JM PAPERS

Time-dependent regularised 13-moment equations with Onsager boundary conditions in the linear regime

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We develop the time-dependent regularised 13-moment equations for general elastic collision models under the linear regime. Detailed derivation shows the proposed equations have super-Burnett order for small Knudsen numbers, and the moment equations enjoy a symmetric structure. A new modification of Onsager boundary conditions is proposed to ensure stability as well as the removal of undesired boundary layers. Numerical examples of one-dimensional channel flows is conducted to verified our model.

Key words: kinetic theory, boundary layer control

1. Introduction

The study of rarefied gas dynamics has evolved over more than a century, where kinetic theory is crucial for accurately describing its fluid mechanics via a microscopic explanation for macroscopic behaviour. The fundamental equation of the kinetic theory, the Boltzmann equation, provides a detailed statistical description of the gas dynamics. The development of Boltzmann solvers has progressed significantly in Bhatnagar, Gross & Krook (1954); Bird (1970); Mieussens (2000); Dimarco & Pareschi (2014); Gamba *et al.* (2017); Dimarco *et al.* (2018); Alekseenko, Martin & Wood (2022); Cai *et al.* (2024*a*), nevertheless, accurately solving the Boltzmann equation for practical problems remains a complex and resource-intensive task mainly due to its high-dimensionality, nonlinear collisions and complex boundary conditions.

Instead of directly solving the Boltzmann equation, many researchers focus on the macroscopic moments of the distribution function and modify classical fluid equations, such as the Navier–Stokes equations, to describe the mechanics of moderately rarefied gases. Two classical techniques used to derive higher-order (in terms of Knudsen number) macroscopic fluid equations from the Boltzmann equation are the Grad's moment method in Grad (1949) and the Chapman–Enskog expansion in Chapman & Cowling (1970). Despite their successes in capturing near-equilibrium effects, the Grad's 13-moment equations may experience a loss of hyperbolicity and unphysical subshocks. Moreover, the second-order Burnett and third-order super-Burnett equations, which are derived from the Chapman–Enskog expansion, suffer from instability. Recent research addresses these limitations by employing various regularisation techniques (Jin & Slemrod 2001; Müller *et al.* 2003; Struchtrup & Torrilhon 2003; Bobylev 2006; Öttinger 2010; Han *et al.* 2019) to enhance the accuracy and stability of the methods across a broader range of rarefied gas dynamics. Besides the regularisation by the above two classical techniques, researchers have also explored alternative ways to address their limitations and derive higher-order equations such as the Onsager-consistent approaches (Agrawal, Kushwaha & Jadhav 2019; Jadhav, Yadav & Agrawal 2023).

In this work we investigate the regularised version of Grad's 13-moment equations proposed in Struchtrup & Torrilhon (2003), which can be interpreted as a Chapman–Enskog-like procedure applied to the Grad's 13 moments. This regularisation, abbreviated as R13, has been developed for both Maxwell (Struchtrup 2005*b*) and non-Maxwell molecules (Struchtrup & Torrilhon 2013; Cai & Wang 2020) and validated across diverse applications (Taheri & Bahrami 2012; Rana, Mohammadzadeh & Struchtrup 2015; Timokhin *et al.* 2017). The R13 equations are attractive since the equations include only second-order derivatives while attaining the super-Burnett order. Here the super-Burnett order means that the super-Burnett equations, which are the result of the Chapman–Enskog expansion up to the third order, can be derived from the R13 equations. Note that the original super-Burnett equations contain fourth-order derivatives, causing significant difficulties in the numerical discretisation and formulation of boundary conditions. Due to the inclusion of corrections from higher-order moments through terms derived from the Chapman–Enskog expansion, the R13 equations can describe various rarefaction effects such as Knudsen boundary layers and heat fluxes from cold areas to hot areas (Rana, Torrilhon & Struchtrup 2013). Also, the R13 equations are equipped with reliable boundary conditions (Torrilhon & Struchtrup 2008; Struchtrup *et al.* 2017) and have been shown to be robust in numerical simulations (Rana *et al.* 2013). Recently in Torrilhon & Sarna (2017), Onsager boundary conditions are proposed to ensure the stability of boundary value problems of linear R13 equations for Maxwell molecules. However, it is not straightforward to generalise these Onsager boundary conditions to non-Maxwell molecules, even in the linear case. The main reason is the loss of a symmetric structure required by the Onsager boundary conditions (see Öttner *et al.* (2023)). To remedy this, in Cai *et al.* (2024*b*), the linear R13 equations for arbitrary elastic collision models were rederived using a different method. The new derivation relies on the simpler form of the Chapman–Enskog expansion for steady-state equations compared with the time-dependent case, so that it cannot be applied directly to dynamic problems.

The purpose of this work is to seek possibilities to generalise the Onsager boundary conditions to time-dependent R13 equations in the linear regime. This also requires new derivations of R13 equations based on the linearised Boltzmann equation for the distribution function f,

$$\frac{\partial f}{\partial t} + \xi_k \frac{\partial f}{\partial x_k} = \frac{1}{Kn} \mathcal{L} f, \tag{1.1}$$

where $\mathcal{L}$ is a self-adjoint negative semidefinite linear operator; x_k and ξ_k are position and velocity variables, respectively; Kn is the Knudsen number defined as the ratio of the mean free path of the molecules to macroscopic length scale. Note that here we have used the summation convention: when the same index appears twice, it is assumed that the sum applied for this index and the range is from 1–3. Due to the linearisation, the model is mainly applicable for fluids with low speeds such as microflows, and numerical experiments show good agreement with results obtained from the direct simulation Monte-Carlo (DSMC) method (see Wu, Reese & Zhang 2014). In order that the Onsager boundary conditions can be applied, the linear moment equations should take the form

$$\mathbf{A}_0 \frac{\partial \boldsymbol{u}}{\partial t} + \mathbf{A}_k \frac{\partial \boldsymbol{u}}{\partial x_k} = \frac{1}{Kn} \mathbf{L} \boldsymbol{u}, \qquad (1.2)$$

where $\mathbf{A}_0$ is the symmetric mass matrix, $\mathbf{A}_k$ is the symmetric discretisation of operator ξ_k and $\mathbf{L}$ is the discretisation of operator $\mathcal{L}$ that is symmetric negative semidefinite. The matrix $\mathbf{A}_0$ is allowed to have zero eigenvalues to cover the parabolic scenarios such as the linearised R13 equations, which has been used to study phenomena including evaporation Claydon *et al.* (2017) and rarefied effects in flows around a sphere Beckmann *et al.* (2018). It should be noted that the symmetric structure in the above matrices plays a key role in obtaining the second law of thermodynamics for our moment equations. The similar idea of maintaining symmetry to comply with thermodynamics has also been applied to the derivation of other moment equations (Singh & Agrawal 2016; Yadav, Jonnalagadda & Agrawal 2023).

When considering thermodynamics of (1.2) within a bounded domain Ω, the entropy production from its boundary should be taken into account. This can be seen by multiplying $\boldsymbol{u}^\intercal$ on (1.2) and integrating over Ω, yielding

$$\frac{\mathrm{d}}{\mathrm{d}t} \int_\Omega \frac{1}{2} \boldsymbol{u}^\intercal \mathbf{A}_0 \boldsymbol{u} \mathrm{d}\boldsymbol{x} + \int_{\partial\Omega} \frac{1}{2} \boldsymbol{u}^\intercal \mathbf{A}_k n_k \boldsymbol{u} \mathrm{d}s = \frac{1}{Kn} \int_\Omega \boldsymbol{u}^\intercal \mathbf{L} \boldsymbol{u} \mathrm{d}\boldsymbol{x} \leqslant 0, \qquad (1.3)$$

where $\boldsymbol{n} = (n_1, n_2, n_3)^\intercal$ denotes the outward normal vector at boundary $\partial\Omega$. Hence, the second law of thermodynamics can be achieved if the flux across the boundary is bounded, i.e.

$$-\boldsymbol{u}^\intercal n_k \mathbf{A}_k \boldsymbol{u} \leqslant \boldsymbol{g}_{ext}^\intercal \mathbf{M} \boldsymbol{g}_{ext} \qquad (1.4)$$

for a given matrix $\mathbf{M}$ and an external source vector $\boldsymbol{g}_{ext} = \boldsymbol{g}_{ext}(t, \boldsymbol{x})$ from boundary conditions. With the above entropic stability, the uniqueness of the solution of (1.2) can be achieved.

The stable boundary conditions are studied in Sarna & Torrilhon (2018) and the authors therein propose a specific form of boundary conditions that fulfils (1.4), which is called the Onsager boundary conditions. To specify these boundary conditions, we can introduce an orthogonal matrix $\mathbf{P}$ that decomposes moments $\boldsymbol{u}$ into two subsets $\boldsymbol{u}_{odd}$ and $\boldsymbol{u}_{even}$ as

$$\mathbf{P}\boldsymbol{u} = \begin{pmatrix} \boldsymbol{u}_{odd} \\ \boldsymbol{u}_{even} \end{pmatrix}, \qquad \mathbf{P} n_k \mathbf{A}_k \mathbf{P}^\intercal = \begin{pmatrix} 0 & \mathbf{A}_{oe} \\ \mathbf{A}_{eo} & 0 \end{pmatrix}. \qquad (1.5)$$

The odd moments $\boldsymbol{u}_{odd}$ consist of quantities that change sign when the normal vector $\boldsymbol{n}$ is flipped, while the even moments $\boldsymbol{u}_{even}$ remain unchanged by this flipping. For example, the normal velocity, shear stress and normal heat flux belong to $\boldsymbol{u}_{odd}$, whereas the density, temperature and tangential velocity belong to $\boldsymbol{u}_{even}$. The anti-diagonal block structure of the matrix in (1.5) is due to the fact that the normal flux of an odd moment corresponds to an even moment, and conversely, the normal flux of an even moment corresponds to

an odd moment. The symmetricity of $\mathbf{A}_k$ implies that the matrix in (1.5) is symmetric and, therefore, $\mathbf{A}_{eo} = \mathbf{A}_{oe}^{\mathsf{T}}$. The Onsager boundary conditions in Sarna & Torrilhon (2018) suggest that, for a full row rank $\mathbf{A}_{oe}$, the following form of boundary conditions

$$\boldsymbol{u}_{odd} = \mathbf{Q}\mathbf{A}_{oe}(\boldsymbol{g}_{ext} - \boldsymbol{u}_{even}), \tag{1.6}$$

with matrix $\mathbf{Q}$ being negative semidefinite, yield (1.4) and, therefore, L^2 stability is obtained. However, as shown in Cai *et al.* (2024*b*), for general collision models, the matrix $\mathbf{A}_{oe}$ can be rank deficient, which requires an extra step that reduces the number of boundary conditions to the rank of $\mathbf{A}_{oe}$. Such a technique is also required in this work.

Two major difficulties were encountered when we tried to derive time-dependent linear R13 equations for general collision models. The first is to obtain the form (1.2) while maintaining the super-Burnett order. To achieve this, instead of the classical approach that uses the stress tensor and the heat flux in the equations, we change them to new variables that better match the order of magnitude method. Such an approach can lead to both the desired order of accuracy and the desired structure of equations, so that the technique introduced in Öttinger *et al.* (2023) and tweaked in Cai *et al.* (2024*b*) can be employed to derive the Onsager boundary conditions. However, the solution exhibits unphysical boundary layers, giving us a second major difficulty in deriving the new model. To address this problem, we revise the original boundary conditions by enforcing equalities setting the coefficients of these boundary layers to zero. Both steady-state and unsteady examples are presented to show the solutions of these new equations.

The rest of this paper is organised as follows. Our linearisation and non-dimensionalisation of the Boltzmann equation and moment equations are introduced in § 2. Section 3 introduces the variables and then shows our main results including the explicit expressions of linear R13 equations with boundary conditions for general elastic collision models. The derivation of R13 equations is given in § 4, where we also demonstrate the super-Burnett order of the model. In § 5 we formulate the boundary conditions, analyse the boundary layers and remove the unwanted layers by fixing the boundary conditions. One-dimensional examples are shown in § 6 to validate our models. We conclude our paper with a brief summary in § 7.

2. Linearisation and non-dimensionalisation

All the derivations in this work will be established on dimensionless and linearised equations. In this section we state our approaches to both linearisation and non-dimensionalisation. Note that each dimensionless variable in this section will be labelled by adding a hat '$\hat{\ }$' on top of the symbol denoting the variable, while such accents will be removed for convenience in other sections.

2.1. *Linearisation and non-dimensionalisation of the Boltzmann equation*

In the original Boltzmann equation, the distribution function $f(\boldsymbol{x}, \boldsymbol{\xi}, t)$ satisfies the following integro-differential equation:

$$\frac{\partial f}{\partial t} + \xi_k \frac{\partial f}{\partial x_k} = Q[f, f] := \int_{\mathbb{R}^3} \int_{\mathbb{S}^2} B(\boldsymbol{\xi} - \boldsymbol{\xi}_1, \boldsymbol{\omega})[f(\boldsymbol{\xi}_1')f(\boldsymbol{\xi}') - f(\boldsymbol{\xi}_1)f(\boldsymbol{\xi})] \, \mathrm{d}\boldsymbol{\omega} \, \mathrm{d}\boldsymbol{\xi}_1. \tag{2.1}$$

Here $B(\cdot, \cdot)$ stands for the collision kernel, and

$$\boldsymbol{\xi}' = \frac{\boldsymbol{\xi} + \boldsymbol{\xi}_1}{2} + \frac{|\boldsymbol{\xi} - \boldsymbol{\xi}_1|}{2}\boldsymbol{\omega}, \qquad \boldsymbol{\xi}_1' = \frac{\boldsymbol{\xi} + \boldsymbol{\xi}_1}{2} - \frac{|\boldsymbol{\xi} - \boldsymbol{\xi}_1|}{2}\boldsymbol{\omega}. \tag{2.2}$$

In this work we are interested in the linear regime where the distribution function is close to a global Maxwellian with density ρ_0, velocity $\boldsymbol{v}_0$, temperature θ_0 and mass of a single molecule m:

$$\mathcal{M}_0(\boldsymbol{\xi}) = \frac{\rho_0}{m(2\pi\theta_0)^{3/2}} \exp\left(-\frac{|\boldsymbol{\xi} - \boldsymbol{v}_0|^2}{2\theta_0}\right). \tag{2.3}$$

We can then introduce a small quantity ϵ and write the distribution function f as

$$f(\boldsymbol{x}, \boldsymbol{\xi}, t) = \mathcal{M}_0(\boldsymbol{\xi})[1 + \epsilon \hat{f}(\hat{\boldsymbol{x}}, \hat{\boldsymbol{\xi}}, \hat{t})], \tag{2.4}$$

where $\hat{\boldsymbol{x}}, \hat{\boldsymbol{\xi}}$ and $\hat{t}$ are dimensionless variables defined by

$$\hat{\boldsymbol{x}} = (\boldsymbol{x} - \boldsymbol{v}_0 t)/L, \qquad \hat{\boldsymbol{\xi}} = (\boldsymbol{\xi} - \boldsymbol{v}_0)/\sqrt{\theta_0}, \qquad \hat{t} = t/(L/\sqrt{\theta_0}). \tag{2.5}$$

Plugging (2.4) into the Boltzmann equation yields

$$\frac{\partial \hat{f}}{\partial \hat{t}} + \hat{\xi}_k \frac{\partial \hat{f}}{\partial \hat{x}_k} = \frac{\rho_0 L}{m\sqrt{\theta_0}} \frac{\mathcal{Q}[\hat{\mathcal{M}}_0, \hat{f}\hat{\mathcal{M}}_0] + \mathcal{Q}[\hat{f}\hat{\mathcal{M}}_0, \hat{\mathcal{M}}_0] + \epsilon \mathcal{Q}[\hat{f}\hat{\mathcal{M}}_0, \hat{f}\hat{\mathcal{M}}_0]}{\hat{\mathcal{M}}_0}, \tag{2.6}$$

where $\hat{\mathcal{M}}_0$ is the dimensionless Maxwellian distribution function

$$\hat{\mathcal{M}}_0(\hat{\boldsymbol{\xi}}) = \frac{1}{(2\pi)^{3/2}} \exp\left(-\frac{|\hat{\boldsymbol{\xi}}|^2}{2}\right). \tag{2.7}$$

The linearised equation can then be obtained by discarding the $O(\epsilon)$ term in (2.6) and defining

$$\hat{\mathcal{L}}[\hat{f}] := \frac{\mathcal{Q}[\hat{\mathcal{M}}_0, \hat{f}\hat{\mathcal{M}}_0] + \mathcal{Q}[\hat{f}\hat{\mathcal{M}}_0, \hat{\mathcal{M}}_0]}{B_0 \hat{\mathcal{M}}_0}, \qquad Kn = \frac{mB_0\sqrt{\theta_0}}{\rho_0 L}. \tag{2.8}$$

Here B_0 is a constant with the same dimension as the collision kernel $B(\cdot, \cdot)$ to guarantee that $\hat{\mathcal{L}}$ is dimensionless, and here we choose B_0 such that

$$\langle \hat{\xi}_1 \hat{\xi}_2, \hat{\mathcal{L}}(\hat{\xi}_1 \hat{\xi}_2) \rangle = -1, \tag{2.9}$$

where the inner product is defined by

$$\langle \hat{f}, \hat{g} \rangle = \int_{\mathbb{R}^3} \hat{f}(\hat{\boldsymbol{\xi}}) \hat{g}(\hat{\boldsymbol{\xi}}) \hat{\mathcal{M}}_0(\hat{\boldsymbol{\xi}}) \, d\hat{\boldsymbol{\xi}}. \tag{2.10}$$

Note that the linearised Boltzmann equation satisfies the linearised H-theorem. In the original Boltzmann equation (2.1), the entropy density and the entropy flux are defined by

$$\eta = -k_B \int_{\mathbb{R}^3} f \log f \, d\boldsymbol{\xi}, \qquad \psi_k = -k_B \int_{\mathbb{R}^3} \xi_k f \log f \, d\boldsymbol{\xi}, \tag{2.11}$$

which satisfy the inequality

$$\frac{\partial \eta}{\partial t} + \frac{\partial \psi_k}{\partial x_k} \geqslant 0, \tag{2.12}$$

indicating the second law of thermodynamics. For the linearised Boltzmann equation, the corresponding definitions are

$$\hat{\eta} = -\int_{\mathbb{R}^3} |\hat{f}|^2 \, d\hat{\boldsymbol{\xi}}, \qquad \hat{\psi}_k = -\int_{\mathbb{R}^3} \xi_k |\hat{f}|^2 \, d\hat{\boldsymbol{\xi}}. \tag{2.13}$$

Since the linearised collision operator $\hat{\mathcal{L}}$ satisfies $\langle \hat{f}, \hat{\mathcal{L}}[\hat{f}] \rangle \leqslant 0$ for any $\hat{f}$, the H-theorem turns out to be the L^2 stability of the linearised Boltzmann equation

$$\frac{\partial \hat{\eta}}{\partial \hat{t}} + \frac{\partial \hat{\psi}_k}{\partial \hat{x}_k} \geqslant 0. \tag{2.14}$$

Later in our derivation of moment equations, this property will be preserved.

2.2. *Linearisation and non-dimensionalisation of the conservation laws*

The laws of mass, momentum and energy conservation can be derived by taking moments of the Boltzmann equation, which yields

$$\frac{\partial \rho}{\partial t} + \frac{\partial (\rho v_j)}{\partial x_j} = 0,$$

$$\frac{\partial (\rho v_i)}{\partial t} + \frac{\partial}{\partial x_j} (\rho v_i v_j + \rho \theta \delta_{ij} + \sigma_{ij}) = 0,$$

$$\frac{\partial}{\partial t} \left(\frac{1}{2} \rho v_i v_i + \frac{3}{2} \rho \theta \right) + \frac{\partial}{\partial x_j} \left(\frac{5}{2} \rho \theta v_j + \frac{1}{2} \rho v_i v_i v_j + \sigma_{ij} v_i + q_j \right) = 0. \tag{2.15}$$

Here σ_{ij} denotes the stress tensor and q_j denotes the heat flux. To linearise these equations, we again assume that the fluid state is close to the equilibrium specified by density ρ_0, velocity $v_{0,i}$ and temperature θ_0, and introduce dimensionless variables $\hat{\rho}$, $\hat{\theta}$, $\hat{v}_i$, $\hat{\sigma}_{ij}$ and $\hat{q}_i$ by

$$\rho = \rho_0 (1 + \epsilon \hat{\rho}), \ \theta = \theta_0 (1 + \epsilon \hat{\theta}), \ v_i = v_{0,i} + \epsilon \sqrt{\theta_0} \hat{v}_i, \ \sigma_{ij} = \epsilon \rho_0 \theta_0 \hat{\sigma}_{ij}, \ q_i = \epsilon \rho_0 \theta_0^{3/2} \hat{q}_i. \tag{2.16}$$

By substituting the above expressions together with (2.5) into the conservation laws, and then dropping all the higher-order terms, we reach the linearised and dimensionless conservation laws:

$$\frac{\partial \hat{\rho}}{\partial \hat{t}} + \frac{\partial \hat{v}_j}{\partial \hat{x}_j} = 0,$$

$$\frac{\partial \hat{v}_i}{\partial \hat{t}} + \frac{\partial \hat{\rho}}{\partial \hat{x}_i} + \frac{\partial \hat{\theta}}{\partial \hat{x}_i} + \frac{\partial \hat{\sigma}_{ij}}{\partial \hat{x}_j} = 0, \tag{2.17}$$

$$\frac{\partial \hat{\theta}}{\partial \hat{t}} + \frac{2}{3} \frac{\partial \hat{v}_j}{\partial \hat{x}_j} + \frac{2}{3} \frac{\partial \hat{q}_j}{\partial \hat{x}_j} = 0.$$

Another approach to derive the same equations is to directly take moments of the linearised Boltzmann equation. The relationship between the dimensionless moments ($\hat{\rho}$, $\hat{\theta}$, etc.) and the dimensionless distribution function $\hat{f}$ is

$$\hat{\rho} = \langle 1, \hat{f} \rangle, \quad \hat{v}_i = \langle \hat{\xi}_i, \hat{f} \rangle, \quad \hat{\theta} = \left\langle \frac{1}{3} |\hat{\boldsymbol{\xi}}|^2 - 1, \hat{f} \right\rangle,$$

$$\hat{\sigma}_{ij} = \left\langle \hat{\xi}_i \hat{\xi}_j - \frac{1}{3} |\hat{\boldsymbol{\xi}}|^2 \delta_{ij}, \hat{f} \right\rangle, \qquad \hat{q}_i = \left\langle \frac{1}{2} |\hat{\boldsymbol{\xi}}|^2 \hat{\xi}_i, \hat{f} \right\rangle. \tag{2.18}$$

Thus, using the fact that $\langle 1, \hat{\mathcal{L}}[\hat{f}] \rangle = \langle \hat{\xi}_i, \hat{\mathcal{L}}[\hat{f}] \rangle = \langle |\hat{\boldsymbol{\xi}}|^2, \hat{\mathcal{L}}[\hat{f}] \rangle = 0$, one can take the inner product of the linearised equation (1.1) and the polynomials 1, $\hat{\xi}_i$ and $|\hat{\boldsymbol{\xi}}|^2$ to obtain the moment equations (2.17).

The two methods to formulate the conservation laws are essentially equivalent, since taking moments and linearising equations are two commutable operations. In our derivation of moment equations to be presented below, we follow the second approach that takes moments of the linearised equations (1.1). Due to the presence of $\hat{\sigma}_{ij}$ and $\hat{q}_i$ in (2.17), our purpose is to find a suitable closure that provides decent approximation to the linearised Boltzmann equation when the Knudsen number Kn is small. Hereafter, the accent ' $\hat{\cdot}$ ' will no longer be added to dimensionless variables.

