_{\mathrm{eq}}(\boldsymbol{c}, J)$ using (4). In the monatomic limit $\delta \to 0$ the distribution f_{eq} becomes a Dirac function at $I \to 0$, while g_{eq} gives nonzero only for values of $J < J_0$. Consequently, all particles are placed in an internal state within $0 \leqslant J < J_0$ and will have zero internal energy, because $(J/J_0)^{2/\delta} \to 0$.

For future reference we also define

$$\rho \frac{3}{2} \theta_{\mathrm{tr}} = \int \frac{m}{2} C^2 f d\boldsymbol{c} dI, \qquad \rho \frac{\delta}{2} \theta_{\mathrm{int}} = \int I f d\boldsymbol{c} dI \tag{7}$$

as the translational and internal temperature. Additionally, we define a dynamic pressure by

$$\Pi = \rho(\theta_{\mathrm{tr}} - \theta) = -\frac{\delta}{3} \rho(\theta_{\mathrm{int}} - \theta) = \frac{\delta}{\delta+3} \rho(\theta_{\mathrm{tr}} - \theta_{\mathrm{int}}), \tag{8}$$

which vanishes in equilibrium, where we have $\theta_{\mathrm{tr}} = \theta_{\mathrm{int}} = \theta$.

B. Polyatomic collision operator and its weak form

In a binary collision the states $(\boldsymbol{c}, I)$ and $(\boldsymbol{c}_\star, I_\star)$ of two particles are converted to postcollisional states $(\boldsymbol{c}', I')$ and $(\boldsymbol{c}'_\star, I'_\star)$ under the constraint of the conservation laws of momentum and total (translational+internal) energy. The collision is parametrized using the Borgnakke-Larsen procedure [11], which is based on the repartition of the total energy $E = \frac{m}{4}|\boldsymbol{u}|^2 + I + I_\star$ in the center-of-mass reference frame defined by $\boldsymbol{u} = \boldsymbol{c} - \boldsymbol{c}_\star$ and $\boldsymbol{h} = (\boldsymbol{c} + \boldsymbol{c}_\star)/2$, and performed using the collision parameters $\boldsymbol{\sigma} \in \mathcal{S}^2$ (unit sphere in $\mathbb{R}^3$) and $(r, R) \in [0, 1]^2$, such that

$$\begin{aligned} \boldsymbol{c}' &= \boldsymbol{h} + \frac{|\boldsymbol{u}'|}{2} \boldsymbol{\sigma}, \quad \boldsymbol{c}'_\star = \boldsymbol{h} - \frac{|\boldsymbol{u}'|}{2} \boldsymbol{\sigma}, \\ \frac{m}{4} |\boldsymbol{u}'|^2 &= RE, \\ I' &= r(1-R)E, \quad I'_\star = (1-r)(1-R)E. \end{aligned} \tag{9}$$

Note that in this setting, the scattering angle χ satisfies

$$\cos \chi = \frac{\boldsymbol{\sigma} \cdot \boldsymbol{u}}{|\boldsymbol{u}|}. \tag{10}$$

The corresponding Boltzmann equation has its easiest form in the state phase space $(\boldsymbol{c}, J)$,

$$\partial_t g + c_i \partial_{x_i} g = \widetilde{Q}(g, g), \tag{11}$$

where the operator reads

$$\begin{aligned} &\widetilde{Q}(g, g)(x, t, \boldsymbol{c}, J) \\ &= \underset{\substack{(\boldsymbol{c}_\star, J_\star) \in \mathbb{R}^3 \times \mathbb{R}^+ \\ (\boldsymbol{\sigma}, r, R) \in \mathcal{S}^2 \times [0,1]^2}}{\int \cdots \int} (g' g'_\star - g g_\star) B \, d\boldsymbol{\sigma} dr dR d\boldsymbol{c}_\star dJ_\star, \end{aligned} \tag{12}$$

with the usual notation for pre- and postcollisional evaluations, e.g., $g' := g(\boldsymbol{x}, t, \boldsymbol{c}', \boldsymbol{J}')$, and a transition probability $B := B(\boldsymbol{c}, \boldsymbol{c}_\star, I(J), I_\star(J_*), r, R, \boldsymbol{\sigma}) \geqslant 0$ supposed to satisfy microreversibility assumptions to be explained below. In the energy phase space, the Boltzmann equation is based on f and uses a transformed operator $Q(f, f)$ which is based on a different measure according to (4),

$$\begin{aligned} Q(f, f)(\boldsymbol{x}, t, \boldsymbol{c}, I) &= \widetilde{Q}(g, g)(x, t, \boldsymbol{c}, J) \varphi(I) \\ &= \int \cdots \int_{\Omega_c} \left(f' f'_\star \frac{\varphi \varphi_\star}{\varphi' \varphi'_\star} - f f_\star \right) \\ &\quad \times B \, d\boldsymbol{\sigma} dr dR d\boldsymbol{c}_\star dI_\star. \end{aligned} \tag{13}$$

Here, we abbreviated the integral limits that have been used in (12) by Ω_c.