3. Linear R13 equations

Here we present the final form of the R13 equations with wall boundary conditions, which is the main conclusion of this paper. Since our selection of the 13 moments is slightly different from classical literature, we introduce our choice of variables before listing out the equations.

3.1. *Choice of variables*

The 13-moment equations were first proposed by Grad (1949), where the distribution function was expanded into an infinite series using Hermite polynomials. The coefficients of the polynomials were regarded as moments, and Grad chose to include the first 13 moments, namely the density (ρ), momentum (ρv_i), pressure ($\rho\theta$), stress tensor (σ_{ij}) and heat flux (q_i), into his equations. In later developments of 13-moment systems, such a choice of the 13 moments becomes a standard and is followed by most works (Myong 1999; Struchtrup & Torrilhon 2003; Zhu *et al.* 2015). In particular, for the regularised 13-moment equations for Maxwell molecules, such a choice of moments matches exactly with the analysis using the order of magnitude method (Struchtrup(2005*b*, Chapter 8). It is seen that for linear equations, these moments, denoted by $\langle \phi_{13}, f \rangle$ with ϕ_{13} being a 13-dimensional vector of polynomials of $\boldsymbol{\xi}$, fully describes the distribution function f up to order $O(Kn)$, which means for any polynomial $r(\boldsymbol{\xi})$ satisfying $\langle \phi_{13}, r \rangle = 0$, the moment $\langle r, f \rangle$ has at least order $O(Kn^2)$ when performing asymptotic analysis. This property leads to the super-Burnett order of R13 equations for Maxwell molecules, meaning that the super-Burnett equations can be derived from the R13 equations by Chapman–Enskog expansion. However, it is also known that this no longer holds for other types of molecules (Struchtrup 2005*a*). Inspired by this fact, in our study of 13-moment equations for general gas molecules, we adopt a different set of variables $\langle \tilde{\phi}_{13}, f \rangle$, such that we can again obtain $\langle r, f \rangle \sim o(Kn)$ once $\langle \tilde{\phi}_{13}, r \rangle = 0$. This will help achieve the super-Burnett order for the moment equations.

The details on the construction of $\tilde{\phi}_{13}$ will be discussed in § 4. Here we only provide some brief information necessary for the formulation of the moment equations. Our 13 moments also include conservative quantities such as the density (ρ), velocity (v_i) and temperature (θ). Note that the velocity and the temperature are conservative only under linear settings. For the remaining 8 moments, they also include a trace-free 2-tensor and a vector like in the classical case. For consistency, we denote the 2-tensor by $\bar{\sigma}_{ij}$ and the vector by $\bar{q}_i$. The relationship between these variables and the stress tensor (σ_{ij}) and the heat flux (q_i) will be given later in this section. The conservative variables ρ, v_i and θ are $O(Kn^0)$ moments, while the higher-order moments $\bar{\sigma}_{ij}$ and $\bar{q}_i$ are $O(Kn)$ moments. Note that the conservative moments are always defined using the distribution function f by

$$(\rho, v_i, \theta) = \left\langle \left(1, \xi_i, \frac{1}{3}\xi_k\xi_k\right), f \right\rangle, \tag{3.1}$$

where the definitions of $\bar{\sigma}_{ij}$ and $\bar{q}_i$ depend on the collision model. When Maxwell molecules are considered, the definitions of $\bar{\sigma}_{ij}$ and $\bar{q}_i$ reduce to those of σ_{ij} and q_i.

3.2. *Moment equations and boundary conditions*

In this section wel list the equations and boundary conditions derived for the aforementioned variables. Like the generalised 13-moment equations derived in Struchtrup (2005*a*), our equations will contain coefficients that depend on the type of gas molecules. In the equations below, these constants will be denoted by k_i and l_i. The equations are

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \boldsymbol{v} = 0, \tag{3.2}$$

$$\frac{\partial \theta}{\partial t} + \frac{2}{3}\nabla \cdot \boldsymbol{v} + \frac{2}{3}k_0\nabla \cdot \bar{\boldsymbol{q}} - k_1 Kn\Delta\theta + k_2 Kn\nabla \cdot (\nabla \cdot \bar{\boldsymbol{\sigma}}) = 0, \tag{3.3}$$

$$\frac{\partial \boldsymbol{v}}{\partial t} + \nabla\rho + \nabla\theta - k_3 Kn\nabla \cdot (\nabla \boldsymbol{v})_{stf} - k_4 Kn\nabla \cdot (\nabla\bar{\boldsymbol{q}})_{stf} + k_5\nabla \cdot \bar{\boldsymbol{\sigma}} = 0, \tag{3.4}$$

$$\frac{\partial \bar{\boldsymbol{q}}}{\partial t} + \frac{5}{2}k_0\nabla\theta - \frac{5}{2}k_4 Kn\nabla \cdot (\nabla \boldsymbol{v})_{stf} - 2k_6 Kn\nabla(\nabla \cdot \bar{\boldsymbol{q}})$$
$$- \frac{12}{5}k_7 Kn\nabla \cdot (\nabla\bar{\boldsymbol{q}})_{stf} + k_8\nabla \cdot \bar{\boldsymbol{\sigma}} = -\frac{1}{Kn}\frac{2}{3}l_1\bar{\boldsymbol{q}}, \tag{3.5}$$

$$\frac{\partial \bar{\boldsymbol{\sigma}}}{\partial t} + 3k_2 Kn\left(\nabla^2\theta\right)_{stf} + 2k_5(\nabla \boldsymbol{v})_{stf} + \frac{4}{5}k_8(\nabla\bar{\boldsymbol{q}})_{stf}$$
$$- 2k_9 Kn\nabla \cdot (\nabla\bar{\boldsymbol{\sigma}})_{stf} - k_{10}Kn\left(\nabla(\nabla \cdot \bar{\boldsymbol{\sigma}})\right)_{stf} = -\frac{1}{Kn}l_2\bar{\boldsymbol{\sigma}}. \tag{3.6}$$

Here $(\cdot)_{stf}$ refers to the symmetric and trace-free part of a given tensor, which is defined entry wisely as $(\cdot)_{ij} \mapsto ((\cdot)_{stf})_{ij} = (\cdot)_{\langle ij\rangle}$ for a matrix and $(\cdot)_{ijk} \mapsto ((\cdot)_{stf})_{ijk} = (\cdot)_{\langle ijk\rangle}$ for a 3-tensor. The detailed definition can be found in Struchtrup (2005*b*). The coefficients k_i and l_i have been computed for gas molecules whose intermolecular potential satisfies inverse power laws. Values for these coefficients for some power indices are given in Appendix B. Although these coefficients look arbitrary, our derivation in § 4 will reveal that they are fully determined by the linearised and non-dimensionalised Boltzmann collision operator, which depends only on the potential energy between two gas molecules. In inverse-power-law models, only two parameters exist: the intensity coefficient of the potential and the power η. After non-dimensionalisation, the intensity coefficient is integrated into the Knudsen number and, thus, η is the only parameter that dictates all the coefficients.

The first three equations (3.2), (3.3) and (3.4) are conservation laws of mass, energy and momentum. By comparing (3.3) and (3.4) with the conservation laws expressed by the stress tensor and the heat flux (see (2.17)), i.e.

$$\frac{\partial \theta}{\partial t} + \frac{2}{3}\nabla \cdot \boldsymbol{v} + \frac{2}{3}\nabla \cdot \boldsymbol{q} = 0, \qquad \frac{\partial \boldsymbol{v}}{\partial t} + \nabla\rho + \nabla\theta + \nabla \cdot \boldsymbol{\sigma} = 0, \tag{3.7}$$

one can observe the relationship between $\bar{\boldsymbol{\sigma}}$, $\bar{\boldsymbol{q}}$ and $\boldsymbol{\sigma}$, $\boldsymbol{q}$:

$$\boldsymbol{\sigma} = k_5\bar{\boldsymbol{\sigma}} - k_4 Kn(\nabla\bar{\boldsymbol{q}})_{stf} - k_3 Kn(\nabla \boldsymbol{v})_{stf}, \quad \boldsymbol{q} = k_0\bar{\boldsymbol{q}} - \frac{3}{2}k_1 Kn\nabla\theta + \frac{3}{2}k_2 Kn\nabla \cdot \bar{\boldsymbol{\sigma}}. \tag{3.8}$$

Such a relationship allows us to calculate the stress tensor and heat flux once (3.2)–(3.6) are solved. We remark that the moment equations (3.2)–(3.6) we derived are Galilean invariant. The detailed proof can be found in Appendix A.

Another important ingredient of the moment equations is the wall boundary conditions, since the linear moment equations are often applied in channel flows, where the boundaries play crucial roles in rarefaction effects. The boundary conditions we present here are derived from the Maxwell boundary conditions for the Boltzmann equation, where the reflected gas flow is a linear combination of specular and diffusive reflections. The accommodation coefficient, denoted by χ, is the parameter describing the proportion of diffusive reflection. For simplicity, we are going to use $\tilde{\chi} = 2\chi/(2 - \chi)$ in our formulation of boundary conditions.

We now focus on a specific point on the wall and let $\boldsymbol{n}$ be the outer unit normal vector at this point. Meanwhile, we let τ_1 and τ_2 be the two tangential unit vectors that are perpendicular to each other. When describing boundary conditions, we temporarily rotate our coordinate system such that the three axes become $\boldsymbol{n}$, τ_1 and τ_2. Correspondingly, the three components of the velocity will be denoted by v_n, v_{τ_1} and v_{τ_2} (similar for $\bar{q}$), and the components of $\bar{\sigma}$ are written by $\bar{\sigma}_{nn}, \bar{\sigma}_{n\tau_1}, \bar{\sigma}_{n\tau_2}, \bar{\sigma}_{\tau_1\tau_1}, \bar{\sigma}_{\tau_1\tau_2}, \bar{\sigma}_{\tau_2\tau_2}$. Moreover, we assume that the temperature and velocity of the wall are θ^W and v_i^W at this point. Under these assumptions, the wall boundary conditions have the following form:

$$v_n = 0, \tag{3.9}$$

$$\bar{q}_n = \tilde{\chi}\left[m_{11}(\theta - \theta^W) + m_{12}\bar{\sigma}_{nn} - m_{13}Kn\frac{\partial \bar{q}_j}{\partial x_j} - m_{14}Kn\frac{\partial \bar{q}_{\langle n}}{\partial x_{n\rangle}} - m_{15}Kn\frac{\partial v_{\langle n}}{\partial x_{n\rangle}} \right], \tag{3.10}$$

$$m_{26}\bar{q}_n + m_{27}Kn\frac{\partial \theta}{\partial x_n} - m_{28}Kn\frac{\partial \bar{\sigma}_{nj}}{\partial x_j} = \tilde{\chi}\left[-m_{21}(\theta - \theta^W) + m_{22}\bar{\sigma}_{nn} + m_{23}Kn\frac{\partial \bar{q}_j}{\partial x_j} \right.$$
$$\left. + m_{24}Kn\frac{\partial \bar{q}_{\langle n}}{\partial x_{n\rangle}} + m_{25}Kn\frac{\partial v_{\langle n}}{\partial x_{n\rangle}} \right], \tag{3.11}$$

$$\bar{\sigma}_{\tau_i n} = \tilde{\chi}\left[m_{31}(v_{\tau_i} - v_{\tau_i}^W) + m_{32}\bar{q}_{\tau_i} - m_{33}Kn\frac{\partial \bar{\sigma}_{\tau_i j}}{\partial x_j} - m_{34}Kn\frac{\partial \bar{\sigma}_{\langle \tau_i n}}{\partial x_{n\rangle}} + m_{35}Kn\frac{\partial \theta}{\partial x_{\tau_i}} \right],$$
$$i = 1, 2, \tag{3.12}$$

$$m_{46}\bar{\sigma}_{\tau_i n} + m_{47}Kn\frac{\partial v_{\langle \tau_i}}{\partial x_{n\rangle}} + m_{48}Kn\frac{\partial \bar{q}_{\langle \tau_i}}{\partial x_{n\rangle}} = -\tilde{\chi}\left[-m_{41}(v_{\tau_i} - v_{\tau_i}^W) + m_{42}\bar{q}_{\tau_i} \right.$$
$$\left. + m_{43}Kn\frac{\partial \bar{\sigma}_{\tau_i j}}{\partial x_j} + m_{44}Kn\frac{\partial \bar{\sigma}_{\langle \tau_i n}}{\partial x_{n\rangle}} - m_{45}Kn\frac{\partial \theta}{\partial x_{\tau_i}} \right], \quad i = 1, 2, \tag{3.13}$$

$$m_{56}\bar{\sigma}_{\tau_i n} + m_{57}Kn\frac{\partial v_{\langle \tau_i}}{\partial x_{n\rangle}} + m_{58}Kn\frac{\partial \bar{q}_{\langle \tau_i}}{\partial x_{n\rangle}} = -\tilde{\chi}\left[-m_{51}(v_{\tau_i} - v_{\tau_i}^W) + m_{52}\bar{q}_{\tau_i} \right.$$
$$\left. + m_{53}Kn\frac{\partial \bar{\sigma}_{\tau_i j}}{\partial x_j} + m_{54}Kn\frac{\partial \bar{\sigma}_{\langle \tau_i n}}{\partial x_{n\rangle}} - m_{55}Kn\frac{\partial \theta}{\partial x_{\tau_i}} \right], \quad i = 1, 2, \tag{3.14}$$

$$m_{66}\bar{q}_n + Kn\left(m_{67}\frac{\partial \bar{\sigma}_{\langle nn}}{\partial x_{n\rangle}} + m_{68}\frac{\partial \bar{\sigma}_{nj}}{\partial x_j} + m_{69}\frac{\partial \theta}{\partial x_n} \right) = -\tilde{\chi}\left[-m_{61}(\theta - \theta^W) + m_{62}\bar{\sigma}_{nn} \right.$$
$$\left. + m_{63}Kn\frac{\partial \bar{q}_j}{\partial x_j} + m_{64}Kn\frac{\partial \bar{q}_{\langle n}}{\partial x_{n\rangle}} + m_{65}Kn\frac{\partial v_{\langle n}}{\partial x_{n\rangle}} \right], \tag{3.15}$$

$$Kn\left(\frac{\partial \bar{\sigma}_{\langle \tau_i \tau_i}}{\partial x_{n\rangle}} + \frac{1}{2}\frac{\partial \bar{\sigma}_{\langle nn}}{\partial x_{n\rangle}} \right) = -\tilde{\chi}m_{71}\left(\bar{\sigma}_{\tau_i \tau_i} + \frac{1}{2}\bar{\sigma}_{nn} \right), \quad i = 1, 2, \tag{3.16}$$

$$Kn\frac{\partial \bar{\sigma}_{\langle \tau_1 \tau_2}}{\partial x_{n\rangle}} = -\tilde{\chi}m_{81}\bar{\sigma}_{\tau_1 \tau_2}. \tag{3.17}$$

In these equations, m_{jk} are constants depending on the molecular interactions. As examples, we consider inverse-power-law models in which the repulsive force between two gas molecules is proportional to the ηth power of the distance between them. For such models, the values of the constants k_i and m_{ij} are tabulated in Appendix B for some power indices.

It will become clear by its derivation that this set of boundary conditions satisfies the general form of L^2-stable boundary conditions (1.6), which implies the second law of thermodynamics. The external contribution $\boldsymbol{g}_{ext}$ is given by the terms with wall velocity v_i^W and wall temperature θ^W.

3.3. *Second law of thermodynamics*

The derivation of the new R13 equations (3.2)–(3.6), to be detailed in the next section, maintains the structure required by (1.2). Therefore, according to (1.3), the second law of thermodynamics is automatically satisfied. In fact, the entropy inequality can also be observed from (3.2) to (3.6) directly by straightforward calculations. Assume that the spatial domain is $\mathbb{R}^3$ and all quantities decay to zero when $\boldsymbol{x}$ tends to infinity. Then, by calculating

$$\int_{\mathbb{R}^3} \left[\rho \cdot (3.1) + \frac{3}{2}\theta \cdot (3.2) + \boldsymbol{v} \cdot (3.3) + \frac{2}{5}\bar{\boldsymbol{q}} \cdot (3.4) + \frac{1}{2}\bar{\boldsymbol{\sigma}} : (3.5) \right] \mathrm{d}\boldsymbol{x}, \qquad (3.18)$$

one obtains

$$\frac{\mathrm{d}}{\mathrm{d}t} \int_{\mathbb{R}^3} \frac{1}{2} \left(\rho^2 + \frac{3}{2}\theta^2 + |\boldsymbol{v}|^2 + \frac{2}{5}|\bar{\boldsymbol{q}}|^2 + \frac{1}{2}\|\bar{\boldsymbol{\sigma}}\|^2 \right) \mathrm{d}\boldsymbol{x} =$$

$$- Kn \int_{\mathbb{R}^3} \left(\frac{3}{2}k_1|\nabla\theta|^2 + k_3\|(\nabla\boldsymbol{v})_{stf}\|^2 + \frac{4}{5}k_6\|\nabla\bar{\boldsymbol{q}}\|^2 + \frac{24}{25}k_7\|(\nabla\bar{\boldsymbol{q}})_{stf}\|^2 \right) \mathrm{d}\boldsymbol{x}$$

$$- Kn \int_{\mathbb{R}^3} \left(k_9\|\|(\nabla\bar{\boldsymbol{\sigma}})_{stf}\|\|^2 + \frac{1}{2}k_{10}|\nabla\cdot\bar{\boldsymbol{\sigma}}|^2 \right) \mathrm{d}\boldsymbol{x} - \frac{1}{Kn} \int_{\mathbb{R}^3} \left(\frac{4}{15}l_1|\bar{\boldsymbol{q}}|^2 + \frac{1}{2}l_2\|\bar{\boldsymbol{\sigma}}\|^2 \right) \mathrm{d}\boldsymbol{x}$$

$$+ 3\,Kn k_2 \int_{\mathbb{R}^3} \nabla\theta \cdot (\nabla\cdot\bar{\boldsymbol{\sigma}})\,\mathrm{d}\boldsymbol{x} - 2\,Kn k_4 \int_{\mathbb{R}^3} (\nabla\boldsymbol{v})_{stf} : (\nabla\bar{\boldsymbol{q}})_{stf}\,\mathrm{d}\boldsymbol{x}, \qquad (3.19)$$

where we have used $|\cdot|$, $\|\cdot\|$ and $\|\|\cdot\|\|$ to denote the Frobenius norms of vectors, 2-tensors and 3-tensors, respectively. We show later (at the end of § 4.3) that

$$\frac{(3k_2)^2}{4} \leqslant \frac{3}{2}k_1 \cdot \frac{1}{2}k_{10}, \qquad k_4^2 \leqslant k_3 \cdot \frac{24}{25}k_7, \qquad (3.20)$$

which yields

$$\left| 3k_2 \int_{\mathbb{R}^3} \nabla\theta \cdot (\nabla\cdot\bar{\boldsymbol{\sigma}})\,\mathrm{d}\boldsymbol{x} \right| \leqslant \int_{\mathbb{R}^3} \left(\frac{3}{2}k_1|\nabla\theta|^2 + \frac{1}{2}k_{10}|\nabla\cdot\bar{\boldsymbol{\sigma}}|^2 \right) \mathrm{d}\boldsymbol{x},$$

$$\left| 2k_4 \int_{\mathbb{R}^3} (\nabla\boldsymbol{v})_{stf} : (\nabla\bar{\boldsymbol{q}})_{stf}\,\mathrm{d}\boldsymbol{x} \right| \leqslant \int_{\mathbb{R}^3} \left(k_3\|(\nabla\boldsymbol{v})_{stf}\|^2 + \frac{24}{25}k_7\|(\nabla\bar{\boldsymbol{q}})_{stf}\|^2 \right) \mathrm{d}\boldsymbol{x}. \qquad (3.21)$$

Thus,

$$\frac{\mathrm{d}}{\mathrm{d}t} \int_{\mathbb{R}^3} \frac{1}{2} \left(\rho^2 + \frac{3}{2}\theta^2 + |\boldsymbol{v}|^2 + \frac{2}{5}|\bar{\boldsymbol{q}}|^2 + \frac{1}{2}\|\bar{\boldsymbol{\sigma}}\|^2 \right) \mathrm{d}\boldsymbol{x} \leqslant$$

$$- Kn \int_{\mathbb{R}^3} \left(\frac{4}{5}k_6\|\nabla\bar{\boldsymbol{q}}\|^2 + k_9\|\|(\nabla\bar{\boldsymbol{\sigma}})_{stf}\|\|^2 \right) \mathrm{d}\boldsymbol{x} - \frac{1}{Kn} \int_{\mathbb{R}^3} \left(\frac{4}{15}l_1|\bar{\boldsymbol{q}}|^2 + \frac{1}{2}l_2\|\bar{\boldsymbol{\sigma}}\|^2 \right) \mathrm{d}\boldsymbol{x}, \qquad (3.22)$$

Since the coefficients k_6, k_9, l_1 and l_2 are all non-negative, the right-hand side of the equation above is non-positive. The entropy density can thus be defined by

$$H = H_0 - \frac{1}{2}\left(\rho^2 + \frac{3}{2}\theta^2 + |\boldsymbol{v}|^2 + \frac{2}{5}|\bar{\boldsymbol{q}}|^2 + \frac{1}{2}\|\bar{\boldsymbol{\sigma}}\|^2\right), \tag{3.23}$$

where H_0 is an arbitrary constant. In the case of Maxwell molecules, this result echos the conclusion in Struchtrup & Torrilhon (2007).

For bounded domains, with boundary conditions (3.9)–(3.17), we can also show that the entropy may increase only due to the incoming fluxes from the boundary. The derivation is similar to the unbounded case, while boundary terms appear when performing integration by parts, for which the boundary conditions need to be applied to make further simplifications. For any bounded domain Ω, the conclusion has the form

$$-\frac{\mathrm{d}}{\mathrm{d}t}\int_{\Omega} H\,\mathrm{d}\boldsymbol{x} \leqslant \int_{\partial\Omega} \theta^W(C_1\theta + C_2\bar{q}_n + C_3\bar{\sigma}_{nn})\,\mathrm{d}s$$
$$+ \int_{\partial\Omega}[v_{\tau_1}^W(C_4 v_{\tau_1} + C_5\bar{q}_{\tau_1} + C_6\bar{\sigma}_{n\tau_1}) + v_{\tau_2}^W(C_4 v_{\tau_2} + C_5\bar{q}_{\tau_2} + C_6\bar{\sigma}_{n\tau_2})]\,\mathrm{d}s, \tag{3.24}$$

where the constants C_1–C_6 depend only on the coefficients in the equations and the boundary conditions. In (3.24) the right-hand side only contains terms related to $\boldsymbol{v}^W$ and θ^W, meaning that the entropy can increase only due to the velocities and temperatures of the walls, which does not violate the second law of thermodynamics.

4. Derivation of R13 equations

In this section we detail our derivation of the time-dependent R13 equations. To begin with, we first explain how the 13 variables used in our equations are chosen based on the collision model.

4.1. *Choice of variables*

As described in the previous section, our choice of the 13 variables is different from Grad's 13-moment equations. To explain how the new variables are defined, we start from the following definition of trace-free moments, which has been utilised in the derivation of steady-state R13 equations (Cai *et al.* 2024*b*):

$$w_{i_1\cdots i_l}^n = \langle \psi_{i_1\cdots i_l}^n, f\rangle. \tag{4.1}$$

Here $\psi_{i_1\cdots i_l}^n$ is a polynomial defined by

$$\psi_{i_1\cdots i_l}^n(\boldsymbol{\xi}) = \bar{L}_n^{(l+1/2)}\left(\frac{|\boldsymbol{\xi}|^2}{2}\right)\xi_{\langle i_1}\cdots\xi_{i_l\rangle}, \tag{4.2}$$

and $\bar{L}_n^{(l+1/2)}$ is the normalised Laguerre polynomial

$$\bar{L}_n^{(l+1/2)}(x) = \sqrt{\frac{\sqrt{\pi}}{2^{l+1}n!\Gamma(n+l+3/2)}}\,x^{-(l+1/2)}\left(\frac{\mathrm{d}}{\mathrm{d}x}-1\right)^n x^{n+l+1/2}. \tag{4.3}$$

These moments can be viewed as generalisations of Grad's 13 moments, and they are related to Grad's moments by

$$\rho = w^0, \quad v_i = \sqrt{3}w_i^0, \quad \theta = -\sqrt{\frac{2}{3}}w^1, \quad \sigma_{ij} = \sqrt{15}w_{ij}^0, \quad q_i = -\sqrt{\frac{15}{2}}w_i^1. \tag{4.4}$$

By taking moments of the Boltzmann equation (1.1), one can derive evolution equations for the moments $w_{i_1 \cdots i_l}^n$:

$$\frac{\partial w_{i_1 \cdots i_l}^n}{\partial t} + \left(\sqrt{2(n+l)+3} \frac{\partial w_{i_1 \cdots i_l j}^n}{\partial x_j} - \sqrt{2n} \frac{\partial w_{i_1 \cdots i_l j}^{n-1}}{\partial x_j} \right)$$

$$+ \frac{l}{2l+1} \left(\sqrt{2(n+l)+1} \frac{\partial w_{\langle i_1 \cdots i_{l-1}}^n}{\partial x_{i_l \rangle}} - \sqrt{2(n+1)} \frac{\partial w_{\langle i_1 \cdots i_{l-1}}^{n+1}}{\partial x_{i_l \rangle}} \right) = \frac{1}{Kn} \sum_{n'=0}^{+\infty} a_{lnn'} w_{i_1 \cdots i_l}^{n'}. \tag{4.5}$$

Here the coefficients $a_{lnn'}$ on the right-hand side are given by

$$a_{lnn'} = \frac{(2l+1)!!}{l!} \langle \psi_{i_1 \cdots i_l}^n, \mathcal{L} \psi_{i_1 \cdots i_l}^{n'} \rangle, \tag{4.6}$$

where we do not take summation over the indices $i_1, \ldots, i_l$, and the choice of these indices does not affect the value of $a_{lnn'}$ due to the rotational invariance of the linearised collision operator. By the self-adjointness of $\mathcal{L}$, one can observe that $a_{lnn'} = a_{ln'n}$. Due to the conservation of mass, momentum and energy, it holds that

$$a_{00n} = a_{0n0} = a_{01n} = a_{0n1} = a_{10n} = a_{1n0} = 0. \tag{4.7}$$

For inverse-power-law models, the computation of these coefficients are provided in Cai & Torrilhon (2015).

To select appropriate moments in our equations, we apply the Chapman–Enskog expansion to the moment equations, which requires assuming that Kn is a small parameter and applying the following asymptotic expansion:

$$w_{i_1 \cdots i_l}^n = w_{i_1 \cdots i_l}^{n|0} + Kn w_{i_1 \cdots i_l}^{n|1} + Kn^2 w_{i_1 \cdots i_l}^{n|2} + Kn^3 w_{i_1 \cdots i_l}^{n|3} + \cdots. \tag{4.8}$$

The conservative variables w^0, w_i^0 and w^1 are regarded as $O(1)$ variables. Straightforward analysis leads to the following results:

$$w^{n|0} = w^{n|1} = 0, \quad n \geqslant 2; \qquad w_i^{n|0} = 0, \quad n \geqslant 1; \tag{4.9}$$

$$w_{i_1 \cdots i_l}^{n|0} = w_{i_1 \cdots i_l}^{n|1} = 0, \quad l = 3; \qquad w_{i_1 \cdots i_l}^{n|0} = w_{i_1 \cdots i_l}^{n|1} = w_{i_1 \cdots i_l}^{n|2} = 0, \quad l \geqslant 4; \tag{4.10}$$

$$w_i^{n|1} = \beta_1^{(1),n} \frac{\partial w^1}{\partial x_i}, \quad n \geqslant 1; \qquad w_{ij}^{n|1} = \beta_2^{(1),n} \frac{\partial w_{\langle i}^0}{\partial x_{j \rangle}}; \tag{4.11}$$

$$w^{n|2} = \gamma_0^{(2),n} \frac{\partial w_j^{1|1}}{\partial x_j}, \quad n \geqslant 2; \qquad w_i^{n|2} = \gamma_{t1}^{(1),n} \frac{\partial w_i^{1|1}}{\partial t} + \gamma_{s1}^{(1),n} \frac{\partial w_{ij}^{0|1}}{\partial x_j}, \quad n \geqslant 2; \tag{4.12}$$

$$w_{ij}^{n|2} = \gamma_{t2}^{(1),n} \frac{\partial w_{ij}^{0|1}}{\partial t} + \gamma_{s2}^{(1),n} \frac{\partial w_{\langle i}^{1|1}}{\partial x_{j \rangle}}, \quad n \geqslant 1; \qquad w_{ijk}^{n|2} = \gamma_3^{(2),n} \frac{\partial w_{\langle ij}^{0|1}}{\partial x_{k \rangle}}. \tag{4.13}$$

The coefficients β and γ are all constants depending on the collision term. Note that (4.11) implies the Navier–Stokes law and the Fourier law, and these equations lead to the following linear relationship between the moments:

$$w_i^{n|1} = \frac{\beta_1^{(1),n}}{\beta_1^{(1),1}} w_i^{1|1}, \quad n \geqslant 1; \qquad w_{ij}^{n|1} = \frac{\beta_2^{(1),n}}{\beta_2^{(1),0}} w_{ij}^{n|0}. \tag{4.14}$$

By the definition of $w_{i_1 \cdots i_l}^n$ (see (4.1)), the above equations indicate that

$$\left\langle \psi_i^n - \frac{\beta_1^{(1),n}}{\beta_1^{(1),1}} \psi_i^1, f \right\rangle \sim O(Kn^2), \quad n \geqslant 1; \qquad \left\langle \psi_{ij}^n - \frac{\beta_2^{(1),n}}{\beta_2^{(1),0}} \psi_{ij}^0, f \right\rangle \sim O(Kn^2).$$

(4.15)

Meanwhile, (4.9) yields

$$\langle \psi^n, f \rangle \sim O(Kn^2), \quad n \geqslant 2; \qquad \langle \psi_{i_1 \cdots i_l}^n, f \rangle \sim O(Kn^2), \quad l \geqslant 3.$$

(4.16)

Recall that we want to choose the 13 variables of the our equations to be $\langle \tilde{\phi}_{13}, f \rangle$ with $\tilde{\phi}_{13}$ satisfying $\langle r, f \rangle \sim o(Kn)$ whenever $\langle \tilde{\phi}_{13}, r \rangle = 0$. A straightforward approach is to select $\tilde{\phi}_{13}$ to be a basis of $(\mathbb{S}^{(2)})^\perp$, with $\mathbb{S}^{(2)}$ being the linear span of all polynomials appearing in (4.15) and (4.16):

$$\mathbb{S}^{(2)} = \mathrm{span}\left\{ \psi_i^n - \frac{\beta_1^{(1),n}}{\beta_1^{(1),1}} \psi_i^1 \,\middle|\, n \geqslant 1 \right\} \oplus \mathrm{span}\left\{ \psi_{ij}^n - \frac{\beta_2^{(1),n}}{\beta_2^{(1),0}} \psi_{ij}^0 \,\middle|\, n \geqslant 0 \right\}$$
$$\oplus \mathrm{span}\{\psi^n \mid n \geqslant 2\} \oplus \mathrm{span}\{\psi_{i_1 \cdots i_l}^n \mid l \geqslant 3\}.$$

(4.17)

This leads to the following choice of $\tilde{\phi}_{13}$:

$$\psi^0, \quad \psi^1, \quad \psi_i^0, \quad \phi_i^1, \quad \phi_{ij}^0.$$

(4.18)

Here ψ^0, ψ^1 and ψ_i^0 correspond to conservative moments, and ϕ_i^1 and ϕ_{ij}^0, corresponding to non-equilibrium variables, are defined by

$$\phi_i^1 = \sum_{n=1}^{+\infty} c_1^{1,n} \psi_i^n, \qquad \phi_{ij}^0 = \sum_{n=0}^{+\infty} c_2^{0,n} \psi_{ij}^n,$$

(4.19)

with the coefficients $c_1^{1,n}$ and $c_2^{0,n}$ satisfying

$$c_1^{1,n} = \frac{\beta_1^{(1),n}}{\beta_1^{(1),1}} c_1^{1,1}, \qquad c_2^{0,n} = \frac{\beta_2^{(1),n}}{\beta_2^{(1),0}} c_2^{0,0}.$$

(4.20)

Thus, the 13 moments in our equations include

$$\rho, \quad \theta, \quad v_i, \quad \bar{q}_i = \langle \phi_i^1, f \rangle, \quad \bar{\sigma}_{ij} = \langle \phi_{ij}^0, f \rangle.$$

(4.21)

In (4.19) the constants $c_1^{1,1}$ and $c_2^{0,0}$ can be chosen as arbitrary non-zero numbers, and here we choose them such that when the collision model reduces Maxwell molecules ($\eta = 5$), $\bar{q}_i$ and $\bar{\sigma}_{ij}$ reduce to q_i and σ_{ij}. More precisely, we choose negative $c_1^{1,1}$ and positive $c_2^{0,0}$ such that

$$\sum_{n=1}^{+\infty} \left(c_1^{1,n}\right)^2 = \frac{15}{2}, \qquad \sum_{n=0}^{+\infty} \left(c_2^{0,n}\right)^2 = 15. \tag{4.22}$$

Note that the definitions of $\bar{q}_i$ and $\bar{\sigma}_{ij}$ depend on the collision model since the coefficients $c_1^{1,n}$ and $c_2^{0,n}$ are determined by $\beta_1^{(1),n}$ and $\beta_2^{(1),0}$, and these constants will vary when the collision model changes.

4.2. *Second-order variables*

To derive a model with the super-Burnett order, second-order moments are needed as auxiliary variables. The choice of these variables also follows the requirement of orthogonality, meaning that we want to find a vector function $\tilde{\psi}(\boldsymbol{\xi})$ such that:

(i) $\langle \tilde{\phi}_{13}, \tilde{\psi} \rangle = 0$;
(ii) for any function $r(\boldsymbol{\xi})$ such that $\langle r, \tilde{\psi} \rangle = 0$, it holds that $\langle r, f \rangle \sim o(Kn^2)$;
(iii) the number of components of $\tilde{\psi}$ should be as low as possible.

To find $\tilde{\psi}$, we need the following linear relationship between the second-order terms of moments:

$$w^{n|2} = d_{02}^n w^{2|2}, \quad n \geqslant 2; \qquad w_i^{n|2} = d_{12}^n w_i^{2|2} + d_{13}^n w_i^{3|2}, \quad n \geqslant 2;$$
$$w_{ij}^{n|2} = d_{21}^n w_{ij}^{1|2} + d_{22}^n w_{ij}^{2|2}, \quad n \geqslant 1; \qquad w_{ijk}^{n|2} = d_{30}^n w_{ijk}^{0|2}, \quad n \geqslant 0, \tag{4.23}$$

where

$$d_{02}^n = \frac{\gamma_0^{(2),n}}{\gamma_0^{(2),2}}, \qquad\qquad d_{30}^n = \frac{\gamma_3^{(2),n}}{\gamma_3^{(2),0}},$$

$$d_{12}^n = \frac{\gamma_{t1}^{(1),n}\gamma_{s1}^{(1),3} - \gamma_{s1}^{(1),n}\gamma_{t1}^{(1),3}}{\gamma_{s1}^{(1),3}\gamma_{t1}^{(1),2} - \gamma_{s1}^{(1),2}\gamma_{t1}^{(1),3}}, \qquad d_{13}^n = \frac{\gamma_{s1}^{(1),n}\gamma_{t1}^{(1),2} - \gamma_{t1}^{(1),n}\gamma_{s1}^{(1),2}}{\gamma_{s1}^{(1),3}\gamma_{t1}^{(1),2} - \gamma_{s1}^{(1),2}\gamma_{t1}^{(1),3}},$$

$$d_{21}^n = \frac{\gamma_{t2}^{(1),n}\gamma_{s2}^{(1),2} - \gamma_{s2}^{(1),n}\gamma_{t2}^{(1),2}}{\gamma_{s2}^{(1),2}\gamma_{t2}^{(1),1} - \gamma_{s2}^{(1),1}\gamma_{t2}^{(1),2}}, \qquad d_{22}^n = \frac{\gamma_{s2}^{(1),n}\gamma_{t2}^{(1),1} - \gamma_{t2}^{(1),n}\gamma_{s2}^{(1),1}}{\gamma_{s2}^{(1),2}\gamma_{t2}^{(1),1} - \gamma_{s2}^{(1),1}\gamma_{t2}^{(1),2}}. \tag{4.24}$$

These equations can be derived from (4.12), (4.13) by cancelling the differential terms. The equations in (4.23) reveal that low-order parts of the moments can be cancelled by linear combinations:

$$w^n - d_{02}^n w^2 \sim o\left(Kn^2\right), \quad n \geqslant 2;$$
$$\left(w_i^n - Kn w_i^{n|1}\right) - d_{12}^n \left(w_i^2 - Kn w_i^{2|1}\right) - d_{13}^n \left(w_i^3 - Kn w_i^{3|1}\right) \sim o\left(Kn^2\right), \quad n \geqslant 2;$$
$$\left(w_{ij}^n - Kn w_{ij}^{n|1}\right) - d_{21}^n \left(w_{ij}^1 - Kn w_{ij}^{1|1}\right) - d_{22}^n \left(w_{ij}^2 - Kn w_{ij}^{2|1}\right) \sim o\left(Kn^2\right), \quad n \geqslant 1;$$
$$w_{ijk}^n - d_{30} w_{ijk}^0 \sim o\left(Kn^2\right), \quad n \geqslant 0. \tag{4.25}$$

Note that the correctness of (4.12) and (4.13) (and thus, (4.23) and (4.25)) replies only on the relation (4.14), and does not require the specific choice of $w_i^{n|1}$ and $w_{ij}^{n|1}$ as described in (4.11). Therefore, in (4.25) we can follow (4.15) to select

$$Knw_i^{n|1} = \left\langle \frac{\beta_1^{(1),n}}{\beta_1^{(1),1}} \psi_i^1, f \right\rangle, \quad n \geqslant 1; \qquad Knw_{ij}^{n|1} = \left\langle \frac{\beta_2^{(1),n}}{\beta_2^{(1),0}} \psi_{ij}^0, f \right\rangle, \quad n \geqslant 0, \quad (4.26)$$

so that we can find a linear space $\mathbb{S}^{(3)}$ such that $\langle r, f \rangle \sim o(Kn^2)$ for all $r \in \mathbb{S}^{(3)}$. The definition of $\mathbb{S}^{(3)}$ is

$$\mathbb{S}^{(3)} = \text{span} \left\{ \psi^n - d_{02}^n \psi^2 \mid n \geqslant 3 \right\}$$

$$\oplus \text{span} \left\{ \left(\psi_i^n - \frac{\beta_1^{(1),n}}{\beta_1^{(1),1}} \psi_i^1 \right) - d_{12}^n \left(\psi_i^2 - \frac{\beta_1^{(1),2}}{\beta_1^{(1),1}} \psi_i^1 \right) - d_{13}^n \left(\psi_i^3 - \frac{\beta_1^{(1),3}}{\beta_1^{(1),1}} \psi_i^1 \right) \,\middle|\, n \geqslant 4 \right\}$$

$$\oplus \text{span} \left\{ \left(\psi_{ij}^n - \frac{\beta_2^{(1),n}}{\beta_2^{(1),0}} \psi_{ij}^0 \right) - d_{21}^n \left(\psi_{ij}^1 - \frac{\beta_2^{(1),1}}{\beta_2^{(1),0}} \psi_{ij}^0 \right) - d_{22}^n \left(\psi_{ij}^2 - \frac{\beta_2^{(1),2}}{\beta_2^{(1),0}} \psi_{ij}^0 \right) \,\middle|\, n \geqslant 3 \right\}$$

$$\oplus \text{span} \left\{ \psi_{ijk}^n - d_{30} \psi_{ijk}^0 \mid n \geqslant 1 \right\} \oplus \text{span} \left\{ \psi_{i_1 \cdots i_l}^n \mid l \geqslant 4 \right\}. \quad (4.27)$$

The second-order variables are chosen to be a basis of $\mathbb{S}^{(2)} \cap (\mathbb{S}^{(3)})^\perp$.

The function space $\mathbb{S}^{(2)} \cap (\mathbb{S}^{(3)})^\perp$ has the form

$$\mathbb{S}^{(2)} \cap (\mathbb{S}^{(3)})^\perp = \text{span}\{\phi^2, \phi_i^2, \phi_i^3, \phi_{ij}^1, \phi_{ij}^2, \phi_{ijk}^0\}, \quad (4.28)$$

where

$$\phi^2 = \sum_{n=2}^{+\infty} c_0^{2,n} \psi^n, \quad \phi_i^2 = \sum_{n=2}^{+\infty} c_1^{2,n} \left(\psi_i^n - \frac{\beta_1^{(1),n}}{\beta_1^{(1),1}} \psi_i^1 \right), \quad \phi_i^3 = \sum_{n=2}^{+\infty} c_1^{3,n} \left(\psi_i^n - \frac{\beta_1^{(1),n}}{\beta_1^{(1),1}} \psi_i^1 \right),$$

$$\phi_{ij}^1 = \sum_{n=1}^{+\infty} c_2^{1,n} \left(\psi_{ij}^n - \frac{\beta_2^{(1),n}}{\beta_2^{(1),0}} \psi_{ij}^0 \right), \quad \phi_{ij}^2 = \sum_{n=1}^{+\infty} c_2^{2,n} \left(\psi_{ij}^n - \frac{\beta_2^{(1),n}}{\beta_2^{(1),0}} \psi_{ij}^0 \right), \quad \phi_{ijk}^0 = \sum_{n=0}^{+\infty} c_3^{0,n} \psi_{ijk}^n.$$

$$(4.29)$$

The coefficients $c_k^{\ell,n}$ can be represented as functions of $\beta_k^{(\ell),n}$, and the details can be found in Appendix D. Here we only emphasise that the choice has been made such that $\langle \phi_i^2, \phi_i^3 \rangle = \langle \phi_{ij}^1, \phi_{ij}^2 \rangle = 0$, and in the case of Maxwell molecules, $\phi_i^{2,3} = \psi_i^{2,3}$ and $\phi_{ij}^{1,2} = \psi_{ij}^{1,2}$. Equation (4.28) indicates that the minimum number of second-order variables is $24 \, (= 1 + 3 + 3 + 5 + 5 + 7)$. These variables will be denoted by

$$u^2 := \langle \phi^2, f \rangle, \qquad u_i^2 := \langle \phi_i^2, f \rangle, \qquad u_i^3 := \langle \phi_i^3, f \rangle,$$
$$u_{ij}^1 := \langle \phi_{ij}^1, f \rangle, \qquad u_{ij}^2 := \langle \phi_{ij}^2, f \rangle, \qquad u_{ijk}^0 := \langle \phi_{ijk}^0, f \rangle. \quad (4.30)$$

REMARK 1. *A similar procedure has been applied in Cai, Torrilhon & Yang (2024b) to obtain second-order variables in the case of steady-state equations. When time derivatives are absent, we have simpler relationships $w_i^{n|2} = d_{12}^n w_i^{2|2}$ and $w_{ij}^{n|2} = d_{21}^n w_{ij}^{1|2}$ in place of (4.23), resulting in only 16 second-order variables. In Struchtrup & Torrilhon (2013), when time-dependent R13 equations were derived for hard-sphere molecules, only* 29 (= 13 + 16) *equations were considered. However, the resulting equations may not hold the symmetry as in (1.2). In this paper we are going to include all the 37 (= 13 + 24) equations in our derivation to achieve the L^2 stability.*

4.3. *Derivation of R13 equations*

By the analysis above, the distribution function f can be separated into four parts according to the order of magnitude

$$f = f^{(0)} + f^{(1)} + f^{(2)} + f^{(r)}, \tag{4.31}$$

where $f^{(k)}$ is the projection of f onto the function space $\mathbb{V}^{(k)}$, defined by

$$\begin{aligned}
\mathbb{V}^{(0)} &= \text{span}\{\psi^0, \psi^1, \psi_i^0\}, & \mathbb{V}^{(1)} &= (\mathbb{V}^{(0)})^\perp \cap (\mathbb{S}^{(2)})^\perp, \\
\mathbb{V}^{(2)} &= \mathbb{S}^{(2)} \cap (\mathbb{S}^{(3)})^\perp, & \mathbb{V}^{(r)} &= \mathbb{S}^{(3)}.
\end{aligned} \tag{4.32}$$

It is clear that $f^{(0)}$, $f^{(1)}$ and $f^{(2)}$ represent, respectively, the zeroth-, first- and second-order parts of f, and $f^{(r)}$ represents the remaining part of f that has order $o(Kn^2)$. For simplicity, we use $\mathcal{P}^{(k)}$ to denote the projection operator onto $\mathbb{V}^{(k)}$. A key observation in our derivation is that the super-Burnett equations can be derived from the following equations without using $f^{(r)}$:

$$\frac{\partial}{\partial t} \begin{pmatrix} f^{(0)} \\ f^{(1)} \\ 0 \end{pmatrix} + \begin{pmatrix} \partial_{x_i} \mathcal{P}^{(0)} \xi_i f^{(0)} + \partial_{x_i} \mathcal{P}^{(0)} \xi_i f^{(1)} + \partial_{x_i} \mathcal{P}^{(0)} \xi_i f^{(2)} \\ \partial_{x_i} \mathcal{P}^{(1)} \xi_i f^{(0)} + \partial_{x_i} \mathcal{P}^{(1)} \xi_i f^{(1)} + \partial_{x_i} \mathcal{P}^{(1)} \xi_i f^{(2)} \\ \partial_{x_i} \mathcal{P}^{(2)} \xi_i f^{(0)} + \partial_{x_i} \mathcal{P}^{(2)} \xi_i f^{(1)} \end{pmatrix}$$
$$= \frac{1}{Kn} \begin{pmatrix} 0 \\ \mathcal{P}^{(1)} \mathcal{L} f^{(1)} + \mathcal{P}^{(1)} \mathcal{L} f^{(2)} \\ \mathcal{P}^{(2)} \mathcal{L} f^{(1)} + \mathcal{P}^{(2)} \mathcal{L} f^{(2)} \end{pmatrix}. \tag{4.33}$$

This form is similar to Grad's moment equations with truncation up to the second order, but the temporal and spatial derivatives of $f^{(2)}$ in the last equation are removed, allowing us to express $f^{(2)}$ using $f^{(0)}$ and $f^{(1)}$ according to the last equation:

$$f^{(2)} = \left[\mathcal{P}^{(2)} \mathcal{L}|_{\mathbb{V}^{(2)}} \right]^{-1} \left(\partial_{x_i} \mathcal{P}^{(2)} \xi_i f^{(0)} + \partial_{x_i} \mathcal{P}^{(2)} \xi_i f^{(1)} - \mathcal{P}^{(2)} \mathcal{L} f^{(1)} \right). \tag{4.34}$$

Thus, the second-order part $f^{(2)}$ can be eliminated from the equations, and the resulting equations contain only $f^{(0)}$ and $f^{(1)}$, which can be represented as 13-moment equations.