To derive the conservative weak form of the collision operator we consider the transformation of precollisional variables $(\boldsymbol{\sigma}, \boldsymbol{c}_\star, \boldsymbol{c}, r, R, J_\star, J)$ into a postcollisional state $(\boldsymbol{\sigma}', \boldsymbol{c}'_\star, \boldsymbol{c}', r', R', J'_\star, J')$ by using (9) and the additional definitions

$$R' = \frac{m}{4E} |\boldsymbol{u}|^2, \quad r' = \frac{I}{I + I_\star}, \quad \boldsymbol{\sigma}' = \frac{\boldsymbol{u}}{|\boldsymbol{u}|}. \tag{14}$$

The measure $d\boldsymbol{\sigma} dr dR d\boldsymbol{c}_\star dJ_\star d\boldsymbol{c} dJ$ on the complete domain of definition $\Omega = \mathbb{R}^3 \times \mathbb{R}^+ \times \Omega_c$ of the integrand of $\tilde{Q}(g, g)$ becomes invariant when multiplied with the function

$$H_\delta(r, R) := [r(1-r)]^{\frac{\delta}{2}-1} (1-R)^{\delta-1} R^{1/2}. \tag{15}$$

If the transition probability $B := B(\boldsymbol{c}, \boldsymbol{c}_\star, I, I_*, r, R, \boldsymbol{\sigma})$ in (13) satisfies the microreversibility according to

$$B'/H'_\delta = B/H_\delta, \tag{16}$$

it will be possible that the microscopic conservation properties of the collisions imply conservation laws of the Boltzmann collision operator. In fact, we can transform the weak form of the collision operator (12) for a test function $\psi(\boldsymbol{c}, J)$, namely

$$Q^{(\psi)} = \int \cdots \int_{\Omega} \psi(\boldsymbol{c}, J)\tilde{Q}(g, g) d\boldsymbol{c} dJ, \tag{17}$$

into the conservative form

$$Q^{(\psi)} = \int \cdots \int_{\Omega} (\psi - \psi') f f_{\star} B \, d\boldsymbol{\sigma} dr dR d\boldsymbol{c}_{\star} dI_{\star} d\boldsymbol{c} dI, \tag{18}$$

where we switched to the energy-based formulation by replacing $g dJ = f dI$ and $g_{\star} dJ_{\star} = f_{\star} dI_{\star}$. The conservative weak form ensures that the operator (12) satisfies conservation laws and the H theorem [18] consistent with the microscopic collision laws and implies the equilibrium distribution (6), which is independent of the underlying phase space. It is also a building block for the collision operator evaluation to be presented in Sec. III.

C. Consistency

Because the microreversibility is different, it is impossible to choose a simple model for the transition probability B as in the monatomic case [10]. Additionally, we also require that the results of the collision operator reduce to the monatomic case for the limit $\delta \to 0$. We first construct a consistent ansatz by matching the collision frequencies. A concrete model will be formulated in Sec. II F.

Following the microreversibility (16) we will use the ansatz

$$B = K_{\delta} H_{\delta}(r, R) \hat{B} \tag{19}$$

with a yet to be specified invariant part satisfying $\hat{B} = \hat{B}'$. The prefactor K_{δ} will be used to achieve consistency for the simplest invariant expression $\hat{B} = \hat{B}^{(0)} = \text{const.}$ In particular, this transition probability has no dependency on relative velocity, as Maxwell molecules, defined as the monatomic-gas interaction potential $1/r^{s-1}$ with $s = 5$ and yielding $\partial_{|\boldsymbol{u}|} B = 0$, and also no dependence on the scattering angle (10), as a variable-hard-sphere model $\partial_{\chi} B = 0$. In the present setting, we require that the total collision frequency

$$\nu_{\text{tot}} = \frac{m}{\rho} \int \cdots \int_{\Omega} f f_{\star} B \, d\boldsymbol{\sigma} dr dR d\boldsymbol{c}_{\star} dI_{\star} d\boldsymbol{c} dI \tag{20}$$

matches the monatomic value $\nu_{\text{tot}} = \frac{\rho}{m} \hat{B}^{(0)}$. We obtain

$$\nu_{\text{tot}} = \frac{\rho}{m} \hat{B}^{(0)} \iint_{(r,R) \in [0,1]^2} K_{\delta} H_{\delta}(r, R) dr dR, \tag{21}$$

where for consistency we set the integral to unity, yielding the constant K_{δ} in the form

$$K_{\delta} = \frac{2\Gamma\left(\delta + \frac{3}{2}\right)}{\sqrt{\pi}\, \Gamma\left(\frac{\delta}{2}\right)^2}. \tag{22}$$