The reason why (4.33) has the super-Burnett order will be detailed in the next subsection. Here we apply this result to derive the R13 equations. The derivation requires explicit formulations of $f^{(0)}$, $f^{(1)}$ and $f^{(2)}$:

$$\begin{aligned}
f^{(0)} &= \rho \psi^0 - \sqrt{\frac{3}{2}} \theta \psi^1 + \sqrt{3} v_i \psi_i^0, \\
f^{(1)} &= \frac{2}{5} \bar{q}_i \phi_i^1 + \frac{1}{2} \bar{\sigma}_{ij} \phi_{ij}^0, \\
f^{(2)} &= u^2 \phi^2 + 3u_i^2 \phi_i^2 + 3u_i^3 \phi_i^3 + \frac{15}{2} u_{ij}^1 \phi_{ij}^1 + \frac{15}{2} u_{ij}^2 \phi_{ij}^2 + \frac{35}{2} u_{ijk}^0 \phi_{ijk}^0.
\end{aligned} \tag{4.35}$$

Then, (4.33) can be converted to moment equations by the Galerkin method. For example, the equation of $\bar{\sigma}_{ij}$ can be obtained by

$$\langle \phi_{ij}^0, f^{(1)} \rangle + \frac{\partial}{\partial x_k} \langle \phi_{ij}^0, \xi_k (f^{(0)} + f^{(1)} + f^{(2)}) \rangle = \langle \phi_{ij}^0, \mathcal{L}(f^{(1)} + f^{(2)}) \rangle, \tag{4.36}$$

and the equation of u_i^2 is

$$\frac{\partial}{\partial x_k} \langle \phi_i^2, \xi_k (f^{(0)} + f^{(1)}) \rangle = \langle \phi_i^2, \mathcal{L}(f^{(1)} + f^{(2)}) \rangle. \tag{4.37}$$

All these inner products can be computed explicitly, and the complete 37-moment equations are

$$\frac{\partial \rho}{\partial t} + \frac{\partial v_j}{\partial x_j} = 0, \tag{4.38}$$

$$\frac{\partial \theta}{\partial t} + \frac{2}{3}\frac{\partial v_j}{\partial x_j} + \frac{2}{3}c_1^{1,1}\frac{\partial \bar{q}_j}{\partial x_j} - \sqrt{\frac{10}{3}}\left(c_1^{2,1}\frac{\partial u_j^2}{\partial x_j} + c_1^{3,1}\frac{\partial u_j^3}{\partial x_j}\right) = 0, \tag{4.39}$$

$$\frac{\partial v_i}{\partial t} + \frac{\partial \rho}{\partial x_i} + \frac{\partial \theta}{\partial x_i} + c_2^{0,0}\frac{\partial \bar{\sigma}_{ij}}{\partial x_j} + \sqrt{15}\left(c_2^{1,0}\frac{\partial u_{ij}^1}{\partial x_j} + c_2^{2,0}\frac{\partial u_{ij}^2}{\partial x_j}\right) = 0, \tag{4.40}$$

$$\frac{\partial \bar{q}_i}{\partial t} + \frac{5}{2}c_1^{1,1}\frac{\partial \theta}{\partial x_i} - \frac{\sqrt{2}}{6}A_{45}\frac{\partial \bar{\sigma}_{ij}}{\partial x_j} - \sqrt{\frac{5}{6}}\left(A_{49}\frac{\partial u_{ij}^1}{\partial x_j} + A_{4,10}\frac{\partial u_{ij}^2}{\partial x_j} + A_{46}\frac{\partial u^2}{\partial x_i}\right)$$
$$= \frac{1}{Kn}\left(\frac{1}{3}\mathscr{L}_1^{(11)}\bar{q}_i - \sqrt{\frac{5}{6}}\mathscr{L}_1^{(12)}u_i^2 - \sqrt{\frac{5}{6}}\mathscr{L}_1^{(13)}u_i^3\right), \tag{4.41}$$

$$\frac{\partial \bar{\sigma}_{ij}}{\partial t} + 2c_2^{0,0}\frac{\partial v_{\langle i}}{\partial x_{j\rangle}} - \frac{2\sqrt{2}}{15}A_{45}\frac{\partial \bar{q}_{\langle i}}{\partial x_{j\rangle}} + \frac{2}{\sqrt{15}}\left(A_{57}\frac{\partial u_{\langle i}^2}{\partial x_{j\rangle}} + A_{58}\frac{\partial u_{\langle i}^3}{\partial x_{j\rangle}} + A_{5,11}\frac{\partial u_{ijk}^0}{\partial x_k}\right)$$
$$= \frac{1}{Kn}\left(\frac{2}{15}\mathscr{L}_2^{(00)}\bar{\sigma}_{ij} + \frac{2}{\sqrt{15}}\mathscr{L}_2^{(01)}u_{ij}^1 + \frac{2}{\sqrt{15}}\mathscr{L}_2^{(02)}u_{ij}^2\right), \tag{4.42}$$

$$-\sqrt{\frac{2}{15}}A_{46}\frac{\partial \bar{q}_j}{\partial x_j} = \frac{1}{Kn}\mathscr{L}_0^{(22)}u^2, \tag{4.43}$$

$$-\sqrt{\frac{15}{2}}c_1^{2,1}\frac{\partial \theta}{\partial x_i} + \sqrt{\frac{1}{15}}A_{57}\frac{\partial \bar{\sigma}_{ij}}{\partial x_j} = \frac{1}{Kn}\left(-\sqrt{\frac{2}{15}}\mathscr{L}_1^{(21)}\bar{q}_i + \mathscr{L}_1^{(22)}u_i^2 + \mathscr{L}_1^{(23)}u_i^3\right), \tag{4.44}$$

$$-\sqrt{\frac{15}{2}}c_1^{3,1}\frac{\partial \theta}{\partial x_i} + \sqrt{\frac{1}{15}}A_{58}\frac{\partial \bar{\sigma}_{ij}}{\partial x_j} = \frac{1}{Kn}\left(-\sqrt{\frac{2}{15}}\mathscr{L}_1^{(31)}\bar{q}_i + \mathscr{L}_1^{(32)}u_i^2 + \mathscr{L}_1^{(33)}u_i^3\right), \tag{4.45}$$

$$\sqrt{15}c_2^{1,0}\frac{\partial v_{\langle i}}{\partial x_{j\rangle}} - \sqrt{\frac{2}{15}}A_{49}\frac{\partial \bar{q}_{\langle i}}{\partial x_{j\rangle}} = \frac{1}{Kn}\left(\sqrt{\frac{1}{15}}\mathscr{L}_2^{(10)}\bar{\sigma}_{ij} + \mathscr{L}_2^{(11)}u_{ij}^1 + \mathscr{L}_2^{(12)}u_{ij}^2\right), \tag{4.46}$$

$$\sqrt{15}c_2^{2,0}\frac{\partial v_{\langle i}}{\partial x_{j\rangle}} - \sqrt{\frac{2}{15}}A_{4,10}\frac{\partial \bar{q}_{\langle i}}{\partial x_{j\rangle}} = \frac{1}{Kn}\left(\sqrt{\frac{1}{15}}\mathscr{L}_2^{(20)}\bar{\sigma}_{ij} + \mathscr{L}_2^{(21)}u_{ij}^1 + \mathscr{L}_2^{(22)}u_{ij}^2\right), \tag{4.47}$$

$$\sqrt{\frac{1}{15}}A_{5,11}\frac{\partial \bar{\sigma}_{\langle ij}}{\partial x_{k\rangle}} = \frac{1}{Kn}\mathscr{L}_3^{(00)}u_{ijk}^0. \tag{4.48}$$

The coefficients A_{ij} are a series of $c_k^{l,n}$, with their expressions provided in Appendix E.

It is now clear that the second-order variables defined in (4.30) can be solved according to (4.43)–(4.48). Plugging the results into (4.39)–(4.42) yields our final equations (3.2)–(3.6). Here we would like to write down the explicit expressions for a few coefficients in (3.2)–(3.6):

$$k_1 = -5 \begin{pmatrix} c_1^{2,1} & c_1^{3,1} \end{pmatrix} \begin{pmatrix} \mathscr{L}_1^{(22)} & \mathscr{L}_1^{(23)} \\ \mathscr{L}_1^{(32)} & \mathscr{L}_1^{(33)} \end{pmatrix}^{-1} \begin{pmatrix} c_1^{2,1} \\ c_1^{3,1} \end{pmatrix}, \tag{4.49}$$

$$k_2 = -\frac{\sqrt{2}}{3} \begin{pmatrix} c_1^{2,1} & c_1^{3,1} \end{pmatrix} \begin{pmatrix} \mathscr{L}_1^{(22)} & \mathscr{L}_1^{(23)} \\ \mathscr{L}_1^{(32)} & \mathscr{L}_1^{(33)} \end{pmatrix}^{-1} \begin{pmatrix} A_{57} \\ A_{58} \end{pmatrix}, \tag{4.50}$$

$$k_3 = -15 \begin{pmatrix} c_2^{1,0} & c_2^{2,0} \end{pmatrix} \begin{pmatrix} \mathscr{L}_2^{(11)} & \mathscr{L}_2^{(12)} \\ \mathscr{L}_2^{(21)} & \mathscr{L}_2^{(22)} \end{pmatrix}^{-1} \begin{pmatrix} c_2^{1,0} \\ c_2^{2,0} \end{pmatrix}, \tag{4.51}$$

$$k_4 = \sqrt{2} \begin{pmatrix} A_{49} & A_{4,10} \end{pmatrix} \begin{pmatrix} \mathscr{L}_2^{(11)} & \mathscr{L}_2^{(12)} \\ \mathscr{L}_2^{(21)} & \mathscr{L}_2^{(22)} \end{pmatrix}^{-1} \begin{pmatrix} c_2^{1,0} \\ c_2^{2,0} \end{pmatrix}, \tag{4.52}$$

$$k_7 = -\frac{5}{36} \begin{pmatrix} A_{49} & A_{4,10} \end{pmatrix} \begin{pmatrix} \mathscr{L}_2^{(11)} & \mathscr{L}_2^{(12)} \\ \mathscr{L}_2^{(21)} & \mathscr{L}_2^{(22)} \end{pmatrix}^{-1} \begin{pmatrix} A_{49} \\ A_{4,10} \end{pmatrix}, \tag{4.53}$$

$$= -\frac{2}{15} \begin{pmatrix} A_{57} & A_{58} \end{pmatrix} \begin{pmatrix} \mathscr{L}_1^{(22)} & \mathscr{L}_1^{(23)} \\ \mathscr{L}_1^{(32)} & \mathscr{L}_1^{(33)} \end{pmatrix}^{-1} \begin{pmatrix} A_{57} \\ A_{58} \end{pmatrix}. \tag{4.54}$$

Since the matrices

$$\begin{pmatrix} \mathscr{L}_1^{(22)} & \mathscr{L}_1^{(23)} \\ \mathscr{L}_1^{(32)} & \mathscr{L}_1^{(33)} \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} \mathscr{L}_2^{(11)} & \mathscr{L}_2^{(12)} \\ \mathscr{L}_2^{(21)} & \mathscr{L}_2^{(22)} \end{pmatrix} \tag{4.55}$$

are symmetric and negative definite, we can obtain (3.20) by the Cauchy–Schwarz inequality, which completes the proof of the H-theorem (3.22).

4.4. *Verification of the super-Burnett order*

To show that (4.33) have super-Burnett order, we rewrite the Boltzmann equation in the form

$$\frac{\partial}{\partial t} \begin{pmatrix} f^{(0)} \\ f^{(1)} \\ f^{(2)} \\ f^{(\mathrm{r})} \end{pmatrix} + \begin{pmatrix} \mathcal{A}^{(00)} & \mathcal{A}^{(01)} & \mathcal{A}^{(02)} & \mathcal{A}^{(0\mathrm{r})} \\ \mathcal{A}^{(10)} & \mathcal{A}^{(11)} & \mathcal{A}^{(12)} & \mathcal{A}^{(1\mathrm{r})} \\ \mathcal{A}^{(20)} & \mathcal{A}^{(21)} & \mathcal{A}^{(22)} & \mathcal{A}^{(2\mathrm{r})} \\ \mathcal{A}^{(\mathrm{r}0)} & \mathcal{A}^{(\mathrm{r}1)} & \mathcal{A}^{(\mathrm{r}2)} & \mathcal{A}^{(\mathrm{rr})} \end{pmatrix} \begin{pmatrix} f^{(0)} \\ f^{(1)} \\ f^{(2)} \\ f^{(\mathrm{r})} \end{pmatrix}$$

$$= \frac{1}{Kn} \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & \mathcal{L}^{(11)} & \mathcal{L}^{(12)} & \mathcal{L}^{(1\mathrm{r})} \\ 0 & \mathcal{L}^{(21)} & \mathcal{L}^{(22)} & \mathcal{L}^{(2\mathrm{r})} \\ 0 & \mathcal{L}^{(\mathrm{r}1)} & \mathcal{L}^{(\mathrm{r}2)} & \mathcal{L}^{(\mathrm{rr})} \end{pmatrix} \begin{pmatrix} f^{(0)} \\ f^{(1)} \\ f^{(2)} \\ f^{(\mathrm{r})} \end{pmatrix}, \tag{4.56}$$

where

$$\mathcal{A}^{(kl)} f^{(l)} = \frac{\partial}{\partial x_i} \mathcal{A}_i^{(kl)} f^{(l)}, \qquad \mathcal{A}_i^{(kl)} = \mathcal{P}^{(k)} \xi_i \mathcal{P}^{(l)}, \qquad \mathcal{L}^{(kl)} f^{(l)} = \mathcal{P}^{(k)} \mathcal{L} f^{(l)}, \tag{4.57}$$

and they satisfy

$$\langle g^{(k)}, \mathcal{A}_i^{(kl)} g^{(l)} \rangle = \langle \mathcal{A}_i^{(lk)} g^{(k)}, g^{(l)} \rangle, \qquad \langle g^{(k)}, \mathcal{L}^{(kl)} g^{(l)} \rangle = \langle \mathcal{L}^{(lk)} g^{(k)}, g^{(l)} \rangle \tag{4.58}$$

for all $g^{(k)} \in \mathbb{V}^{(k)}$ and $g^{(l)} \in \mathbb{V}^{(l)}$.

It is well known that the super-Burnett equations can be derived via three Maxwellian iterations applied to the Boltzmann equation, which begin with the initial value

$$f_0^{(1)} = f_0^{(2)} = f_0^{(r)} = 0, \tag{4.59}$$

and proceeds from the jth iteration to the $(j+1)$th iteration according to

$$\frac{\partial}{\partial t} \begin{pmatrix} f_j^{(1)} \\ f_j^{(2)} \\ f_j^{(r)} \end{pmatrix} + \begin{pmatrix} \mathcal{A}^{(10)} & \mathcal{A}^{(11)} & \mathcal{A}^{(12)} & \mathcal{A}^{(1r)} \\ \mathcal{A}^{(20)} & \mathcal{A}^{(21)} & \mathcal{A}^{(22)} & \mathcal{A}^{(2r)} \\ \mathcal{A}^{(r0)} & \mathcal{A}^{(r1)} & \mathcal{A}^{(r2)} & \mathcal{A}^{(rr)} \end{pmatrix} \begin{pmatrix} f^{(0)} \\ f_j^{(1)} \\ f_j^{(2)} \\ f_j^{(r)} \end{pmatrix} = \frac{1}{Kn} \begin{pmatrix} \mathcal{L}^{(11)} & \mathcal{L}^{(12)} & \mathcal{L}^{(1r)} \\ \mathcal{L}^{(21)} & \mathcal{L}^{(22)} & \mathcal{L}^{(2r)} \\ \mathcal{L}^{(r1)} & \mathcal{L}^{(r2)} & \mathcal{L}^{(rr)} \end{pmatrix} \begin{pmatrix} f_{j+1}^{(1)} \\ f_{j+1}^{(2)} \\ f_{j+1}^{(r)} \end{pmatrix}. \tag{4.60}$$

The super-Burnett equations can be written in the form

$$\frac{\partial f^{(0)}}{\partial t} + \mathcal{A}^{(00)} f^{(0)} + \mathcal{A}^{(01)} f_3^{(1)} + \mathcal{A}^{(02)} f_3^{(2)} + \mathcal{A}^{(02)} f_3^{(3)} = 0. \tag{4.61}$$

To show that (4.33) have the super-Burnett order, we just need to demonstrate that the derivation of super-Burnett equations does not involve any operators that do not appear in (4.33). Below, we carry out the derivation step by step in the following subsections.

4.4.1. *First Maxwellian iteration*

Setting $j = 0$ in (4.60) and using the initial data $f_0^{(1)} = f_0^{(2)} = f_0^{(r)} = 0$, we obtain

$$\begin{pmatrix} \mathcal{A}^{(10)} f^{(0)} \\ \mathcal{A}^{(20)} f^{(0)} \\ \mathcal{A}^{(r0)} f^{(0)} \end{pmatrix} = \frac{1}{Kn} \begin{pmatrix} \mathcal{L}^{(11)} & \mathcal{L}^{(12)} & \mathcal{L}^{(1r)} \\ \mathcal{L}^{(21)} & \mathcal{L}^{(22)} & \mathcal{L}^{(2r)} \\ \mathcal{L}^{(r1)} & \mathcal{L}^{(r2)} & \mathcal{L}^{(rr)} \end{pmatrix} \begin{pmatrix} f_1^{(1)} \\ f_1^{(2)} \\ f_1^{(r)} \end{pmatrix}. \tag{4.62}$$

By Gaussian elimination,

$$\begin{pmatrix} \mathcal{A}^{(10)} f^{(0)} \\ [\mathcal{A}^{(20)} - \mathcal{L}^{(21)}(\mathcal{L}^{(11)})^{-1}\mathcal{A}^{(10)}] f^{(0)} \\ [\mathcal{A}^{(r0)} - \mathcal{L}^{(r1)}(\mathcal{L}^{(11)})^{-1}\mathcal{A}^{(10)}] f^{(0)} \end{pmatrix} = \frac{1}{Kn} \begin{pmatrix} \mathcal{L}^{(11)} & \mathcal{L}^{(12)} & \mathcal{L}^{(1r)} \\ & \mathcal{L}_*^{(22)} & \mathcal{L}_*^{(2r)} \\ & \mathcal{L}_*^{(r2)} & \mathcal{L}_*^{(rr)} \end{pmatrix} \begin{pmatrix} f_1^{(1)} \\ f_1^{(2)} \\ f_1^{(r)} \end{pmatrix}, \tag{4.63}$$

where

$$\mathcal{L}_*^{(22)} = \mathcal{L}^{(22)} - \mathcal{L}^{(21)}(\mathcal{L}^{(11)})^{-1}\mathcal{L}^{(12)}, \qquad \mathcal{L}_*^{(2r)} = \mathcal{L}^{(2r)} - \mathcal{L}^{(21)}(\mathcal{L}^{(11)})^{-1}\mathcal{L}^{(1r)},$$
$$\mathcal{L}_*^{(r2)} = \mathcal{L}^{(r2)} - \mathcal{L}^{(r1)}(\mathcal{L}^{(11)})^{-1}\mathcal{L}^{(12)}, \qquad \mathcal{L}_*^{(rr)} = \mathcal{L}^{(rr)} - \mathcal{L}^{(r1)}(\mathcal{L}^{(11)})^{-1}\mathcal{L}^{(1r)}. \tag{4.64}$$

Note that throughout the iterations, we always have $f_j^{(2)} \sim o(Kn)$ and $f_j^{(r)} \sim o(Kn^2)$, which requires

$$\mathcal{A}^{(20)} - \mathcal{L}^{(21)}(\mathcal{L}^{(11)})^{-1}\mathcal{A}^{(10)} = \mathcal{A}^{(r0)} - \mathcal{L}^{(r1)}(\mathcal{L}^{(11)})^{-1}\mathcal{A}^{(10)} = 0. \tag{4.65}$$

Thus, the result of the first Maxwellian iteration can be written as

$$f_1^{(1)} = Kn(\mathcal{L}^{(11)})^{-1}\mathcal{A}^{(10)} f^{(0)}, \qquad f_1^{(2)} = 0, \qquad f_1^{(r)} = 0. \tag{4.66}$$

For simplicity, we define $\mathcal{S}_1^{(10)} = (\mathcal{L}^{(11)})^{-1}\mathcal{A}^{(10)}$, so that $f_1^{(1)} = Kn\mathcal{S}_1^{(10)} f^{(0)}$.

4.4.2. *Second Maxwellian iteration*

Setting $j = 0$ in (4.60) and using the result of the first Maxwellian iteration, we get

$$
\frac{\partial}{\partial t} \begin{pmatrix} Kn\mathcal{S}_1^{(10)} f^{(0)} \\ 0 \\ 0 \end{pmatrix} + \begin{pmatrix} \left(\mathcal{A}^{(10)} + Kn\mathcal{A}^{(11)}\mathcal{S}_1^{(10)} \right) f^{(0)} \\ \left(\mathcal{A}^{(20)} + Kn\mathcal{A}^{(21)}\mathcal{S}_1^{(10)} \right) f^{(0)} \\ \left(\mathcal{A}^{(r0)} + Kn\mathcal{A}^{(r1)}\mathcal{S}_1^{(10)} \right) f^{(0)} \end{pmatrix}
$$
$$
= \frac{1}{Kn} \begin{pmatrix} \mathcal{L}^{(11)} & \mathcal{L}^{(12)} & \mathcal{L}^{(1r)} \\ \mathcal{L}^{(21)} & \mathcal{L}^{(22)} & \mathcal{L}^{(2r)} \\ \mathcal{L}^{(r1)} & \mathcal{L}^{(r2)} & \mathcal{L}^{(rr)} \end{pmatrix} \begin{pmatrix} f_2^{(1)} \\ f_2^{(2)} \\ f_2^{(r)} \end{pmatrix}. \tag{4.67}
$$

Next, we perform the following operations.

(i) Replace the time derivative with the spatial derivative using

$$
\frac{\partial f^{(0)}}{\partial t} + \mathcal{A}^{(00)} f^{(0)} = O(Kn), \tag{4.68}
$$

where the $O(Kn)$ part can be discarded and it does not affect the order of accuracy.