We will see below that this gives consistency also for more general transition probabilities. Note that Ref. [18] also integrates out the energies of the collision partners in the transition probability in order to arrive at a consistent total cross section.

D. Frozen internal states

Inspired by typical relaxation models [19,20], we assume that a fraction of collisions will not change the internal energy, i.e., $I' = I$ and $I'_{\star} = I_{\star}$, which implies nonchanging internal states and consequently $|\boldsymbol{u}'| = |\boldsymbol{u}|$. In this case, the Borgnakke-Larsen procedure cannot be applied and the usual parametrization with the direction $\boldsymbol{\sigma} \in \mathcal{S}^2$ is used instead,

$$\boldsymbol{c}' = \boldsymbol{h} + \frac{|\boldsymbol{u}|}{2}\boldsymbol{\sigma}, \quad \boldsymbol{c}'_{\star} = \boldsymbol{h} - \frac{|\boldsymbol{u}|}{2}\boldsymbol{\sigma}. \tag{23}$$

The resulting collision operator would have the form

$$\begin{aligned} &Q^{(\text{frozen})}(f, f)(\boldsymbol{x}, t, \boldsymbol{c}, I) \\ &\quad = \int \ldots \int_{\substack{(\boldsymbol{c}_{\star}, I_{\star}) \in \mathbb{R}^3 \times \mathbb{R}^+ \\ \boldsymbol{\sigma} \in \mathcal{S}^2}} \left(f' f'_{\star}\big|_{\substack{I' = I \\ I'_{\star} = I_{\star}}} - f f_{\star} \right) \overline{B} \, d\boldsymbol{\sigma} d\boldsymbol{c}_{\star} dI_{\star}, \end{aligned} \tag{24}$$

where $\overline{B} := \overline{B}(\boldsymbol{c}, \boldsymbol{c}_{\star}, I, I_{\star}, \boldsymbol{\sigma})$ is the transition probability for a frozen collision, that satisfies monatomiclike microreversibility, i.e., $\overline{B}(\boldsymbol{c}, \boldsymbol{c}_{\star}, I, I_{\star}, \boldsymbol{\sigma}) = \overline{B}(\boldsymbol{c}', \boldsymbol{c}'_{\star}, I, I_{\star}, \boldsymbol{\sigma}') = \overline{B}(\boldsymbol{c}_{\star}, \boldsymbol{c}, I_{\star}, I, -\boldsymbol{\sigma})$.

A frozen collision is also equivalent to choosing the parameter values $r = r'$ and $R = R'$ with the definitions (14) as can be seen from (9). Hence, this can be included into the full operator (13) by replacing the transition probability B by

$$B^{(\text{frozen})}(\boldsymbol{c}, \boldsymbol{c}_{\star}, I, I_{\star}, r, R, \boldsymbol{\sigma}) = \overline{B}\, \delta_{r-r'} \delta_{R-R'}, \tag{25}$$

with Dirac δ functions at zero, such that the procedure (9) reduces to the frozen case. For a constant $\overline{B} = \overline{B}^{(0)}$ the total collision frequency now reduces to $\nu^{(\text{frozen})} = \frac{\rho}{m} \overline{B}^{(0)}$ which is also consistent with the monatomic case.

E. The Boltzmann equation

For the evolution of the distribution function $f := f(\boldsymbol{x}, t, \boldsymbol{c}, I) \geqslant 0$ defined in the phase space $d\boldsymbol{c} dI$ describing a polyatomic gas, we propose the following Boltzmann equation,

$$\partial_t f + c_i \partial_{x_i} f = \omega Q(f, f) + (1 - \omega) Q^{(\text{frozen})}(f, f), \tag{26}$$

where the collision operator convexly combines the pure polyatomic operator (13) and the frozen one (24) with a weight $0 \leqslant \omega \leqslant 1$.

Alternatively, one may view the Boltzmann equation (26) as the usual polyatomic one (13) with the transition probability

$$B = \omega K_{\delta} H(r, R) \hat{B} + (1 - \omega) \delta_{r-r'} \delta_{R-R'} \overline{B} \tag{27}$$

that encompasses a nonfrozen and frozen transition probability.