(ii) Apply Gaussian elimination and (4.65) to obtain

$$
\begin{pmatrix} \left[\mathcal{A}^{(10)} + Kn\mathcal{A}^{(11)}\mathcal{S}_1^{(10)} - Kn\mathcal{S}_1^{(10)}\mathcal{A}^{(00)} \right] f^{(0)} \\ Kn \left[\mathcal{A}^{(21)}\mathcal{S}_1^{(10)} - \mathcal{L}^{(21)}(\mathcal{L}^{(11)})^{-1} \left(\mathcal{A}^{(11)}\mathcal{S}_1^{(10)} - \mathcal{S}_1^{(10)}\mathcal{A}^{(00)} \right) \right] f^{(0)} \\ Kn \left[\mathcal{A}^{(r1)}\mathcal{S}_1^{(10)} - \mathcal{L}^{(r1)}(\mathcal{L}^{(11)})^{-1} \left(\mathcal{A}^{(11)}\mathcal{S}_1^{(10)} - \mathcal{S}_1^{(10)}\mathcal{A}^{(00)} \right) \right] f^{(0)} \end{pmatrix}
$$
$$
= \frac{1}{Kn} \begin{pmatrix} \mathcal{L}^{(11)} & \mathcal{L}^{(12)} & \mathcal{L}^{(1r)} \\ & \mathcal{L}_*^{(22)} & \mathcal{L}_*^{(2r)} \\ & \mathcal{L}_*^{(r2)} & \mathcal{L}_*^{(rr)} \end{pmatrix} \begin{pmatrix} f_2^{(1)} \\ f_2^{(2)} \\ f_2^{(r)} \end{pmatrix}. \tag{4.69}
$$

(iii) Apply Gaussian elimination again to eliminate $\mathcal{L}_*^{(r2)}$. Then the last equation in the system becomes

$$
Kn\mathcal{B}^{(r0)} f^{(0)} = \frac{1}{Kn} \left(\mathcal{L}_*^{(rr)} - \mathcal{L}_*^{(r2)}(\mathcal{L}_*^{(22)})^{-1}\mathcal{L}_*^{(2r)} \right) f_2^{(r)}, \tag{4.70}
$$

with

$$
\mathcal{B}^{(r0)} = \left(\mathcal{A}^{(r1)} - \mathcal{L}_*^{(r2)}(\mathcal{L}_*^{(22)})^{-1}\mathcal{A}^{(21)} \right) \mathcal{S}_1^{(10)}
$$
$$
- \left(\mathcal{L}^{(r1)} - \mathcal{L}_*^{(r2)}(\mathcal{L}_*^{(22)})^{-1}\mathcal{L}^{(21)} \right) (\mathcal{L}^{(11)})^{-1} \left(\mathcal{A}^{(11)}\mathcal{S}_1^{(10)} - \mathcal{S}_1^{(10)}\mathcal{A}^{(00)} \right). \tag{4.71}
$$

Due to the fact that $f_2^{(r)} \sim o(Kn^2)$, the operator $\mathcal{B}^{(r0)}$ has to be zero, and thus $f_2^{(r)} = 0$, and $f_2^{(1)}$ and $f_2^{(2)}$ can be solved from (4.69). The results are

$$
f_2^{(1)} = Kn\mathcal{S}_1^{(10)} f^{(0)} - Kn^2(\mathcal{L}^{(11)})^{-1}\mathcal{L}^{(12)}(\mathcal{L}_*^{(22)})^{-1}\mathcal{A}^{(11)}\mathcal{S}_1^{(10)} f^{(0)} + Kn^2 \left(\mathcal{L}^{(11)} \right)^{-1}
$$
$$
\times \left(\mathcal{I} - \mathcal{L}^{(12)}(\mathcal{L}_*^{(22)})^{-1}\mathcal{L}^{(21)}(\mathcal{L}^{(11)})^{-1} \right) \left(\mathcal{A}^{(11)}\mathcal{S}_1^{(10)} - \mathcal{S}_1^{(10)}\mathcal{A}^{(00)} \right) f^{(0)}, \tag{4.72}
$$
$$
f_2^{(2)} = Kn^2(\mathcal{L}_*^{(22)})^{-1} \left[\mathcal{A}^{(21)}\mathcal{S}_1^{(10)} - \mathcal{L}^{(21)}(\mathcal{L}^{(11)})^{-1} \left(\mathcal{A}^{(11)}\mathcal{S}_1^{(10)} - \mathcal{S}_1^{(10)}\mathcal{A}^{(00)} \right) \right] f^{(0)}. \tag{4.73}
$$

For conciseness, below we write these equations in the following simpler form:

$$f_2^{(1)} = Kn\mathcal{S}_1^{(10)} f^{(0)} + Kn^2 \mathcal{S}_2^{(10)} f^{(0)}, \qquad f_2^{(2)} = Kn^2 \mathcal{S}_2^{(20)} f^{(0)}. \qquad (4.74)$$

4.4.3. *Third Maxwellian iteration*

Similarly, the third Maxwellian iteration requires to find $f_3^{(1)}$, $f_3^{(2)}$ and $f_3^{(3)}$ from (4.60) with $j = 2$. However, for the purpose of deriving super-Burnett equations, only the first equation is needed. Here we rewrite this equation below:

$$\frac{\partial}{\partial t} \left(Kn\mathcal{S}_1^{(10)} f^{(0)} + Kn^2 \mathcal{S}_2^{(20)} f^{(0)} \right)$$
$$+ \mathcal{A}^{(10)} f^{(0)} + Kn\mathcal{A}^{(11)} \mathcal{S}_1^{(10)} f^{(0)} + Kn^2 \left(\mathcal{A}^{(11)} \mathcal{S}_2^{(10)} + \mathcal{A}^{(12)} \mathcal{S}_2^{(20)} \right) f^{(0)}$$
$$= \frac{1}{Kn} \left(\mathcal{L}^{(11)} f_3^{(1)} + \mathcal{L}^{(12)} f_3^{(2)} + \mathcal{L}^{(1r)} f_3^{(r)} \right). \qquad (4.75)$$

Further simplification again requires the time derivatives to be replaced without affecting the order of magnitude. This can be done by using

$$\frac{\partial}{\partial t} \left(Kn\mathcal{S}_1^{(10)} f^{(0)} + Kn^2 \mathcal{S}_2^{(20)} f^{(0)} \right) = -Kn\mathcal{S}_1^{(10)} \mathcal{A}^{(00)} f^{(0)}$$
$$- Kn^2 (\mathcal{S}_1^{(10)} \mathcal{A}^{(01)} \mathcal{S}_1^{(10)} + \mathcal{S}_2^{(20)} \mathcal{A}^{(00)}) f^{(0)} + O(Kn^3), \qquad (4.76)$$

which leads to

$$\mathcal{L}^{(11)} f_3^{(1)} + \mathcal{L}^{(12)} f_3^{(2)} + \mathcal{L}^{(1r)} f_3^{(r)} = Kn\mathcal{A}^{(10)} f^{(0)} + Kn^2 \left(\mathcal{A}^{(11)} \mathcal{S}_1^{(10)} - \mathcal{S}_1^{(10)} \mathcal{A}^{(00)} \right) f^{(0)}$$
$$+ Kn^3 \left(\mathcal{A}^{(11)} \mathcal{S}_2^{(10)} + \mathcal{A}^{(12)} \mathcal{S}_2^{(20)} - \mathcal{S}_2^{(20)} \mathcal{A}^{(00)} - \mathcal{S}_1^{(10)} \mathcal{A}^{(01)} \mathcal{S}_1^{(10)} \right) f^{(0)}. \qquad (4.77)$$

4.4.4. *Super-Burnett equations*

By the adjointness (4.58) and the equalities (4.65), we have

$$\mathcal{A}^{(02)} = \mathcal{A}^{(01)} (\mathcal{L}^{(11)})^{-1} \mathcal{L}^{(12)}, \qquad \mathcal{A}^{(0r)} = \mathcal{A}^{(01)} (\mathcal{L}^{(11)})^{-1} \mathcal{L}^{(1r)}. \qquad (4.78)$$

Thus, the super-Burnett equations (4.61) can be reformulated as

$$\frac{\partial f^{(0)}}{\partial t} + \mathcal{A}^{(00)} f^{(0)} + \mathcal{A}^{(01)} (\mathcal{L}^{(11)})^{-1} \left(\mathcal{L}^{(11)} f_3^{(1)} + \mathcal{L}^{(12)} f_3^{(2)} + \mathcal{L}^{(1r)} f_3^{(r)} \right) = 0. \quad (4.79)$$

The final super-Burnett equations can be found by plugging (4.77) into the above equation.

Such a derivation of super-Burnett equations shows that the final equations depend only on the operators

$$\mathcal{A}^{(00)}, \mathcal{A}^{(01)}, \mathcal{A}^{(02)}, \mathcal{A}^{(10)}, \mathcal{A}^{(11)}, \mathcal{A}^{(12)}, \mathcal{A}^{(20)}, \mathcal{A}^{(21)}, \mathcal{L}^{(11)}, \mathcal{L}^{(12)}, \mathcal{L}^{(21)}, \mathcal{L}^{(22)}, \quad (4.80)$$

and the operators

$$\mathcal{A}^{(0r)}, \mathcal{A}^{(1r)}, \mathcal{A}^{(22)}, \mathcal{A}^{(2r)}, \mathcal{A}^{(r0)}, \mathcal{A}^{(r1)}, \mathcal{A}^{(r2)}, \mathcal{A}^{(rr)}, \mathcal{L}^{(1r)}, \mathcal{L}^{(2r)}, \mathcal{L}^{(r1)}, \mathcal{L}^{(r2)}, \mathcal{L}^{(rr)} \quad (4.81)$$

do not appear in the final equations. Therefore, we can set these operators to be zero, and the resulting equations still have the super-Burnett order. Meanwhile, the time derivative $\partial_t f_2$ does not participate in the derivation, which can also be set to zero without affecting the super-Burnett order.

5. Onsager boundary conditions

In microflows, boundary conditions play a key role in describing the rarefaction effect. In this work we focus mainly on the wall boundary condition, and we restrict ourselves to Maxwell's accommodation model in Maxwell (1879), where it is assumed that all gas molecules hitting the wall are reflected either specularly or diffusively, according to the accommodation coefficient of the wall, which specifies the probability of diffusive reflection. In this section we follow the notation used in (3.9)–(3.17) and use n, τ_1 and τ_2 instead of 1, 2 and 3 as indices of vectors or tensors. Thus, Maxwell's wall boundary conditions for the Boltzmann equation (1.1) can be formulated as

$$f(\xi_n, \xi_{\tau_1}, \xi_{\tau_2}) = \chi f_W(\xi_n, \xi_{\tau_1}, \xi_{\tau_2}) + (1 - \chi) f(-\xi_n, \xi_{\tau_1}, \xi_{\tau_2}), \qquad \xi_n < 0. \tag{5.1}$$

Here χ is the accommodation coefficient, and we have omitted the spatial and temporal variables since the boundary condition is valid for any boundary point $\boldsymbol{x}$ and time t, and there are no spatial or temporal derivatives involved. The function f_W describes the diffusive reflection, which depends on the wall velocity $\boldsymbol{v}_W$ and the wall temperature θ_W. Under the linearised setting, it has the form

$$f_W(\boldsymbol{\xi}) = \rho_W + v_{W,\tau_1}\xi_{\tau_1} + v_{W,\tau_2}\xi_{\tau_2} + \frac{1}{2}\theta_W(|\boldsymbol{\xi}|^2 - 3), \tag{5.2}$$

where

$$\rho_W = \sqrt{2\pi}\langle(\xi_n)_+, f\rangle - \frac{\theta_W}{2}, \tag{5.3}$$

which is chosen such that $\langle \xi_n, f \rangle = 0$, meaning that the normal component of the velocity is zero.

In Cai *et al.* (2024b), the boundary condition (5.1) has been equivalently reformulated to

$$\mathcal{P}_{odd}f = \frac{2\chi}{2 - \chi}\mathcal{P}_{odd}\mathcal{C}(f_W - \mathcal{P}_{even}f), \tag{5.4}$$

where

$$\mathcal{P}_{odd}g(\xi_n, \xi_{\tau_1}, \xi_{\tau_2}) = \frac{g(\xi_n, \xi_{\tau_1}, \xi_{\tau_2}) - g(-\xi_n, \xi_{\tau_1}, \xi_{\tau_2})}{2}, \tag{5.5}$$

$$\mathcal{P}_{even}g(\xi_n, \xi_{\tau_1}, \xi_{\tau_2}) = \frac{g(\xi_n, \xi_{\tau_1}, \xi_{\tau_2}) + g(-\xi_n, \xi_{\tau_1}, \xi_{\tau_2})}{2}, \tag{5.6}$$

$$\mathcal{C}g(\xi_n, \xi_{\tau_1}, \xi_{\tau_2}) = \begin{cases} g(\xi_n, \xi_{\tau_1}, \xi_{\tau_2}) & \text{if } \xi_n < 0, \\ 0 & \text{if } \xi_n > 0. \end{cases} \tag{5.7}$$

Such formulation of the boundary condition better fits Grad's theory of boundary conditions for moment equations (Grad 1949), where it is required that all boundary conditions should only be imposed on odd moments. A direct application of Galerkin's method on (5.4) leads to Grad's boundary conditions. However, these boundary conditions may not satisfy the stability requirement (1.4). Our boundary conditions (3.9)–(3.17) are based on the theory of Onsager boundary conditions developed in Sarna & Torrilhon (2018), Öttinger *et al.* (2023) and Cai *et al.* (2024b), which can be demonstrated to satisfy the general form (1.6). In particular, we follow the formulation in Cai *et al.* (2024b) that rewrites (5.4) as

$$\mathcal{P}_{odd}f = \frac{2\chi}{2 - \chi}\mathcal{S}\xi_n(f_W - \mathcal{P}_{even}f), \tag{5.8}$$

where $\mathcal{S} = \mathcal{P}_{odd}\mathcal{C}\xi_n^{-1}$. Thus, the operator $(2\chi/(2-\chi))\mathcal{S}$ corresponds to the negative semidefinite matrix $\mathbf{Q}$, and ξ_n corresponds to the matrix $\mathbf{A}_{oe}$. More details on the discretisation will be given in the following subsections.

REMARK 2. *Note that existing Onsager boundary conditions such as those derived in Sarna & Torrilhon (2018) and Cai et al. (2024b) cannot be directly applied to our systems. The primary reason is that our system generally requires more boundary conditions than previous R13 equations, due to a larger number of moments considered in our derivation. For instance, the boundary conditions for R13 equations with Maxwell molecules consist of 10 equations at each boundary point (Sarna & Torrilhon 2018). However, in our system, the equations of θ and $\boldsymbol{v}$ become parabolic, requiring three more boundary conditions to determine the solution. This motivates us to derive the boundary conditions from scratch and guarantee reliable matching between the equations and boundary conditions.*

5.1. *Onsager boundary conditions*

The abstract form of the R13 equations (4.33) shows that all operators in the Boltzmann equation are approximated by operators in $\mathbb{V} = \mathbb{V}^{(0)} \oplus \mathbb{V}^{(1)} \oplus \mathbb{V}^{(2)}$. If we rewrite the Boltzmann equation (1.1) as

$$\frac{\partial}{\partial t}(\mathcal{I}f) + \frac{\partial}{\partial x_k}(\xi_k f) = \frac{1}{Kn}\mathcal{L}f, \tag{5.9}$$

then the identity operator $\mathcal{I}$ is approximated by $\mathcal{P}^{(01)} := \mathcal{P}^{(0)} + \mathcal{P}^{(1)}$, the velocity operator ξ_k is approximated by

$$\mathcal{A}_k = \mathcal{P}^{(01)}\xi_k\mathcal{P}^{(01)} + \mathcal{P}^{(2)}\xi_k\mathcal{P}^{(01)} + \mathcal{P}^{(01)}\xi_k\mathcal{P}^{(2)} \tag{5.10}$$

and the collision operator $\mathcal{L}$ is approximated by $(\mathcal{P}^{(1)} + \mathcal{P}^{(2)})\mathcal{L}(\mathcal{P}^{(1)} + \mathcal{P}^{(2)})$. Similarly, when deriving boundary conditions for moment equations, operators in (5.8) are also approximated by using operators on $\mathbb{V}$.

We first study the operator $\mathcal{P}_{even}$, which extracts the even part of a function with respect to ξ_n. The discretisation of $\mathcal{P}_{even}$ is simply its restriction on $\mathbb{V}$. Note that all the basis functions of $\mathbb{V}$ are given in (4.35), from which it is not difficult to observe that

$$\mathbb{V}_{even} := \mathcal{P}_{even}\mathbb{V} = \text{span}\{\psi^0, \psi^1, \psi_{\tau_1}^0, \psi_{\tau_2}^0; \phi_{\tau_1}^1, \phi_{\tau_2}^1, \phi_{\tau_1\tau_1}^0, \phi_{\tau_2\tau_2}^0, \phi_{\tau_1\tau_2}^0; \phi^2, \phi_{\tau_1}^2, \phi_{\tau_2}^2,$$
$$\phi_{\tau_1}^3, \phi_{\tau_2}^3, \phi_{\tau_1\tau_1}^1, \phi_{\tau_2\tau_2}^1, \phi_{\tau_1\tau_2}^1, \phi_{\tau_1\tau_1}^2, \phi_{\tau_2\tau_2}^2, \phi_{\tau_1\tau_2}^2, \phi_{\tau_1\tau_1\tau_1}^0, \phi_{\tau_1\tau_1\tau_2}^0, \phi_{\tau_1\tau_2\tau_2}^0, \phi_{\tau_2\tau_2\tau_2}^0\}. \tag{5.11}$$

It is clear that $f_W \in \mathbb{V}_{even}$. Thus, the velocity operator ξ_n should be discretised as the restriction of $\mathcal{A}_n$ on $\mathbb{V}_{even}$. We denote its range by $\mathbb{V}_{odd} := \mathcal{A}_n\mathbb{V}_{even}$. By straightforward calculation,

$$\mathbb{V}_{odd} = \text{span}\left\{\psi_n^0; \phi_n^1, \phi_{n\tau_1}^0, \phi_{n\tau_2}^0; \phi_{n\tau_1}^1, \phi_{n\tau_2}^1, \phi_{n\tau_1}^2, \phi_{n\tau_2}^2, \phi_{n\tau_1\tau_2}^0, \phi_{n\tau_1\tau_1}^0 + \frac{1}{2}\phi_{nnn}^0, \phi_n^2 \right.$$
$$\left. + \frac{c_1^{3,1}}{c_1^{2,1}}\phi_n^3, \mu_1\phi_{nnn}^0 + \mu_2\left(\phi_n^3 - \frac{c_1^{3,1}}{c_1^{2,1}}\phi_n^2\right)\right\}, \tag{5.12}$$

where

$$\mu_1 = 3A_{5,11}\left[1 + \left(\frac{c_1^{3,1}}{c_1^{2,1}}\right)^2\right], \qquad \mu_2 = 2\left(A_{58} - \frac{c_1^{3,1}}{c_1^{2,1}}A_{57}\right). \tag{5.13}$$

Note that the basis functions listed in (5.12) are orthogonal basis functions, and the orthogonality will simplify our derivations of boundary conditions. The discretisation the operator $\mathcal{S}$ is then a straightforward application of Galerkin's method with the subspace $\mathbb{V}_{odd}$.

We would like to comment that $\mathbb{V}_{odd} \oplus \mathbb{V}_{even}$ is only a proper subspace of $\mathbb{V}$, or equivalently, $\mathbb{V}_{odd} \neq \mathcal{P}_{odd}\mathbb{V}$. The reason is that the operator $\mathcal{A}_n$ has a null space being a subspace of $\mathcal{P}_{odd}\mathbb{V}$. This can be seen by focusing on the x_n derivatives in (4.44), (4.45) and (4.48), and find that by the linear combination

$$
A_{5,11}\left(c_1^{3,1} \times (4.29) - c_1^{2,1} \times (4.30)\right) - \frac{5}{3}\left(c_1^{3,1}A_{57} - c_1^{2,1}A_{58}\right) \times (4.33) \tag{5.14}
$$

the x_n derivative will be cancelled out. This indicates that

$$
\mathcal{A}_n\left(3A_{5,11}\left(c_1^{3,1}\phi_n^2 - c_1^{2,1}\phi_n^3\right) - \frac{175}{6}\left(c_1^{3,1}A_{57} - c_1^{2,1}A_{58}\right)\phi_{nnn}^0\right) = 0, \tag{5.15}
$$

which reveals the null space of $\mathcal{A}_n$. The function space $\mathbb{V}_{odd}$ defined in (5.12) is orthogonal to the null space of $\mathcal{A}_n$.

Practically, all the boundary conditions are written as

$$
\langle \phi_{odd}^i, f_{odd} \rangle = \frac{2\chi}{2 - \chi}\sum_j \frac{\langle \phi_{odd}^i, \mathcal{C}\xi_n^{-1}\phi_{odd}^j\rangle\langle \phi_{odd}^j, \mathcal{A}_n(f_W - f_{even})\rangle}{\langle \phi_{odd}^j, \phi_{odd}^j\rangle}, \quad j = 1, \ldots, 12, \tag{5.16}
$$

where ϕ_{odd}^j refers to the jth basis function of $\mathbb{V}_{odd}$ (see (5.12)), and f_{odd} and f_{even} are, respectively, the projection of f onto the function space $\mathbb{V}_{odd}$ and $\mathbb{V}_{even}$. Note that this formula requires the orthogonality of the basis $\{\phi_{odd}^j\}$. Calculation of the integrals in (5.16) requires specifying the collision model. Here we only provide the general form

$$
\begin{pmatrix} v_n \\ \bar{q}_n \\ u_n^2 + \frac{c_1^{3,1}}{c_1^{2,1}}u_n^3 \\ \bar{\sigma}_{\tau_1 n} \\ \bar{\sigma}_{\tau_2 n} \\ u_{\tau_1 n}^1 \\ u_{\tau_2 n}^1 \\ u_{\tau_1 n}^2 \\ u_{\tau_2 n}^2 \\ u_{nnn}^0 + \frac{\mu_2}{\mu_1}\left(u_n^3 - \frac{c_1^{3,1}}{c_1^{2,1}}u_n^2\right) \\ u_{\tau_1\tau_1 n}^0 + \frac{1}{2}u_{nnn}^0 \\ u_{\tau_1\tau_2 n}^0 \end{pmatrix} = \frac{2\chi}{2 - \chi}Z \begin{pmatrix} V_n \\ \bar{Q}_n \\ U_n^2 + \frac{c_1^{3,1}}{c_1^{2,1}}U_n^3 \\ \bar{\Sigma}_{\tau_1 n} \\ \bar{\Sigma}_{\tau_2 n} \\ U_{\tau_1 n}^1 \\ U_{\tau_2 n}^1 \\ U_{\tau_1 n}^2 \\ U_{\tau_2 n}^2 \\ U_{nnn}^0 + \frac{\mu_2}{\mu_1}\left(U_n^3 - \frac{c_1^{3,1}}{c_1^{2,1}}U_n^2\right) \\ U_{\tau_1\tau_1 n}^0 + \frac{1}{2}U_{nnn}^0 \\ U_{\tau_1\tau_2 n}^0 \end{pmatrix}, \tag{5.17}
$$

where the capitalised variables are given by

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$$V_n = (\rho^W - \rho) + (\theta^W - \theta) - c_2^{0,0}\bar{\sigma}_{nn} - \sqrt{15}(c_2^{1,0}u_{nn}^1 + c_2^{2,0}u_{nn}^2),$$

$$\bar{Q}_n = \frac{5}{2}c_1^{1,1}(\theta^W - \theta) + \frac{\sqrt{2}}{6}A_{45}\bar{\sigma}_{nn} + \sqrt{\frac{5}{6}}(A_{46}u^2 + A_{49}u_{nn}^1 + A_{4,10}u_{nn}^2),$$

$$U_n^2 = \frac{\sqrt{15}}{3}\left(\frac{\sqrt{2}}{2}c_1^{2,1}(\theta - \theta^W) - \frac{1}{15}A_{57}\bar{\sigma}_{nn}\right),$$

$$U_n^3 = \frac{\sqrt{15}}{3}\left(\frac{\sqrt{2}}{2}c_1^{3,1}(\theta - \theta^W) - \frac{1}{15}A_{58}\bar{\sigma}_{nn}\right),$$

$$\bar{\Sigma}_{\tau_i n} = c_2^{0,0}\left(v_{\tau_i}^W - v_{\tau_i}\right) + \frac{\sqrt{2}}{15}A_{45}\bar{q}_{\tau_i} - \frac{1}{\sqrt{15}}\left(A_{57}u_{\tau_i}^2 + A_{58}u_{\tau_i}^3 + 2A_{5,11}u_{\tau_i nn}^0\right), \quad i = 1, 2,$$

$$U_{\tau_i n}^1 = \frac{\sqrt{15}}{15}\left(c_2^{1,0}(v_{\tau_i}^W - v_{\tau_i}) + \frac{\sqrt{2}}{15}A_{49}\bar{q}_{\tau_i}\right), \quad i = 1, 2,$$

$$U_{\tau_i n}^2 = \frac{\sqrt{15}}{15}\left(c_2^{2,0}(v_{\tau_i}^W - v_{\tau_i}) + \frac{\sqrt{2}}{15}A_{4,10}\bar{q}_{\tau_i}\right), \quad i = 1, 2,$$

$$U_{\tau_i \tau_j n}^0 = \frac{2\sqrt{15}}{1575}A_{5,11}\left(\frac{2}{5}\delta_{ij}\bar{\sigma}_{nn} - \bar{\sigma}_{\tau_i \tau_j}\right), \quad i, j = 1, 2,$$

$$U_{nnn}^0 = -\frac{2\sqrt{15}}{875}A_{5,11}\bar{\sigma}_{nn}, \tag{5.18}$$

and the structure of the matrix Z is ("$*$" means a non-zero entry)

$$Z = \begin{pmatrix} * & * & * & 0 & 0 & 0 & 0 & 0 & 0 & * & * & 0 \\ * & * & * & 0 & 0 & 0 & 0 & 0 & 0 & * & * & 0 \\ * & * & * & 0 & 0 & 0 & 0 & 0 & 0 & * & * & 0 \\ 0 & 0 & 0 & * & 0 & * & 0 & * & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & * & 0 & * & 0 & * & 0 & 0 & 0 \\ 0 & 0 & 0 & * & 0 & * & 0 & * & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & * & 0 & * & 0 & * & 0 & 0 & 0 \\ 0 & 0 & 0 & * & 0 & * & 0 & * & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & * & 0 & * & 0 & * & 0 & 0 & 0 \\ * & * & * & 0 & 0 & 0 & 0 & 0 & 0 & * & * & 0 \\ * & * & * & 0 & 0 & 0 & 0 & 0 & 0 & * & * & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & * \end{pmatrix} = \begin{pmatrix} z_0 & \zeta_0^\mathsf{T} \\ \zeta_1 & Z_1 \end{pmatrix}. \tag{5.19}$$

The matrix Z is the discrete form of the operator $\mathcal{S} = \mathcal{P}_{odd}\mathcal{C}\xi_n^{-1}$, and is therefore similar to a symmetric and positive definite matrix. To complete the derivation, we still need to take into account the condition $v_n = \langle \xi_n, f \rangle = 0$, since V_n depends on ρ_W (see (5.3)), which has to be determined by this condition. Instead of solving ρ_W, an equivalent way is to solve V_n from the first equation of (5.17), and then plug the result into other equations. Such an equivalence is due to the fact that ρ^W appears only in V_n in all the quantities defined in (5.18). This leads to boundary conditions that have the same form as (5.17), but the matrix Z is replaced by

$$\begin{pmatrix} 0 & 0 \\ 0 & Z_1 - z_0^{-1}\zeta_1\zeta_0^\mathsf{T} \end{pmatrix}. \tag{5.20}$$

Since the Schur complement of a symmetric and positive definite matrix is still symmetric and positive definite, we can guarantee that the above matrix can still be viewed as a positive semidefinite operator.