F. Collision model

Mathematical analysis reveals that only very few, specific functional dependences of the transition probability will yield well-posedness of the resulting Boltzmann equation with a pure polyatomic operator. Recent results [9,15] rely on the multiplicative splitting

$$B = b(\cos\chi) \tilde{B}(|\boldsymbol{u}|, I, I_{\star}, r, R), \tag{28}$$

where the function b takes care of the dependency on the scattering angle (10) and $\tilde{B}$ includes the influence of translational and internal energy of the collision. For the energy part it is known that a standard variable-hard-sphere ansatz proportional to $|\boldsymbol{u}|^\zeta$ is insufficient to match experimental data [21] and does not satisfy the assumptions from the mathematical analysis [15]. A mathematically feasible dependency of the transition probability is E^ζ with the total energy of the collision E, however, this model does not show enough flexibility in terms of free parameters. An additive combination of relative speed and internal energy is possible [15] as a geometric means of pre- and postcollisional quantities scaled by total energy E. We suggest to use the dependency

$$B_{\zeta,\eta} = b(\cos\chi)\left(\frac{|\boldsymbol{u}'|^\zeta|\boldsymbol{u}|^\zeta}{(\frac{4}{m}E)^{\zeta/2}} + \eta\frac{(I'I)^{\zeta/2} + (I'_\star I_\star)^{\zeta/2}}{(mE)^{\zeta/2}}\right) \tag{29}$$

with the constant parameters $\zeta \geqslant 0$ and $\eta \geqslant 0$, and $|\boldsymbol{u}'|, I', I'_*$ from (9). The contributions from internal energies are scaled such that $\eta = 1$ resembles a splitting of the total energy, but other values of $\eta \geqslant 0$ are also allowed, according to (16).

In this paper, we propose to use (29) both as the nonfrozen probability $\hat{B}$ and frozen probability $\overline{B}$ in (27), with the same exponent ζ but different parameters η and η_f such that we have

$$B = \omega K_\delta H(r,R)B_{\zeta,\eta} + (1-\omega)\delta_{r-r'}\delta_{R-R'}B_{\zeta,\eta_\mathrm{f}}\big|_{\substack{I'=I\\ I'_\star = I_\star}} \tag{30}$$

with a weight $0 \leqslant \omega \leqslant 1$. The dimensionless parameters $\eta \geqslant 0$ and $\eta_\mathrm{f} \geqslant 0$ control the influence of the internal energies, while the exponent ζ will determine the temperature dependency of viscosity. The function b is assumed to be constant in this paper, i.e., we set

$$b(\cos\chi) = \mathcal{B} = \mathrm{const}, \tag{31}$$

following the variable-hard-sphere (VHS) model [19]. The factor $\mathcal{B}$ is constant but with the dimension $\frac{\text{volume}}{\text{time}\times\text{velocity}^\zeta}$. Using a reference temperature θ_R and density ρ_R we can define a reference collision frequency $\nu_\mathrm{R} = (\rho_\mathrm{R}/m)\theta_\mathrm{R}^{\zeta/2}\mathcal{B}$ of the polyatomic VHS gas (pVHS). Note that due to consistency, the limit $\delta \to 0$ of the weak form (18) will result in the weak form of a monatomic VHS gas with $B = \mathcal{B}|\boldsymbol{u}|^\zeta$ independently of the values of ω, η, and η_f.

III. EVALUATION

A. Distribution expansion

The evaluation of the collision operator will be conducted in the energy phase space. We assume a polynomial expansion [20,22,23] of order M based on scaled variables $\boldsymbol{\xi} = \boldsymbol{C}/\theta^{1/2}$ and $\iota = I/(m\theta)$ and write

$$f_M(\boldsymbol{c}, I)d\boldsymbol{c}dI = \sum_{\beta=0}^{M} w_\beta\phi_\beta(\boldsymbol{\xi},\iota)f_0(\boldsymbol{\xi},\iota)d\boldsymbol{\xi}d\iota, \tag{32}$$

with

$$f_0(\boldsymbol{\xi},\iota) = \frac{\frac{\rho}{m}}{(2\pi)^{3/2}\Gamma\left(\frac{\delta}{2}\right)}\iota^{\frac{\delta}{2}-1}e^{-\frac{1}{2}\xi^2-\iota} \tag{33}$$

the scaled local equilibrium distribution as the kernel. The coefficients w_α follow from projections with suitable dual polynomials ψ_α,

$$w_\alpha = \iint_{\mathbb{R}^3\times\mathbb{R}^+}\psi_\alpha(\boldsymbol{\xi},\iota)f_M d\boldsymbol{c}dI, \tag{34}$$

which can be related to classical moments. Using $\psi := \psi_\alpha$ in (18) the weak form can be written

$$Q^{(\psi_\alpha)} = \sum_{\beta_1,\beta_2} Q^{(\alpha)}_{\beta_1\beta_2}w_{\beta_1}w_{\beta_2}, \tag{35}$$

with coefficients

$$Q^{(\alpha)}_{\beta_1\beta_2} = \int\cdots\int_\Omega(\psi_\alpha - \psi'_\alpha)\frac{1}{2}(\phi_{\beta_1}\phi^\star_{\beta_2} + \phi_{\beta_2}\phi^\star_{\beta_1}) \times f_0 f_0^\star B\, d(\boldsymbol{\sigma}, r, R, \boldsymbol{\xi}_\star, \iota_\star)d\boldsymbol{\xi}d\iota. \tag{36}$$

The evaluation of this integral is easily accessible by computer algebra software and we provide a publicly available straightforward implementation [16,24].

B. Example production terms

We choose polynomials in (32) that represent the gas variables density ρ, velocity v_i, and total temperature θ, as well as dynamic pressure Π, deviatoric stress tensor σ_{ij}, translational heat flux q_i, and internal heat flux s_i (see also Refs. [12,25]).

When restricted to these variables, the projection over velocity-internal energy space $\mathbb{R}^3 \times \mathbb{R}^+$ of the homogeneous Boltzmann equation with a quadratic collision operator can be written in tensor notation as

$$\partial_t\Pi = -\nu\left(P^{(0)}_\Pi\Pi + P^{(1)}_\Pi\frac{\Pi\,\Pi}{\rho\theta} + P^{(2)}_\Pi\frac{\sigma_{ij}\sigma_{ij}}{\rho\theta} + P^{(3)}_\Pi\frac{q_iq_i}{\rho\theta^2} + P^{(4)}_\Pi\frac{s_is_i}{\rho\theta^2} + P^{(5)}_\Pi\frac{q_is_i}{\rho\theta^2}\right), \tag{37}$$

$$\partial_t\sigma_{ij} = -\nu\left(P^{(0)}_\sigma\sigma_{ij} + P^{(1)}_\sigma\frac{\Pi\sigma_{ij}}{\rho\theta} + P^{(2)}_\sigma\frac{\sigma_{k\langle i}\sigma_{j\rangle k}}{\rho\theta} + P^{(3)}_\sigma\frac{q_{\langle i}q_{j\rangle}}{\rho\theta^2} + P^{(4)}_\sigma\frac{s_{\langle i}s_{j\rangle}}{\rho\theta^2} + P^{(5)}_\sigma\frac{q_{\langle i}s_{j\rangle}}{\rho\theta^2}\right), \tag{38}$$

$$\partial_t q_i = -\nu\left(P^{(0)}_q q_i + P^{(1)}_q s_i + P^{(2)}_q\frac{\Pi q_i}{\rho\theta} + P^{(3)}_q\frac{\Pi s_i}{\rho\theta} + P^{(4)}_q\frac{\sigma_{ij}q_j}{\rho\theta} + P^{(5)}_q\frac{\sigma_{ij}s_j}{\rho\theta}\right), \tag{39}$$

$$\partial_t s_i = -\nu\left(P^{(0)}_s s_i + P^{(1)}_s q_i + P^{(2)}_s\frac{\Pi s_i}{\rho\theta} + P^{(3)}_s\frac{\Pi q_i}{\rho\theta} + P^{(4)}_s\frac{\sigma_{ij}s_j}{\rho\theta} + P^{(5)}_s\frac{\sigma_{ij}q_j}{\rho\theta}\right), \tag{40}$$

where we suppressed the conservation laws and introduced the collision frequency $\nu = \nu_\mathrm{R}(\rho/\rho_\mathrm{R})(\theta/\theta_\mathrm{R})^{\zeta/2} = (\rho/m)\theta^{\zeta/2}\mathcal{B}$. Note that angle brackets $\langle\cdot,\cdot\rangle$ around the indices indicate a symmetric, trace-free tensor [20]. The 24 coefficients can be easily computed using the code in Ref. [16] and the pVHS model (30) with (29). Note that for the monatomic limit $\delta \to 0$, we find for the coefficients of stress and translational

TABLE I. Coefficients for nonlinear production terms in (37)–(40) evaluated for a pVHS gas with $\delta = 2$ and viscosity exponent $r_{\text{visc}} = 0.75$ ($\zeta = 1/2$) corresponding to nitrogen.