Such boundary conditions satisfy all the properties required by the L^2 stability. However, spurious boundary layers are observed in the solution, which will be detailed in the next subsection.

5.2. *One-dimensional problems and spurious boundary layers*

To show the boundary layers in the solution, we consider the steady-state one-dimensional flow in which

$$v_2 = v_3 = \bar{q}_2 = \bar{q}_3 = \bar{\sigma}_{13} = \bar{\sigma}_{23} = 0, \qquad \bar{\sigma}_{22} = \bar{\sigma}_{33}. \tag{5.21}$$

These conditions come from the assumption that the distribution function satisfies $f(\boldsymbol{x}, \xi_1, \xi_2, \xi_3, t) = \tilde{f}(\boldsymbol{x}, \xi_1, \sqrt{\xi_2^2 + \xi_3^2}, t)$ for every $\boldsymbol{x}$ and t, meaning that f is axisymmetric about the axis $\xi_2 = \xi_3 = 0$. Under this assumption, only five variables remain and the equations have the form

$$\frac{\partial v}{\partial x} = 0, \tag{5.22}$$

$$\frac{2}{3}\frac{\partial v}{\partial x} + \frac{2}{3}k_0\frac{\partial \bar{q}}{\partial x} - k_1 Kn\frac{\partial^2 \theta}{\partial x^2} + k_2 Kn\frac{\partial^2 \bar{\sigma}}{\partial x^2} = 0, \tag{5.23}$$

$$\frac{\partial \rho}{\partial x} + \frac{\partial \theta}{\partial x} - \frac{2}{3}k_3 Kn\frac{\partial^2 v}{\partial x^2} - \frac{2}{3}k_4 Kn\frac{\partial^2 \bar{q}}{\partial x^2} + k_5\frac{\partial \bar{\sigma}}{\partial x} = 0, \tag{5.24}$$

$$\frac{5}{2}k_0\frac{\partial \theta}{\partial x} - \frac{5}{3}k_4 Kn\frac{\partial^2 v}{\partial x^2} - 2k_6 Kn\frac{\partial^2 \bar{q}}{\partial x^2} - \frac{8}{5}k_7 Kn\frac{\partial^2 \bar{q}}{\partial x^2} + k_8\frac{\partial \bar{\sigma}}{\partial x} = -\frac{2}{3}\frac{1}{Kn}l_1\bar{q}, \tag{5.25}$$

$$2k_2 Kn\frac{\partial^2 \theta}{\partial x^2} + \frac{4}{3}k_5\frac{\partial v}{\partial x} + \frac{8}{15}k_8\frac{\partial \bar{q}}{\partial x} - \frac{6}{5}k_9 Kn\frac{\partial^2 \bar{\sigma}}{\partial x^2} - \frac{2}{3}k_{10} Kn\frac{\partial^2 \bar{\sigma}}{\partial x^2} = -\frac{1}{Kn}l_2\bar{\sigma}. \tag{5.26}$$

Here time derivatives have been removed so that the solution of the equations correspond to the steady state of the fluid. In the one-dimensional case, the boundary conditions are reduced to

$$v = 0, \tag{5.27}$$

$$\bar{q} = s_n\tilde{\chi}\left[\hat{m}_{11}(\theta - \theta^W) + \hat{m}_{12}\bar{\sigma} - \hat{m}_{13}Kn\frac{\partial \bar{q}}{\partial x} - \frac{2}{3}\hat{m}_{14}Kn\frac{\partial \bar{q}}{\partial x} - \frac{2}{3}\hat{m}_{15}Kn\frac{\partial v}{\partial x}\right], \tag{5.28}$$

$$\hat{m}_{26}\bar{q} + \hat{m}_{27}Kn\frac{\partial \theta}{\partial x} - \hat{m}_{28}Kn\frac{\partial \bar{\sigma}}{\partial x}$$

$$= s_n\tilde{\chi}\left[-\hat{m}_{21}(\theta - \theta^W) + \hat{m}_{22}\bar{\sigma} + \hat{m}_{23}Kn\frac{\partial \bar{q}}{\partial x} + \frac{2}{3}\hat{m}_{24}Kn\frac{\partial \bar{q}}{\partial x} + \frac{2}{3}\hat{m}_{25}Kn\frac{\partial v}{\partial x}\right], \tag{5.29}$$

$$-\hat{m}_{66}\bar{q} - Kn\left(\frac{3}{5}\hat{m}_{67}\frac{\partial \bar{\sigma}}{\partial x} + \hat{m}_{68}\frac{\partial \bar{\sigma}}{\partial x} + \hat{m}_{69}\frac{\partial \theta}{\partial x}\right)$$

$$= s_n\tilde{\chi}\left[-\hat{m}_{61}(\theta - \theta^W) + \hat{m}_{62}\bar{\sigma} + \hat{m}_{63}Kn\frac{\partial \bar{q}}{\partial x} + \frac{2}{3}\hat{m}_{64}Kn\frac{\partial \bar{q}}{\partial x} + \frac{2}{3}\hat{m}_{65}Kn\frac{\partial v}{\partial x}\right], \tag{5.30}$$

where $s_n = 1$ at the right boundary and $s_n = -1$ at the left boundary. The coefficient $\hat{m}_{ij}$ is computed from the Onsager boundary conditions (5.17), which are not equal to the m_{ij} in our final boundary conditions, as shown in (3.9)–(3.17).

The one-dimensional equations (5.22)–(5.30) can be solved analytically. First, it is straightforward to get $v(x) = 0$ from (5.22) and (5.27). Second, by noting that variable ρ only appears in (5.24), we can solve other equations and then plug other variables into (5.24). Third, (5.23) reveals that $\partial \bar{q}/\partial x = (3/2k_0)Kn(k_1(\partial^2\theta/\partial x^2)) - (k_2(\partial^2\bar{\sigma}/\partial x^2))$, which indicates that

$$\bar{q}(x) = \frac{3}{2k_0}Kn\left(k_1\frac{\partial \theta}{\partial x} - k_2\frac{\partial \bar{\sigma}}{\partial x}\right) + C_{\bar{q}}, \tag{5.31}$$

with the constant $C_{\bar{q}}$ to be determined. Plugging $\bar{q}(x)$ into (5.25) and integrating the equation, we find that

$$Kn^2\left(-k_6 - \frac{4}{5}k_7\right)\frac{3}{k_0}\left(k_1\frac{\partial^2\theta}{\partial x^2} - k_2\frac{\partial^2\bar{\sigma}}{\partial x^2}\right) + \frac{5}{2}k_0\theta + k_8\bar{\sigma} = -\frac{l_1}{k_0}(k_1\theta - k_2\bar{\sigma}) + C_{\bar{q}}^1 x + C_{\bar{q}}^2, \tag{5.32}$$

where $C_{\bar{q}}^1 = -(2l_1/3Kn)C_{\bar{q}}$ and $C_{\bar{q}}^2$ are two constants to be determined. Similarly, plugging (5.31) into (5.26) yields

$$2k_2 Kn\frac{\partial^2\theta}{\partial x^2} + \frac{4k_8}{5k_0}Kn\left(k_1\frac{\partial^2\theta}{\partial x^2} - k_2\frac{\partial^2\bar{\sigma}}{\partial x^2}\right) - \left(\frac{6}{5}k_9 + \frac{2}{3}k_{10}\right)Kn\frac{\partial^2\bar{\sigma}}{\partial x^2} = -\frac{1}{Kn}l_2\bar{\sigma}. \tag{5.33}$$

We can then define

$$\xi = Kn\frac{\partial \theta}{\partial x}, \qquad \xi' = Kn\frac{\partial \bar{\sigma}}{\partial x}, \tag{5.34}$$

and reformulate (5.32) and (5.33) as

$$Kn\begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ -\left(k_6 + \frac{4}{5}k_7\right)\frac{3k_1}{k_0} & \left(k_6 + \frac{4}{5}k_7\right)\frac{3k_2}{k_0} & 0 & 0 \\ 2k_2 + \frac{4k_8k_1}{5k_0} & -\left(\frac{6}{5}k_9 + \frac{2}{3}k_{10} + \frac{4k_8k_2}{5k_0}\right) & 0 & 0 \end{pmatrix}\frac{\partial}{\partial x}\begin{pmatrix} \xi \\ \xi' \\ \theta \\ \bar{\sigma} \end{pmatrix}$$
$$+ \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & \frac{5}{2}k_0 + \frac{l_1k_1}{k_0} & k_8 - \frac{l_1k_2}{k_0} \\ 0 & 0 & 0 & l_2 \end{pmatrix}\begin{pmatrix} \xi \\ \xi' \\ \theta \\ \bar{\sigma} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ C_{\bar{q}}^1 x + C_{\bar{q}}^2 \\ 0 \end{pmatrix}. \tag{5.35}$$

By multiplying the inverse of the matrix in front of the first-order derivatives, the above equation has the following structure:

$$Kn\frac{\partial}{\partial x}\begin{pmatrix} \xi \\ \xi' \\ \theta \\ \bar{\sigma} \end{pmatrix} + \begin{pmatrix} 0 & 0 & b_{11} & b_{12} \\ 0 & 0 & b_{21} & b_{22} \\ -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix}\begin{pmatrix} \xi \\ \xi' \\ \theta \\ \bar{\sigma} \end{pmatrix} = \begin{pmatrix} c_1(C_{\bar{q}}^1 x + C_{\bar{q}}^2) \\ c_2(C_{\bar{q}}^1 x + C_{\bar{q}}^2) \\ 0 \\ 0 \end{pmatrix}. \tag{5.36}$$

In general, given the following ordinary differential equation (ODE) system

$$Kn\frac{\partial g}{\partial x} + Ag = r(x), \tag{5.37}$$

η	λ_1	λ_2
5	9.1287×10^{-1}	–
7	9.2648×10^{-1}	1.2696×10^{1}
10	9.2989×10^{-1}	7.6747
17	9.2904×10^{-1}	5.6909
∞	9.2248×10^{-1}	4.2387

Table 1. Eigenvalues in the general solution (5.40) for some inverse-power-law models with power index η.

its solution is

$$g(x) = e^{-Ax/Kn}g(0) + \frac{1}{Kn}\int_0^x e^{A(s-x)/Kn}r(s)\mathrm{d}s. \tag{5.38}$$

In our case, the matrix in (5.36) has four distinct eigenvalues $\pm\lambda_1$ and $\pm\lambda_2$ with

$$\lambda_j = \frac{\sqrt{(-1)^j\sqrt{b_{11}^2 - 2b_{22}b_{11} + b_{22}^2 + 4b_{12}b_{21}} - b_{11} - b_{22}}}{\sqrt{2}}, \qquad j = 1, 2. \tag{5.39}$$

The solution of (5.36) therefore has the form

$$\kappa_1 \sinh\left(\frac{\lambda_1 x}{Kn}\right) + \kappa_2 \cosh\left(\frac{\lambda_1 x}{Kn}\right) + \kappa_3 \sinh\left(\frac{\lambda_2 x}{Kn}\right) + \kappa_4 \cosh\left(\frac{\lambda_2 x}{Kn}\right) + \kappa_5 x + \kappa_6, \tag{5.40}$$

where the hyperbolic sines and cosines denote the Knudsen layers. Since $\lambda_1 \neq \lambda_2$, two boundary layers will be present in the general solution. In particular, when the magnitude of the eigenvalues is large or the Knudsen number is small, the solution would exhibit boundary layers.

For Maxwell molecules ($\eta = 5$), the above procedure of solving one-dimensional equations can be further simplified from the third step (see (5.31). By noting that $k_1 = k_2 = 0$, one can get $\partial\bar{q}/\partial x = 0$ and therefore, (5.31) becomes $\bar{q}(x) = C_{\bar{q}}$. Equation (5.33) becomes a second-order ODE for $\bar{\sigma}$, so that the general solution of $\bar{\sigma}(x)$ contains only one boundary layer. Furthermore, (5.32) is in absence of second-order derivatives, and thus,

$$\theta(x) = \frac{2}{5k_0}\left(C_{\bar{q}}^1 x + C_{\bar{q}}^2 - k_8\bar{\sigma}(x)\right), \tag{5.41}$$

showing that the boundary layer of θ has the same thickness as that of $\bar{\sigma}$. In general, when the type of molecules gets closer to Maxwell molecules, the second boundary layer will get thinner, which explains why there is only one boundary layer left for Maxwell molecules.

The thinness of the second boundary layer also indicates the largeness of the corresponding eigenvalue λ_2. To illustrate the magnitude of eigenvalues, we compute them according to (5.39) for various inverse-power-law models and summarise the results in table 1. For Maxwell molecules, only λ_1 is provided. The table clearly shows that all models share one similar eigenvalue λ_1 and each of the non-Maxwell cases has an additional larger eigenvalue λ_2. This eigenvalue λ_2 approaches infinity when η tends to 5.

The one-dimensional solutions on the domain $(-0.5, 0.5)$, with Knudsen number $Kn = 0.2$ and accommodation coefficients $\chi = 1$, are depicted in figure 1. The figure verifies that the larger eigenvalue λ_2 in non-Maxwell cases induces additional boundary layers compared with the Maxwell solutions. These boundary layers are non-physical according to previous results (see Hu, Yang & Cai 2020; Cai *et al.* 2024*b*) for the same problem.

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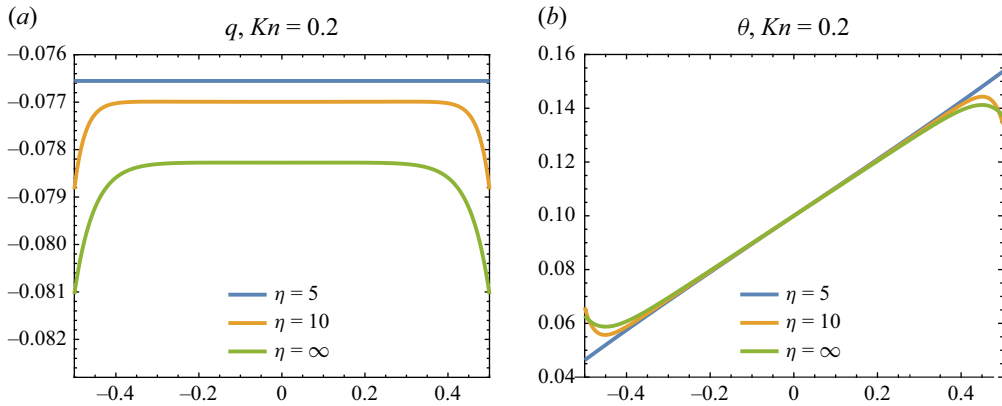
Figure 1. Plots of $\bar{q}$ and θ for the one-dimensional problem (5.22)–(5.30). Results are shown for (a) $\theta^W = 0$ and (b) $\theta^W = 0.2$.

In the next subsection we propose a revision to the Onsager boundary conditions derived in § 5.1 to remove the boundary layers, leading to our final boundary conditions (3.9)–(3.17).

5.3. *Removal of undesired boundary layers*

Our discussion will be based on the following general form of one-dimensional symmetric hyperbolic equations:

$$\begin{pmatrix} 0 & \mathbf{A}_{oe} \\ \mathbf{A}_{eo} & 0 \end{pmatrix} \frac{\partial}{\partial x} \begin{pmatrix} \boldsymbol{u}_o \\ \boldsymbol{u}_e \end{pmatrix} = \begin{pmatrix} \mathbf{L}_{oo} & 0 \\ 0 & \mathbf{L}_{ee} \end{pmatrix} \begin{pmatrix} \boldsymbol{u}_o \\ \boldsymbol{u}_e \end{pmatrix}. \tag{5.42}$$

Here $\mathbf{A}_{eo} = \mathbf{A}_{oe}^{\mathsf{T}}$, and $\mathbf{L}_{oo}$ and $\mathbf{L}_{ee}$ are symmetric and negative semidefinite matrices. As noted in § 5.1, the operator $\mathcal{A}_n$ has a non-trivial null space being a subspace of $\mathcal{P}_{odd}\mathbb{V}$. Accordingly, in order to mimic this property, we assume that the matrix $\mathbf{A}_{oe}$ is rank deficient, and its singular value decomposition is

$$\mathbf{A}_{oe} = \begin{pmatrix} \mathbf{U}_1 & \mathbf{U}_2 \end{pmatrix} \begin{pmatrix} \boldsymbol{\Lambda}_r & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} \mathbf{V}_1^{\mathsf{T}} \\ \mathbf{V}_2^{\mathsf{T}} \end{pmatrix}, \tag{5.43}$$

where r denotes the rank of $\mathbf{A}_{oe}$ and

$$\boldsymbol{\Lambda}_r = \begin{pmatrix} \lambda_1 & 0 & \cdots & 0 \\ 0 & \lambda_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \lambda_r \end{pmatrix}, \qquad \lambda_1 \geqslant \lambda_2 \geqslant \cdots \geqslant \lambda_r > 0. \tag{5.44}$$

Inspired by the preliminary section in Jiang, Sun & Toh (2013), we define

$$\boldsymbol{v}_o = \mathbf{U}_1^{\mathsf{T}} \boldsymbol{u}_o, \quad \boldsymbol{v}_e = \mathbf{V}_1^{\mathsf{T}} \boldsymbol{u}_e. \tag{5.45}$$

By straightforward calculation, it can be shown that $\boldsymbol{v}_o$ and $\boldsymbol{v}_e$ satisfy the differential equations

$$\frac{\partial}{\partial x} \begin{pmatrix} \boldsymbol{v}_o \\ \boldsymbol{v}_e \end{pmatrix} = \begin{pmatrix} 0 & \boldsymbol{\Lambda}_r^{-1} \tilde{\mathbf{L}}_{ee} \\ \boldsymbol{\Lambda}_r^{-1} \tilde{\mathbf{L}}_{oo} & 0 \end{pmatrix} \begin{pmatrix} \boldsymbol{v}_o \\ \boldsymbol{v}_e \end{pmatrix}, \tag{5.46}$$

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where

$$\tilde{\mathbf{L}}_{oo} = \mathbf{U}_1^\mathsf{T} \mathbf{L}_{oo} \mathbf{U}_1 - \mathbf{U}_1^\mathsf{T} \mathbf{L}_{oo} \mathbf{U}_2 (\mathbf{U}_2^\mathsf{T} \mathbf{L}_{oo} \mathbf{U}_2)^{-1} \mathbf{U}_2^\mathsf{T} \mathbf{L}_{oo} \mathbf{U}_1,$$
$$\tilde{\mathbf{L}}_{ee} = \mathbf{V}_1^\mathsf{T} \mathbf{L}_{ee} \mathbf{V}_1 - \mathbf{V}_1^\mathsf{T} \mathbf{L}_{ee} \mathbf{V}_2 (\mathbf{V}_2^\mathsf{T} \mathbf{L}_{ee} \mathbf{V}_2)^{-1} \mathbf{V}_2^\mathsf{T} \mathbf{L}_{ee} \mathbf{V}_1. \tag{5.47}$$

It is obvious that $\tilde{\mathbf{L}}_{oo}$ and $\tilde{\mathbf{L}}_{ee}$ are Schur complements of negative semidefinite matrices, and therefore, are also negative semidefinite matrices. Note that here we require the invertibility of $\mathbf{U}_2^\mathsf{T} \mathbf{L}_{oo} \mathbf{U}_2$ and $\mathbf{V}_2^\mathsf{T} \mathbf{L}_{ee} \mathbf{V}_2$, which is satisfied in the R13 equations derived in previous sections.

The following lemma reveals the eigenpairs of the matrix in (5.46).

LEMMA 1. *If $\{\lambda, (\mathbf{r}_o^\mathsf{T}, \mathbf{r}_e^\mathsf{T})^\mathsf{T}\}$ is an eigenpair of the matrix in (5.46), then $\{-\lambda, (-\mathbf{r}_o^\mathsf{T}, \mathbf{r}_e^\mathsf{T})^\mathsf{T}\}$ is also an eigenpair of it.*

Proof. From

$$\begin{pmatrix} 0 & \boldsymbol{\Lambda}_r^{-1} \tilde{\mathbf{L}}_{ee} \\ \boldsymbol{\Lambda}_r^{-1} \tilde{\mathbf{L}}_{oo} & 0 \end{pmatrix} \begin{pmatrix} \mathbf{r}_o \\ \mathbf{r}_e \end{pmatrix} = \lambda \begin{pmatrix} \mathbf{r}_o \\ \mathbf{r}_e \end{pmatrix}, \tag{5.48}$$

one sees that $\boldsymbol{\Lambda}_r^{-1} \tilde{\mathbf{L}}_{ee} \mathbf{r}_e = \lambda \mathbf{r}_o$ and $\boldsymbol{\Lambda}_r^{-1} \tilde{\mathbf{L}}_{oo} \mathbf{r}_o = \lambda \mathbf{r}_e$. Then

$$\begin{pmatrix} 0 & \boldsymbol{\Lambda}_1^{-1} \tilde{\mathbf{L}}_{ee} \\ \boldsymbol{\Lambda}_1^{-1} \tilde{\mathbf{L}}_{oo} & 0 \end{pmatrix} \begin{pmatrix} -\mathbf{r}_o \\ \mathbf{r}_e \end{pmatrix} = \begin{pmatrix} \boldsymbol{\Lambda}_r^{-1} \tilde{\mathbf{L}}_{ee} \mathbf{r}_e \\ -\boldsymbol{\Lambda}_r^{-1} \tilde{\mathbf{L}}_{oo} \mathbf{r}_o \end{pmatrix} = \begin{pmatrix} \lambda \mathbf{r}_o \\ -\lambda \mathbf{r}_e \end{pmatrix} = -\lambda \begin{pmatrix} -\mathbf{r}_o \\ \mathbf{r}_e \end{pmatrix}, \tag{5.49}$$

which completes the proof. $\qquad\square$

By the above lemma, the eigenvalue decomposition of the matrix in (5.46) is

$$\begin{pmatrix} 0 & \boldsymbol{\Lambda}_r^{-1} \tilde{\mathbf{L}}_{ee} \\ \boldsymbol{\Lambda}_r^{-1} \tilde{\mathbf{L}}_{oo} & 0 \end{pmatrix} = \mathbf{R}_r \begin{pmatrix} \tilde{\lambda}_1 & & & & \\ & -\tilde{\lambda}_1 & & & \\ & & \ddots & & \\ & & & \tilde{\lambda}_r & \\ & & & & -\tilde{\lambda}_r \end{pmatrix} \mathbf{R}_r^{-1}, \tag{5.50}$$

where $\tilde{\lambda}_1 \geqslant \tilde{\lambda}_2 \geqslant \cdots \geqslant \tilde{\lambda}_s > 0 = \tilde{\lambda}_{s+1} = \cdots = \tilde{\lambda}_r$ for some $s \leqslant r$, and

$$\mathbf{R}_r = \begin{pmatrix} \mathbf{R}_s & \mathbf{R}_0 \end{pmatrix} \tag{5.51}$$

with

$$\mathbf{R}_s = \begin{pmatrix} \mathbf{r}_{o1} & -\mathbf{r}_{o1} & \dots & \mathbf{r}_{os} & -\mathbf{r}_{os} \\ \mathbf{r}_{e1} & \mathbf{r}_{e1} & \dots & \mathbf{r}_{es} & \mathbf{r}_{es} \end{pmatrix}. \tag{5.52}$$

For simplicity, we define $\mathbf{L}_r^\mathsf{T} = \mathbf{R}_r^{-1}$ so that $\mathbf{L}_r$ has the form $\begin{pmatrix} \mathbf{L}_s & \mathbf{L}_0 \end{pmatrix}$ with

$$\mathbf{L}_s = \begin{pmatrix} \mathbf{l}_{o1} & -\mathbf{l}_{o1} & \dots & \mathbf{l}_{os} & -\mathbf{l}_{os} \\ \mathbf{l}_{e1} & \mathbf{l}_{e1} & \dots & \mathbf{l}_{es} & \mathbf{l}_{es} \end{pmatrix}. \tag{5.53}$$

If we assume the simulation domain is $(0, 1)$ without loss of generality, the solution of such a linear system has the form

$$v(x) = \begin{pmatrix} v_o(x) \\ v_e(x) \end{pmatrix} = \mathbf{R}_r \begin{pmatrix} e^{\tilde{\lambda}_1 x} & & & & \\ & e^{-\tilde{\lambda}_1 x} & & & \\ & & \ddots & & \\ & & & e^{\tilde{\lambda}_r x} & \\ & & & & e^{-\tilde{\lambda}_r x} \end{pmatrix} \mathbf{L}_r^\mathsf{T} v(0)$$

$$= \sum_{j=1}^{s} \left(e^{\tilde{\lambda}_j x} \begin{pmatrix} r_{oj} \\ r_{ej} \end{pmatrix} (l_{oj}^\mathsf{T}, l_{ej}^\mathsf{T}) + e^{-\tilde{\lambda}_j x} \begin{pmatrix} -r_{oj} \\ r_{ej} \end{pmatrix} (-l_{oj}^\mathsf{T}, l_{ej}^\mathsf{T}) \right) v(0) + \mathbf{R}_0 \mathbf{L}_0^\mathsf{T} v(0)$$

$$= \sum_{j=1}^{s} \left(2 \cosh(\tilde{\lambda}_j x) \begin{pmatrix} r_{oj} l_{oj}^\mathsf{T} v_o(0) \\ r_{ej} l_{ej}^\mathsf{T} v_e(0) \end{pmatrix} + 2 \sinh(\tilde{\lambda}_j x) \begin{pmatrix} r_{oj} l_{ej}^\mathsf{T} v_e(0) \\ r_{ej} l_{oj}^\mathsf{T} v_o(0) \end{pmatrix} \right) + \mathbf{R}_0 \mathbf{L}_0^\mathsf{T} v(0).$$

$$(5.54)$$

The rank r for Maxwell molecules is 3 less than the rank of the non-Maxwell cases. In fact, for non-Maxwell gases, the values of λ_r, λ_{r-1} and λ_{r-2} are very close to 0, and thus $\tilde{\lambda}_{1,2,3} \gg 1$, which exhibits additional boundary layers. Note that when the system is reduced to the one-dimensional case as in § 5.2, only one large eigenvalue is left.

To remove the boundary layers in the non-Maxwell cases, we revise the boundary condition to eliminate the corresponding terms in (5.54). For simplicity, we only introduce the removal of the boundary layer associated with $\tilde{\lambda}_1$. The other two layers are removed similarly. The idea is to enforce the following equalities in our boundary conditions:

$$l_{o1}^\mathsf{T} v_o(0) = l_{o1}^\mathsf{T} v_o(1) = 0. \tag{5.55}$$

This is sufficient to get rid of the terms involving $\cosh(\tilde{\lambda}_1 x)$ and $\sinh(\tilde{\lambda}_1 x)$ in (5.54). The reason will be explained as follows.

We can follow (5.54) to write the solution using boundary conditions at $x = 1$ as

$$v(x) = \sum_{j=1}^{r} \left(2 \cosh(\tilde{\lambda}_j (x-1)) \begin{pmatrix} r_{oj} l_{oj}^\mathsf{T} v_o(1) \\ r_{ej} l_{ej}^\mathsf{T} v_e(1) \end{pmatrix} + 2 \sinh(\tilde{\lambda}_j (x-1)) \begin{pmatrix} r_{oj} l_{ej}^\mathsf{T} v_e(1) \\ r_{ej} l_{oj}^\mathsf{T} v_o(1) \end{pmatrix} \right)$$
$$+ \mathbf{R}_0 \mathbf{L}_0^\mathsf{T} v(1). \tag{5.56}$$

Plugging the following equalities into (5.56) gives

$$\cosh(\tilde{\lambda}_1 (x-1)) = \cosh(\tilde{\lambda}_1 x) \cosh(-\tilde{\lambda}_1) + \sinh(\tilde{\lambda}_1 x) \sinh(-\tilde{\lambda}_1),$$
$$\sinh(\tilde{\lambda}_1 (x-1)) = \sinh(\tilde{\lambda}_1 x) \cosh(-\tilde{\lambda}_1) + \cosh(\tilde{\lambda}_1 x) \sinh(-\tilde{\lambda}_1), \tag{5.57}$$

and matching the coefficients of $\cosh(\tilde{\lambda}_1 x)$ and $\sinh(\tilde{\lambda}_1 x)$ in (5.54), one can show that

$$\begin{pmatrix} r_{o1}(l_{o1}^\mathsf{T} v_o(1) \cosh(-\tilde{\lambda}_1) + l_{e1}^\mathsf{T} v_e(1) \sinh(-\tilde{\lambda}_1)) \\ r_{e1}(l_{e1}^\mathsf{T} v_e(1) \cosh(-\tilde{\lambda}_1) + l_{o1}^\mathsf{T} v_o(1) \sinh(-\tilde{\lambda}_1)) \end{pmatrix} = \begin{pmatrix} r_{o1} l_{o1}^\mathsf{T} v_o(0) \\ r_{e1} l_{e1}^\mathsf{T} v_e(0) \end{pmatrix},$$
$$\begin{pmatrix} r_{o1}(l_{o1}^\mathsf{T} v_o(1) \sinh(-\tilde{\lambda}_1) + l_{e1}^\mathsf{T} v_e(1) \cosh(-\tilde{\lambda}_1)) \\ r_{e1}(l_{e1}^\mathsf{T} v_e(1) \sinh(-\tilde{\lambda}_1) + l_{o1}^\mathsf{T} v_o(1) \cosh(-\tilde{\lambda}_1)) \end{pmatrix} = \begin{pmatrix} r_{o1} l_{e1}^\mathsf{T} v_e(0) \\ r_{e1} l_{o1}^\mathsf{T} v_o(0) \end{pmatrix}. \tag{5.58}$$

We can now apply $l_{o1}^\mathsf{T} v_o(0) = l_{o1}^\mathsf{T} v_o(1) = 0$ to the above equation, and it is not difficult to derive $l_{e1}^\mathsf{T} v_e(0) = l_{e1}^\mathsf{T} v_e(1) = 0$. Therefore, all the terms involving $\cosh(\tilde{\lambda}_1 x)$ and $\sinh(\tilde{\lambda}_1 x)$

in (5.54) or (5.56) disappear so that the corresponding boundary layers are not present in the solution.

The above derivation shows that (5.55) is a sufficient condition to suppress boundary layers. Moreover, it is straightforward to generalise such a condition to multidimensional cases by imposing $\boldsymbol{l}_{o1}^{\mathsf{T}} \boldsymbol{v}_o = 0$ for $\boldsymbol{v}_o$ at all boundary points. Recall that the Onsager boundary conditions take a form of (1.6), which can be reformulated as

$$\boldsymbol{v}_o = \tilde{\boldsymbol{Q}} \boldsymbol{\Lambda} (\tilde{\boldsymbol{g}}_{ext} - \boldsymbol{v}_e). \tag{5.59}$$

To impose $\boldsymbol{l}_{o1}^{\mathsf{T}} \boldsymbol{v}_o = 0$, we choose to modify the symmetric matrix $\tilde{\boldsymbol{Q}}$ such that

$$\boldsymbol{l}_{o1}^{\mathsf{T}} \tilde{\boldsymbol{Q}} = 0. \tag{5.60}$$

However, (5.60) is an underdetermined linear system. To make it uniquely solvable, we add the following constraints.

(i) The revised $\tilde{\boldsymbol{Q}}$ must be symmetric.
(ii) An element of $\tilde{\boldsymbol{Q}}$ should remain zero if it is zero for all non-Maxwell gas molecules.
(iii) An element $Q_{ij} = 2\chi/2 - \chi \langle \phi_{odd}^i, \mathcal{C}\xi_n^{-1} \phi_{odd}^j \rangle / \langle \phi_{odd}^j, \phi_{odd}^j \rangle$ (refer to (5.16)) of $\tilde{\boldsymbol{Q}}$ should remain unchanged if both ϕ_{odd}^i and ϕ_{odd}^j belong to $\mathbb{V}_{odd} \cap (\mathbb{V}_{modified})^{\perp}$, where

$$\mathbb{V}_{modified} = \text{span} \left\{ \phi_{n\tau_1}^2, \phi_{n\tau_2}^2, \phi_n^2 + \frac{c_1^{3,1}}{c_1^{2,1}} \phi_n^3 \right\} \tag{5.61}$$

is a subspace of the $\mathbb{V}_{odd}$ in (5.12).

The rationale for proposing constraint (iii) is that $\mathbb{V}_{modified} = \emptyset$ in the case of Maxwell gas, which does not exhibit any non-physical boundary layers. The additional basis functions in $\mathbb{V}_{modified}$ introduce these layers in the non-Maxwell cases. Therefore, we only modify those elements deduced from $\mathbb{V}_{modified}$.

After imposing these conditions, the matrix $\tilde{\boldsymbol{Q}}$ is uniquely determined. Currently, we do not have theoretical guarantee of the semidefiniteness of the revised $\tilde{\boldsymbol{Q}}$, but this turns out to be true in all cases done in our tests. The symmetry and semidefiniteness of $\tilde{\boldsymbol{Q}}$ indicates that the structure (1.6) is well maintained after the modification, and thus, does not ruin the L^2 stability or the second law of thermodynamics.

To demonstrate the effect of this modification, we reconsider the example described in § 5.2, with the boundary conditions changed to the new ones introduced in this section by replacing $\hat{m}_{ij}$ with m_{ij} in (5.27)–(5.30). The results are plotted in figure 2. A comparison with figure 1 clearly demonstrates that the non-physical boundary layers have been removed.

6. One-dimensional simulations

In this section we apply our model to the example for one-dimensional channel flows in Hu *et al.* (2020) and Cai *et al.* (2024*b*). We show the analytic solutions of the steady-state equations of our model and make a comparison with the results computed by DSMC from Bird's code (Bird 1994) in § 6.1. After that, the numerical solutions of our time-dependent model will be demonstrated in § 6.2 using the finite element method.

The gas flow between two infinitely large parallel plates is considered in the one-dimensional channel flows. Both of the two plates are perpendicular to the x_2 axis, and the
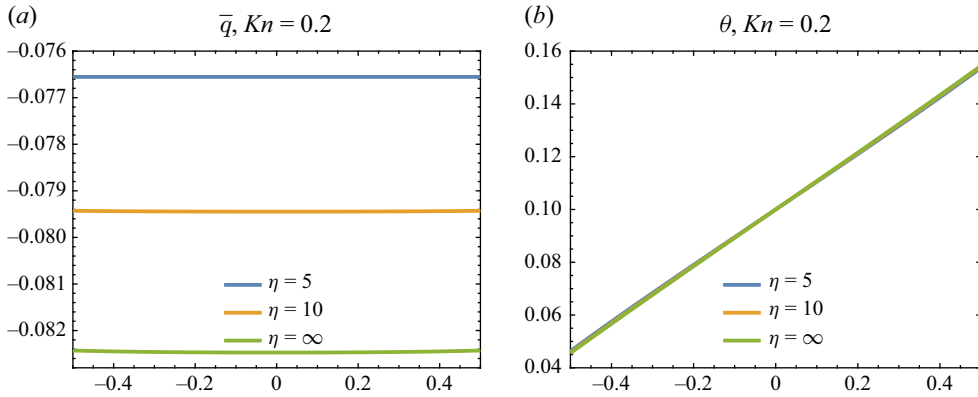
Figure 2. Plots of $\bar{q}$ and θ for the one-dimensional problem (5.22)–(5.30) with modified coefficient $\hat{m}_{ij} \rightarrow m_{ij}$. Results are shown for (a) $\theta^W = 0$ and (b) $\theta^W = 0.2$.

two plates are assumed to move along the x_1 axis with constant velocities. The distance of the two plates is taken as 1, and the coordinates are established such that the simulation domain is $x_2 \in (-0.5, 0.5)$. The temperature and velocity of the left plates ($x_2 = -0.5$) are denoted as θ_l^W and v_l^W, respectively, and similarly, the temperature and velocity of the right plates ($x_2 = 0.5$) are denoted as θ_r^W and v_r^W, respectively. Under this setting, all the moments are functions only of x_2, and therefore, the moment equations for the one-dimensional channel flows can be obtained via dropping all partial derivatives with respect to x_1 and x_3. Furthermore, as two plates move along the x_1 axis, the distribution function enjoys symmetry $f(\boldsymbol{x}, \xi_1, \xi_2, \xi_3, t) = f(\boldsymbol{x}, \xi_1, \xi_2, -\xi_3, t)$ so that the moments that are odd in ξ_3 vanish. As a result,

$$v_3 = \bar{q}_3 = \bar{\sigma}_{13} = \bar{\sigma}_{23} = 0. \qquad (6.1)$$

Therefore, in the one-dimensional channel flows, the 13 moments are reduced to 9 moments: ρ, θ, v_1, v_2, $\bar{q}_1$, $\bar{q}_2$, $\bar{\sigma}_{11}$, $\bar{\sigma}_{12}$, $\bar{\sigma}_{22}$. In addition, both plates are assumed to be completely diffusive, where the accommodation coefficient is always chosen as $\chi = 1$.

6.1. Steady-state examples

To compare with the example in §§ 5.2 and 5.3, we consider a steady-state problem here. In fact, (5.22)–(5.26) can be regarded as a portion of the one-dimensional steady-state channel flow considered here by using the following replacements: $x \rightarrow x_2$, $v \rightarrow v_2$, $\bar{q} \rightarrow \bar{q}_2$ and $\bar{\sigma} \rightarrow \bar{\sigma}_{22}$. Boundary conditions (5.27)–(5.30) also share the same form of boundary conditions considered here by using the above replacements. We adopt the coefficients $\theta_l^W = 0$ and $\theta_r^W = 0.2$, consistent with the example presented in § 5.2.

To compare our solutions with the DSMC results, we show the results by using the Knudsen number $\overline{Kn}$ defined by the ratio of the mean free path to the characteristic length as in Bird (1994). The relationship between $\overline{Kn}$ and the parameter Kn in this paper is

$$Kn = \sqrt{\frac{\pi}{2}} \frac{15\overline{Kn}}{(5 - 2\omega)(7 - 2\omega)}, \qquad \omega = \frac{1}{2} + \frac{2}{\eta - 1}. \qquad (6.2)$$

Moreover, we plot the actual heat flux q_2 instead of $\bar{q}_2$ (see (3.8)) in this example, since q_2 is obtained from the DSMC results. To observe the effect of the Knudsen number, we choose two different $\overline{Kn}$ and plot the results for both original and fixed boundary conditions in figures 3 and 4. Our results are depicted as the blue, yellow and green solid
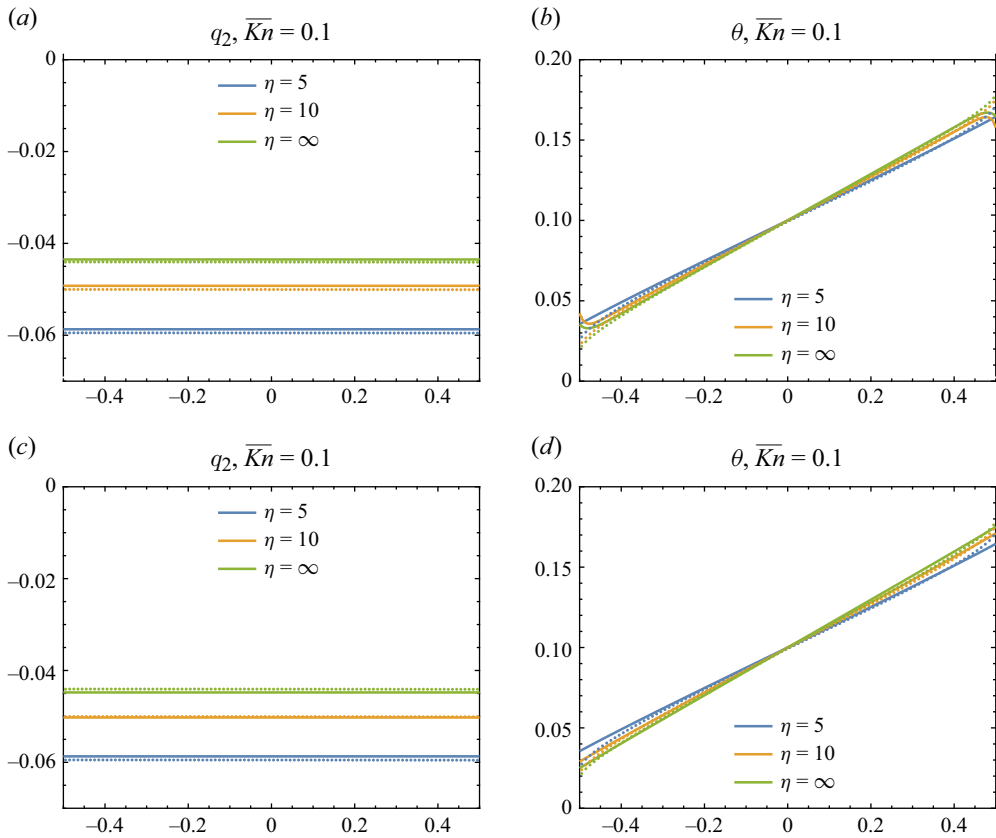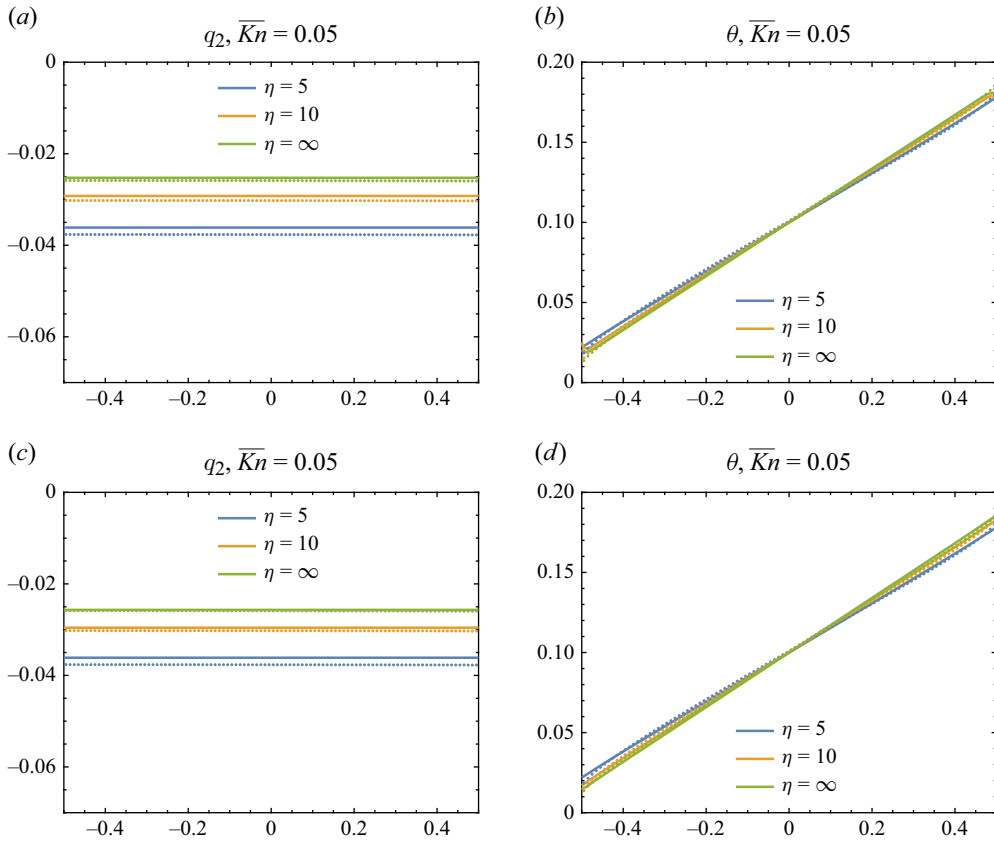
Figure 3. Results of the steady-state example when $\overline{Kn} = 0.1$. (*a, b*) Coefficients $\hat{m}_{ij}$ are used, (*b, c*) modified coefficients m_{ij} are used. The DSMC solutions are given by dotted lines of the same colours.

lines corresponding to $\eta = 5$, 10 and ∞. The relevant solutions obtained by DSMC are presented by dotted lines of the same colours.

The solids lines of the R13 equations generally agree with the dotted lines of the DSMC results, and this agreement is more pronounced for smaller *Kn*, which validates our equations. Moreover, as the DSMC results display no boundary layer, the effectiveness of our modified Onsager boundary conditions is again validated by the successful removal of the undesired boundary layers. Furthermore, compared with the results in figure 1, the width of the undesired boundary layers decreases as the Knudsen number decreases, which is consistent with our analysis of the solution in (5.40). Also, it can be observed that the temperature jump gets more significant as the Knudsen number increases.

6.2. *Time-dependent examples*

After validating the steady-state equations, it would be more compelling to verify the derived model in the time-dependent case, as this is the primary focus of this work. However, it would be challenging to obtain the analytic time-dependent solution, therefore, we aim to solve the time-dependent equations using the finite element method.

The numerical set-up is described as follows. We use a uniform mesh with a mesh size of $1/1000$ and apply the finite element method with piecewise linear functions. The Crank–Nicolson method is used for temporal discretisation with a uniform time step

Figure 4. Results of steady-state example when $\overline{Kn} = 0.05$. (*a, b*) Coefficients $\hat{m}_{ij}$ are used, (*b, c*) modified coefficients m_{ij} are used. The DSMC solutions are given by dotted lines of the same colours.

of $1/4000$. The initial value for θ is set to $(\theta_l^W + \theta_r^W)/2$, while the initial values for all other moments are set to 0. Boundary coefficients are taken from Cai *et al.* (2024*b*), which will be specified in the following two cases.