$P_\Pi^{(0)}$	$\frac{717}{649}\eta\omega + \frac{929}{876}\omega$
$P_\Pi^{(1)}$	$\frac{149}{1124}\omega - \frac{383}{1981}\eta\omega$
$P_\Pi^{(2)}$	$\frac{7}{990}\omega$
$P_\Pi^{(3)}$	$\frac{3}{943}\omega$
$P_\Pi^{(4)}$	0
$P_\Pi^{(5)}$	$-\frac{5}{943}\omega$
$P_\sigma^{(0)}$	$\frac{478}{649}\eta\omega + \frac{395}{569}\eta_{\text{f}}(1-\omega) - \frac{183}{1463}\omega + 1$
$P_\sigma^{(1)}$	$-\frac{286}{2071}\eta\omega - \frac{220}{857}\eta_{\text{f}}(1-\omega) - \frac{121}{1010}\omega + \frac{11}{48}$
$P_\sigma^{(2)}$	$-\frac{7}{484}\eta_{\text{f}}(1-\omega) - \frac{13}{794}\omega + \frac{1}{21}$
$P_\sigma^{(3)}$	$-\frac{3}{922}\eta_{\text{f}}(1-\omega) - \frac{5}{1204}\omega + \frac{3}{280}$
$P_\sigma^{(4)}$	$\frac{11}{1638}\eta_{\text{f}}(1-\omega) + \frac{5}{672}\omega - \frac{5}{672}$
$P_\sigma^{(5)}$	$\frac{1}{922}\eta_{\text{f}}(1-\omega) + \frac{1}{280}\omega - \frac{1}{280}$
$P_q^{(0)}$	$\frac{1154}{1343}\eta\omega + \frac{367}{793}\eta_{\text{f}}(1-\omega) + \frac{319}{1181}\omega + \frac{2}{3}$
$P_q^{(1)}$	$-\frac{659}{1193}\eta\omega - \frac{631}{1190}\omega$
$P_q^{(2)}$	$-\frac{324}{2011}\eta\omega - \frac{97}{706}\eta_{\text{f}}(1-\omega) + \frac{25}{322}\omega + \frac{1}{24}$
$P_q^{(3)}$	$\frac{29}{540}\eta\omega - \frac{188}{821}\eta_{\text{f}}(1-\omega) - \frac{119}{1300}\omega + \frac{5}{72}$
$P_q^{(4)}$	$-\frac{18}{889}\eta_{\text{f}}(1-\omega) - \frac{47}{1065}\omega + \frac{1}{15}$
$P_q^{(5)}$	$-\frac{23}{1499}\eta\omega + \frac{79}{1725}\eta_{\text{f}}(1-\omega) + \frac{32}{551}\omega - \frac{1}{72}$
$P_s^{(0)}$	$\frac{1241}{1049}\eta\omega + \frac{279}{305}\eta_{\text{f}}(1-\omega) + \frac{57}{181}\omega + \frac{115}{144}$
$P_s^{(1)}$	$-\frac{213}{964}\eta\omega - \frac{298}{1405}\omega$
$P_s^{(2)}$	$-\frac{109}{877}\eta\omega - \frac{39}{955}\eta_{\text{f}}(1-\omega) - \frac{35}{792}\omega + \frac{371}{2365}$
$P_s^{(3)}$	$\frac{29}{700}\eta\omega - \frac{16}{653}\eta_{\text{f}}(1-\omega) - \frac{191}{1801}\omega + \frac{253}{2688}$
$P_s^{(4)}$	$\frac{29}{1050}\eta\omega - \frac{9}{551}\eta_{\text{f}}(1-\omega) - \frac{39\omega}{788} + \frac{63}{1004}$
$P_s^{(5)}$	$\frac{12}{943}\omega$

heat flux,

$$\lim_{\delta\to 0} P_\sigma^{(0)} = \sqrt{\pi}\frac{2^{\zeta+4}}{15}\Gamma\left(\frac{\zeta+7}{2}\right), \tag{41}$$

$$\lim_{\delta\to 0} P_q^{(0)} = \sqrt{\pi}\frac{2^{\zeta+5}}{45}\Gamma\left(\frac{\zeta+7}{2}\right), \tag{42}$$

for any values of ω, η, and η_{f}, which are the expressions obtained for a monatomic VHS gas [19,20]. Expressions consistent with the monatomic case also hold for all other coefficients.

Table I displays the form of the coefficients for the specific gas $\delta = 2$ and $\zeta = 1/2$ in an exemplary way. The parameter choice corresponds to nitrogen N_2 in the temperature range of approximately 293–373 K [22]. In the table, the dependency on the parameters ω, η, and η_{f} is explicit, while generally real valued coefficients are approximated by rationals with accuracy 10^{-6}. Also the values are scaled such that $P_\sigma^{(0)} = 1$ when $\omega = 0$ and $\eta_{\text{f}} = 0$. We can observe that the production for dynamic pressure vanishes in the frozen case, $\omega = 0$, as well as the linear cross-coupling terms for the heat fluxes, which is independent of the choice of the transition probability (29). The influence of the internal heat flux on stress vanishes in the completely nonfrozen case, $\omega = 1$.

C. Prandtl number

The explicit form of the production terms allows to conduct the first iteration of the Chapman-Enskog expansion [22,26]. The transport terms for (37)–(40) have been presented elsewhere [6,23]. We only consider the linear, leading-order terms of the transfer equations for the stress tensor,

$$2\rho\theta\partial_{\langle i}v_{j\rangle} = -\nu P_\sigma^{(0)}\sigma_{ij}, \tag{43}$$

and for translational and internal heat fluxes,

$$\frac{5}{2}\rho\theta\partial_i\theta = -\nu\big(P_q^{(0)}q_i + P_q^{(1)}s_i\big), \tag{44}$$

$$\frac{\delta}{2}\rho\theta\partial_i\theta = -\nu\big(P_s^{(0)}s_i + P_s^{(1)}q_i\big), \tag{45}$$

and compute for the stress tensor and total heat flux $q_i^{(\text{tot})} = q_i + s_i$,

$$\sigma_{ij} = -2\frac{\rho\theta}{\nu}\frac{1}{P_\sigma^{(0)}}\partial_{\langle i}v_{j\rangle}, \tag{46}$$

$$q_i^{(\text{tot})} = -\frac{\rho\theta}{\nu}\frac{5\big(P_s^{(0)} - P_s^{(1)}\big) + \delta\big(P_q^{(0)} - P_q^{(1)}\big)}{2\big(P_q^{(0)}P_s^{(0)} - P_q^{(1)}P_s^{(1)}\big)}\partial_i\theta, \tag{47}$$

as a first-order contribution. From these we readily identify the transport coefficients of viscosity μ and heat conductivity κ which depend only on temperature as $\mu, \kappa \sim \theta^{r_{\text{visc}}}$ with an exponent of $r_{\text{visc}} = 1 - \zeta/2$. We find for the Prandtl number [20]

$$\text{Pr} = \frac{(5+\delta)\mu}{2\kappa} \tag{48}$$

$$= \frac{(5+\delta)\big(P_q^{(0)}P_s^{(0)} - P_q^{(1)}P_s^{(1)}\big)}{\big[5\big(P_s^{(0)} - P_s^{(1)}\big) + \delta\big(P_q^{(0)} - P_q^{(1)}\big)\big]P_\sigma^{(0)}}, \tag{49}$$

which depends on the model parameters ω, η, and η_{f}, as well as internal energy degeneracy δ and exponent ζ. Note that fixing Pr still leaves freedom in the choice of those parameters. We also remark that due to consistency, we obtain $\text{Pr} = 2/3$ in the monatomic limit $\delta \to 0$.

The formula of Eucken [4,20] for the Prandtl number has been derived originally in Ref. [27] based on plausible heuristics related to frozen collisions and constant transition probabilities. The result reads

$$\text{Pr} = \frac{2(\delta+5)}{2\delta+15}, \tag{50}$$

which also reduces to the monatomic case when $\delta \to 0$. In agreement with the assumptions of Eucken, the Prandtl number (49) of the pVHS model reduces exactly to the Eucken expression, if we restrict the collisions to the frozen case $\omega = 0$ with a reduced influence of the internal energies $\eta_{\text{f}} = 0$ as well as choosing the exponent $\zeta = 0$. This finding clarifies the restricted validity of the Eucken formula.

In fact, for a general exponent ζ the reduced frozen case $\omega = \eta_{\text{f}} = 0$ gives

$$\text{Pr}^{(\text{frozen})} = \frac{2(\delta+5)}{\delta\big(2+\frac{4}{5}\zeta\big)\frac{2\zeta+2\delta+7}{\zeta+2\delta+7} + 15}, \tag{51}$$

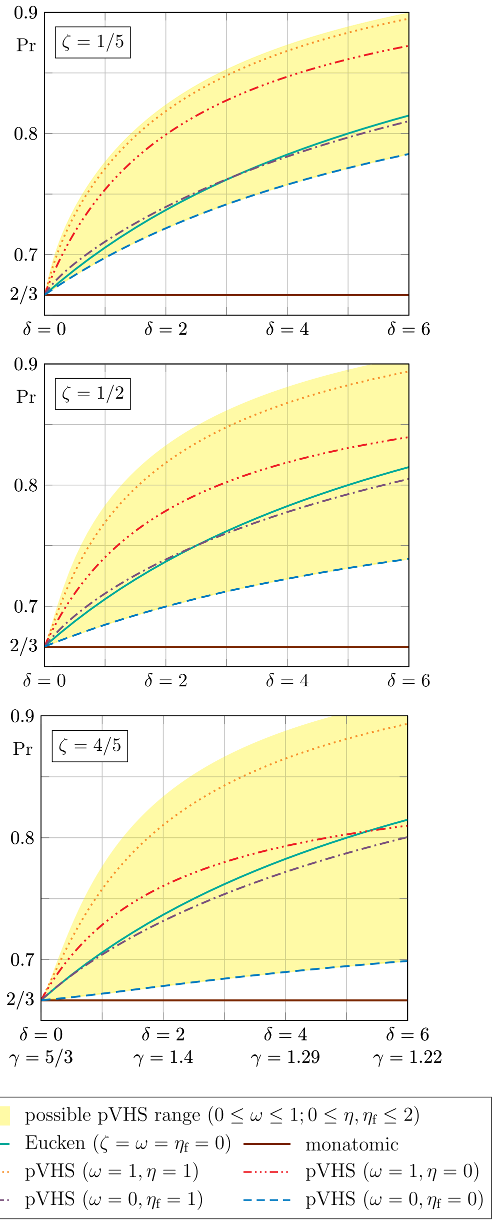

FIG. 1. Possible Prandtl numbers for pVHS gases with different adiabatic coefficients γ for three fixed viscosity exponents, namely $\zeta = 1/5, 1/2, 4/5$, corresponding to $r_{\text{visc}} = 0.9, 0.75, 0.6$, respectively. For a specific gas, the value of ζ would be fixed by the temperature dependence of the viscosity, and the value of δ follows from the adiabatic coefficient. The Prandtl number can then be adjusted by the parameters ω, η, η_f. Here, several choices are possible and the pVHS model allows us to match additional physical properties.

which can be viewed as a generalization of the formula by Eucken to particle models with nonconstant dependence on the relative velocity in the transition probability, $\zeta \geqslant 0$, hence, viscosity exponents $r_{\text{visc}} \leqslant 1$.

However, formula (51) is still restricted and could be varied further by choosing different values for $0 \leqslant \omega \leqslant 1$, η, $\eta_f \geqslant 0$. In particular, the combination of frozen and nonfrozen collisions in the pVHS model allows us to construct many other values for Pr. To demonstrate the wealth of the modeling flexibility of the pVHS model we display the range of the Prandtl number for specific cases of $\zeta = 1/5, 1/2, 4/5$ when varying the parameters $0 \leqslant \omega \leqslant 1$, $0 \leqslant \eta, \eta_f \leqslant 2$ as the yellow background in Fig. 1. Table I is based on the exponent $\zeta = 1/2$ and the curves in Fig. 1 can be obtained from the expressions in the table and (49). The values of the Eucken formula (50) are displayed as a solid green curve to demonstrate the difference from expression (51), shown as a dashed blue curve ($\omega = 0$, $\eta_f = 0$) in the plot. The nonfrozen part of the model tends to give values greater than Eucken, while the frozen part produces smaller values for Pr.

D. Discussion and outlook

The presented results open many possibilities for further investigations. The explicit and accessible nature of the collision operator allows us to compute transport coefficients and moment equations in order to increase the predictivity of polyatomic gas flow models especially in the rarefied or microscopic regime [5,9,12]. Its flexibility, due to a set of model parameters such as $\mathcal{B}$, ω, η, η_f, permits the additional matching of gas properties, such as relaxation times and collision frequencies, beyond the Prandtl number. The collision operator can also be used as a basis to derive, validate, and improve BGK models [13] for polyatomic gases.

The collision model itself may be further refined. It is straightforward to include a nonconstant scattering angle dependency for the transition probability and, hence, use more realistic interaction potentials. Additionally, the averaging between frozen and nonfrozen collisions could be temperature dependent, allowing additional flexibility to adjust to the experimental data. Similarly, the internal degrees of freedom δ could be chosen to depend on temperature or relative velocity, which would model a nonpolytropic gas character.

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