6.2.1. *Couette flow*

In the planar Couette flow, the two plates move in opposite directions and maintain the same temperature. We choose $\theta_l^W = \theta_r^W = 0$ and $v_l^W = -v_r^W = -0.2$. Results are depicted in figure 5, where non-physical boundary layers can still be observed in the solution of time-dependent equations using the previous Onsager boundary conditions, although the width of these layers is very thin in this example. These thin layers are successfully removed at various time steps using our modified boundary conditions.

6.2.2. *Fourier flow*

In the planar Fourier flow, the two plates are stationary, implying that $v_l^W = v_r^W = 0$, and the gas dynamics between the plates are driven by the temperature difference. We set $\theta_l^W = 0$ and $\theta_r^W = 0.2$. The results in figure 6 demonstrate that the previous Onsager boundary conditions produce non-physical boundary layers, which can be eliminated using our modified boundary conditions. Additionally, these layers are more pronounced
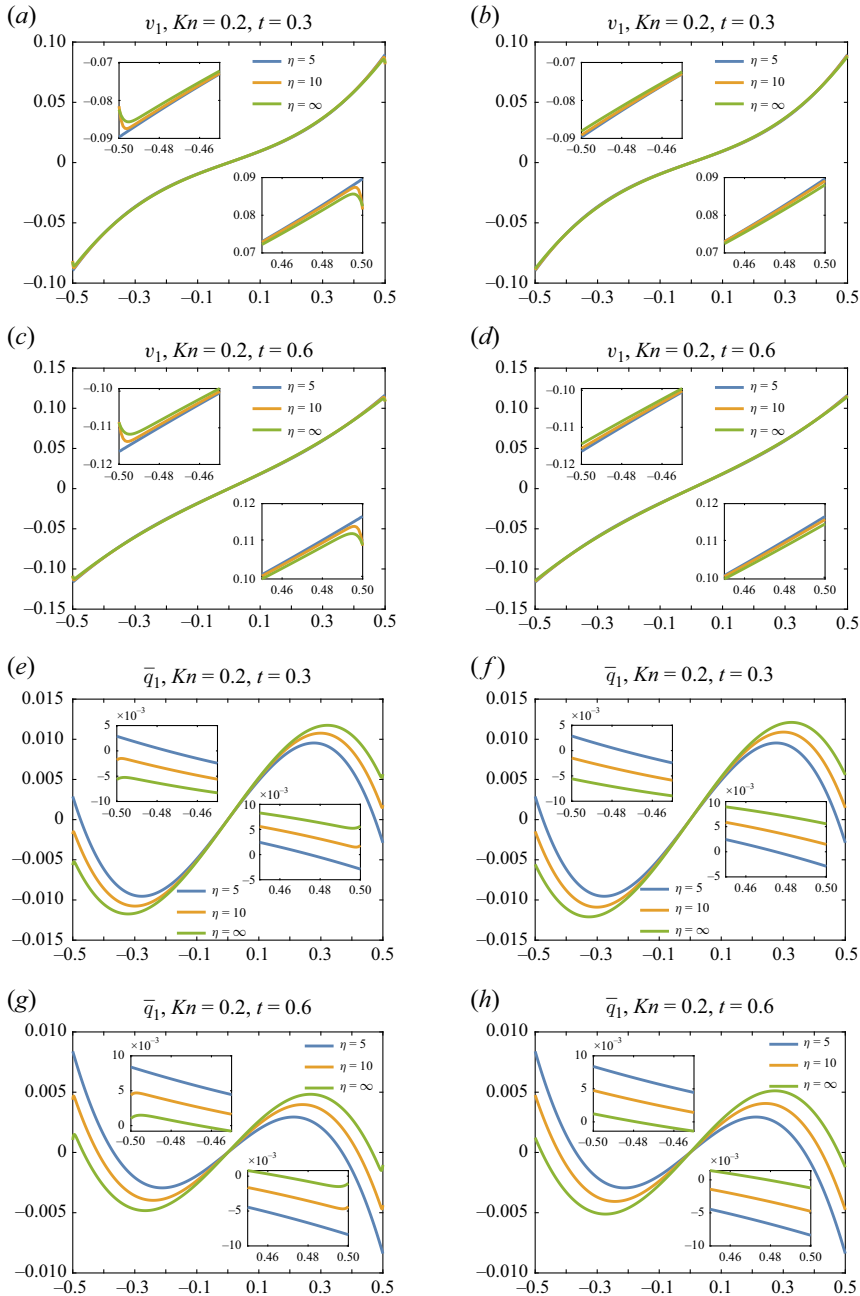
Figure 5. Results of the Couette flow. (*a–d*) Onsager boundary conditions are used. (*e–h*) Our modified boundary conditions are used.

for longer computational times, suggesting our modified boundary conditions would be more important in long-time simulations of the proposed R13 equations.

7. Conclusion

This work provides a new perspective of the derivation of time-dependent regularised 13-moment equations from linear kinetic equation under general elastic collision models.

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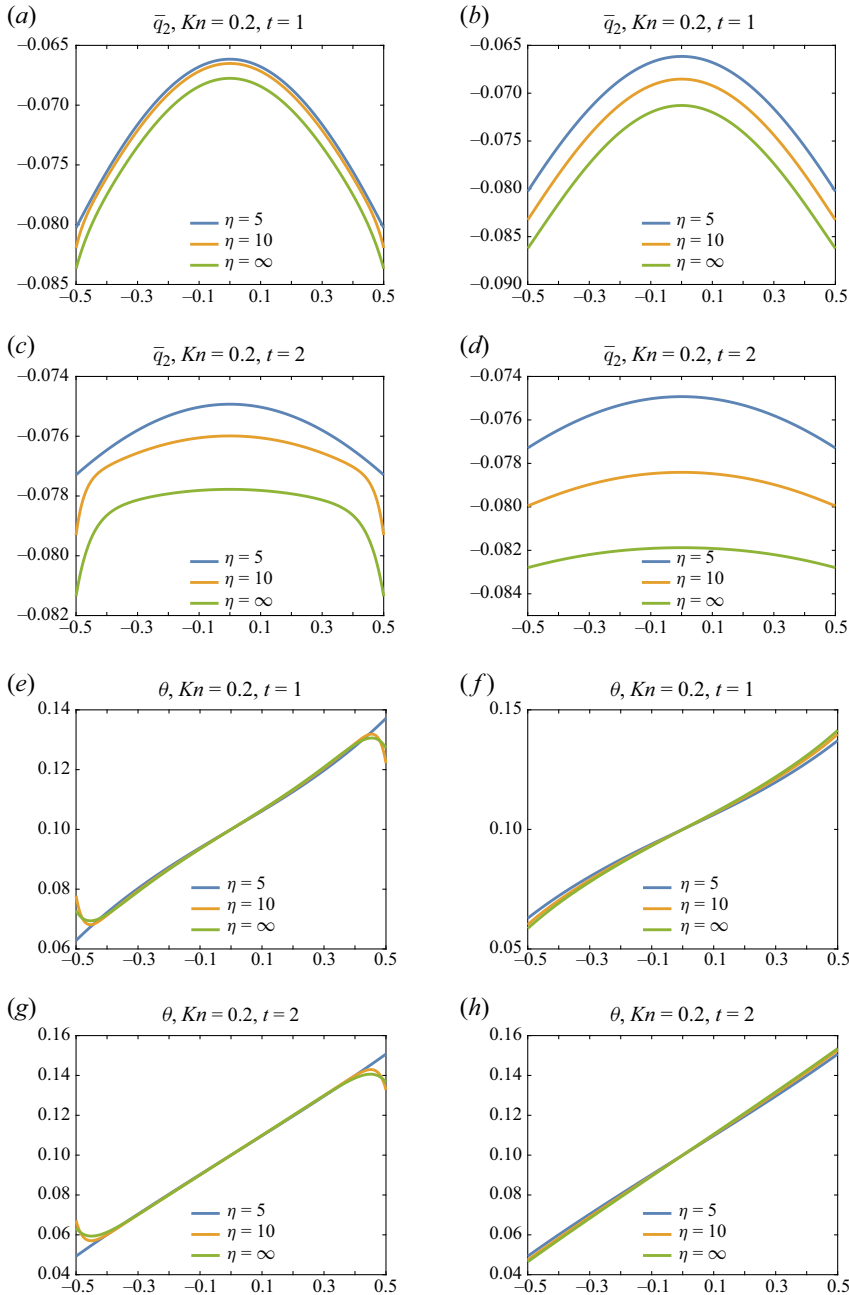
Figure 6. Results of the Fourier flow. (*a–d*) Previous Onsager boundary conditions are used. (*e–h*) Our modified boundary conditions are used.

Compared with previous works such as Hu *et al.* (2020) and Cai *et al.* (2024*b*), our equations possess not only the super-Burnett order, but also a symmetric structure that is useful for deriving Onsager boundary conditions. In the linear regime, our equations can well approximate the Boltzmann equation with moderate Knudsen numbers and preserve the conservation laws and the dissipation of entropy. Another contribution of this work is

the technique to remove undesired boundary layers, which needs to be applied since these layers are obviously unphysical.

Due to the symmetry of the equations and the Onsager boundary conditions, we expect that our equations also admit a symmetric weak form, which extends the weak form of R13 equations for Maxwell molecules (Theisen & Torrilhon (2021)). We are currently working on the finite element methods for our equations in the multidimensional case. Note that it is claimed in Rana *et al.* (2013) that R13 equations can provide satisfactory predictions up to Knudsen number 0.5, and this needs to be tested for our equations with modified boundary conditions in multidimensional applications. Meanwhile, the work on applying this approach to nonlinear kinetic equations is also ongoing.

Funding. Zhenning Cai was supported by the Academic Research Fund of the Ministry of Education of Singapore under grant A-8002392-00-00.

Declaration of interests. The author reports no conflict of interest.

Appendix A. Galilean invariance of moment equations

To demonstrate the Galilean invariance of our moment equations, we need to prove the following invariant properties.

i. Translational invariance: given any $\boldsymbol{v}_{ref} \in \mathbb{R}^3$, under translation

$$\boldsymbol{x}' = \boldsymbol{x} + t\boldsymbol{v}_{ref}, \ \rho'(\boldsymbol{x}', t) = \rho(\boldsymbol{x}, t), \ \theta'(\boldsymbol{x}', t) = \theta(\boldsymbol{x}, t),$$
$$\boldsymbol{v}'(\boldsymbol{x}, t) = \boldsymbol{v}(\boldsymbol{x}', t) + \boldsymbol{v}_{ref}, \ \bar{\boldsymbol{q}}'(\boldsymbol{x}', t) = \bar{\boldsymbol{q}}(\boldsymbol{x}, t), \ \bar{\boldsymbol{\sigma}}'(\boldsymbol{x}', t) = \bar{\boldsymbol{\sigma}}(\boldsymbol{x}, t), \quad (A.1)$$

(3.2)–(3.6) retain their form.
ii. Rotational invariance: given any orthogonal matrix $\mathbf{R} \in \mathbb{R}^{3\times 3}$, under rotation

$$\boldsymbol{x}' = \mathbf{R}\boldsymbol{x}, \ \rho'(\boldsymbol{x}', t) = \rho(\boldsymbol{x}, t), \ \theta'(\boldsymbol{x}', t) = \theta(\boldsymbol{x}, t),$$
$$\boldsymbol{v}'(\boldsymbol{x}', t) = \mathbf{R}\boldsymbol{v}(\boldsymbol{x}, t), \ \bar{\boldsymbol{q}}'(\boldsymbol{x}', t) = \mathbf{R}\bar{\boldsymbol{q}}(\boldsymbol{x}, t), \ \bar{\boldsymbol{\sigma}}'(\boldsymbol{x}', t) = \mathbf{R}\bar{\boldsymbol{\sigma}}(\boldsymbol{x}, t)\mathbf{R}^{\mathsf{T}}, \quad (A.2)$$

(3.2)–(3.6) retain their form.

Since the equations rely solely on the derivatives of $\boldsymbol{v}$ rather than on $\boldsymbol{v}$ itself, the translational invariance can be readily verified in our linear equations. Consequently, we focus on the proof of the rotational invariance in this appendix.

For (3.2), we have

$$\frac{\partial v_i'}{\partial x_i'} = \frac{\partial v_i'}{\partial x_k}\frac{\partial x_k}{\partial x_i'} = R_{ij}\frac{\partial v_j}{\partial x_k}R_{ik} = \frac{\partial v_j}{\partial x_k}\delta_{jk} = \frac{\partial v_j}{\partial x_j}, \quad (A.3)$$

which implies that $\nabla_{\boldsymbol{x}'} \cdot \boldsymbol{v}' = \nabla_{\boldsymbol{x}} \cdot \boldsymbol{v}$. Therefore, (3.2) retains its form under the rotational transformation.

For (3.3), we first calculate the derivative of $\bar{\sigma}$ as

$$\frac{\partial \bar{\sigma}_{ij}'}{\partial x_j'} = \frac{\partial \bar{\sigma}_{ij}'}{\partial x_k}\frac{\partial x_k}{\partial x_j'} = R_{il}R_{jl'}\frac{\partial \bar{\sigma}_{ll'}}{\partial x_k}R_{jk} = R_{il}\delta_{kl'}\frac{\partial \bar{\sigma}_{ll'}}{\partial x_k} = R_{il}\frac{\partial \bar{\sigma}_{lk}}{\partial x_k}, \quad (A.4)$$

and then we arrive at the relationship

$$\frac{\partial^2 \bar{\sigma}_{ij}'}{\partial x_i'\partial x_j'} = R_{il}\frac{\partial^2 \bar{\sigma}_{lk}}{\partial x_k\partial x_{k'}}R_{ik'} = \frac{\partial^2 \bar{\sigma}_{lk}}{\partial x_k\partial x_{k'}}\delta_{lk'} = \frac{\partial^2 \bar{\sigma}_{k'k}}{\partial x_k\partial x_{k'}}, \quad (A.5)$$

which implies that $\nabla_{x'} \cdot (\nabla_{x'} \cdot \bar{\sigma}') = \nabla_x \cdot (\nabla_x \cdot \bar{\sigma})$. Similar to (A.3), we can prove that $\nabla_{x'} \cdot \bar{q}' = \nabla_x \cdot \bar{q}$. In addition, $\Delta_{x'}\theta' = \Delta_x\theta$ according to the rotational invariance of the Laplacian operator. As a result, (3.3) is also rotational invariant.

For (3.4), one can easily see that

$$\frac{\partial \boldsymbol{v}'}{\partial \boldsymbol{x}'} = \mathbf{R}\frac{\partial \boldsymbol{v}}{\partial \boldsymbol{x}}, \quad \nabla_{x'}\rho' = \mathbf{R}\nabla_x\rho, \quad \nabla_{x'}\theta' = \mathbf{R}\nabla_x\theta. \tag{A.6}$$

In addition, we have $\nabla_{x'} \cdot \bar{\sigma}' = \mathbf{R}\nabla_x \cdot \bar{\sigma}$ by (A.4). For the term $\nabla \cdot (\nabla \boldsymbol{v})_{stf}$, we use the fact that

$$(\nabla \boldsymbol{v})_{stf} = \frac{1}{2}(\nabla \boldsymbol{v} + (\nabla \boldsymbol{v})^{\mathsf{T}}) - \frac{1}{3}\mathrm{tr}(\nabla \boldsymbol{v})I,$$
$$\nabla_{x'}\boldsymbol{v}' = \mathbf{R}\nabla_x\boldsymbol{v}\mathbf{R}^T \tag{A.7}$$

and the cyclic property of trace operator to show that $(\nabla_{x'}\boldsymbol{v}')_{stf} = \mathbf{R}(\nabla_x\boldsymbol{v})_{stf}\mathbf{R}^T$. Therefore, we have

$$\frac{\partial}{\partial x'_j}[(\nabla_{x'}\boldsymbol{v}')_{stf}]_{ij} = R_{jk}\frac{\partial}{\partial x_k}R_{il}[(\nabla_x\boldsymbol{v})_{stf}]_{ll'}R_{jl'} = R_{il}\frac{\partial}{\partial x_k}[(\nabla_x\boldsymbol{v})_{stf}]_{lk}, \tag{A.8}$$

which implies that $\nabla_{x'} \cdot (\nabla_{x'}\boldsymbol{v}')_{stf} = \mathbf{R}\nabla_x \cdot (\nabla_x\boldsymbol{v})_{stf}$. Similarly, we can prove such a relationship for $\bar{q}$. Combining these two equalities of $\boldsymbol{v}$ and $\bar{q}$ in conjunction with (A.4) and (A.6), we have verified the rotational invariance of (3.4). The rotational invariance of (3.5) can be similarly proved as (3.4).

For (3.6), similar to (A.7), one can prove that $\nabla_{x'}\bar{q}' = \mathbf{R}\nabla_x\bar{q}\mathbf{R}^T$ and $(\nabla_{x'}\bar{\sigma}')_{stf} = \mathbf{R}(\nabla_x\bar{\sigma})_{stf}\mathbf{R}^T$. For the term $(\nabla(\nabla \cdot \bar{\sigma}))_{stf}$, it holds that

$$[\nabla_{x'}(\nabla_{x'} \cdot \bar{\sigma}')]_{ij} = \frac{\partial^2 \bar{\sigma}'_{ik}}{\partial x'_j \partial x'_k} = R_{jk'}R_{il}R_{kl}R_{kl''}\frac{\partial^2 \bar{\sigma}_{ll'}}{\partial x_{k'}\partial x_{l''}}$$
$$= R_{jk'}R_{il}\delta_{ll''}\frac{\partial^2 \bar{\sigma}_{ll'}}{\partial x_{k'}\partial x_{l''}} = R_{il}\frac{\partial^2 \bar{\sigma}_{ll'}}{\partial x_{k'}\partial x_l}R_{jk'}, \tag{A.9}$$

which implies that $(\nabla_{x'}(\nabla_{x'} \cdot \bar{\sigma}'))_{stf} = \mathbf{R}(\nabla_x(\nabla_x \cdot \bar{\sigma}))_{stf}\mathbf{R}^{\mathsf{T}}$ upon using the formula of $(\cdot)_{stf}$ in (A.7). Furthermore, it is evident that $(\nabla_{x'}^2\theta')_{stf} = \mathbf{R}(\nabla_x^2\theta)_{stf}\mathbf{R}^{\mathsf{T}}$. Therefore, the rotational invariance of (3.6) has been verified.

Overall, our moment equations (3.2)–(3.6) satisfy the rotational invariance and, by encompassing the translational invariance, consequently satisfy the Galilean invariance.

Appendix B. Tables of coefficients in the inverse-power-law model

Table 2 lists the coefficients k_i and l_i of the moment equations in (3.2)–(3.6) for some choices of parameter η in the inverse-power-law model, and tables 3 and 4 list the coefficients m_{ij} of the corresponding boundary conditions (3.9)–(3.17).

Appendix C. Computation of the coefficients β and γ in the asymptotic analysis

This appendix establishes the relationship between the coefficients $a_{lnn'}$ and β and γ in (4.9)–(4.13). For any fixed l, we consider $a_{lnn'}$ as an infinite matrix. We can then define $b_{lnn'}^{(n_0)}$ as the inverse of a submatrix of $a_{lnn'}$:

$$\sum_{n'=n_0}^{+\infty} a_{lnn'}b_{ln'n''}^{(n_0)} = \delta_{nn''}, \quad \text{for all } n, n'' = n_0, n_0 + 1, \ldots. \tag{C.1}$$

η	k_0	k_1	k_2	k_3	k_4
5	1	0	0	0	0
7	9.9785×10^{-1}	3.0773×10^{-3}	1.2550×10^{-5}	2.6072×10^{-3}	4.8885×10^{-2}
10	9.9396×10^{-1}	8.7436×10^{-3}	4.5818×10^{-5}	7.4080×10^{-3}	8.1805×10^{-2}
17	9.8883×10^{-1}	1.6341×10^{-2}	1.0021×10^{-4}	1.3840×10^{-2}	1.1124×10^{-1}
∞	9.7971×10^{-1}	3.0261×10^{-2}	2.0798×10^{-4}	2.5607×10^{-2}	1.5056×10^{-1}

η	k_5	k_6	k_7	k_8	k_9
5	1	1	1	1	1
7	9.9794×10^{-1}	8.9911×10^{-1}	9.7119×10^{-1}	8.6773×10^{-1}	9.6577×10^{-1}
10	9.9420×10^{-1}	8.4173×10^{-1}	9.5624×10^{-1}	7.7962×10^{-1}	9.4997×10^{-1}
17	9.8926×10^{-1}	7.9687×10^{-1}	9.4576×10^{-1}	7.0221×10^{-1}	9.4062×10^{-1}
∞	9.8041×10^{-1}	7.4535×10^{-1}	9.3584×10^{-1}	6.0171×10^{-1}	9.3491×10^{-1}

η	k_{10}	l_1	l_2
5	0	1	1
7	2.8590×10^{-7}	9.9420×10^{-1}	9.9545×10^{-1}
10	1.1896×10^{-6}	9.8385×10^{-1}	9.8727×10^{-1}
17	2.8475×10^{-6}	9.7049×10^{-1}	9.7666×10^{-1}
∞	6.3621×10^{-6}	9.4741×10^{-1}	9.5812×10^{-1}

Table 2. Coefficients in moment equations (3.2)–(3.6) for some power indices η in the inverse-power-law model.

Due to the conservation of mass, momentum and energy, the quantities $b_{0nn'}^{(0)}$, $b_{0nn'}^{(1)}$ and $b_{1nn'}^{(0)}$ do not exist (see (4.7)). Since the collision operator $\mathcal{L}$ is negative semidefinite and has a kernel of five dimensions, all other coefficients $b_{lnn'}^{(n_0)}$ with non-negative l, n, n' and n_0 are well defined. These coefficients have been defined in Cai *et al.* (2024*b*) where R13 equations for steady-state flows are derived.

In practice, the infinite matrices $a_{lnn'}$ are truncated and $b_{lnn'}^{(n_0)}$ are obtained by taking the inverse directly. Then the coefficients β and γ in (4.9)–(4.13) are given by

$$\beta_1^{(1),n} = b_{11n}^{(1)}, \qquad \beta_2^{(1),n} = b_{20n}^{(0)},$$

$$\gamma_0^{(2),n} = \sum_{n'=2}^{+\infty} \frac{b_{0nn'}^{(2)}\left(\sqrt{2n'+3}\,b_{11n'}^{(1)} - \sqrt{2n'}\,b_{11,n'-1}^{(1)}\right)}{b_{111}^{(1)}},$$

$$\gamma_{t1}^{(1),n} = \sum_{n'=2}^{\infty} \frac{b_{1nn'}^{(2)} b_{11n'}^{(1)}}{b_{111}^{(1)}}, \qquad \gamma_{s1}^{(1),n} = \sum_{n'=2}^{\infty} \frac{b_{1nn'}^{(2)}\left(\sqrt{2n'+5}\,b_{20n'}^{(0)} - \sqrt{2n'}\,b_{20,n'-1}^{(0)}\right)}{b_{200}^{(0)}},$$

$$\gamma_{t2}^{(1),n} = \sum_{n'=2}^{\infty} \frac{b_{2nn'}^{(1)} b_{20n'}^{(0)}}{b_{200}^{(0)}}, \qquad \gamma_{s2}^{(1),n} = \frac{2}{5}\sum_{n'=1}^{\infty} \frac{b_{2nn'}^{(1)}\left(\sqrt{2n'+5}\,b_{11n'}^{(1)} - \sqrt{2(n'+1)}\,b_{11,n'+1}^{(1)}\right)}{b_{111}^{(1)}},$$

$$\gamma_3^{(2),n} = \frac{3}{7}\sum_{n'=0}^{+\infty} \frac{b_{3nn'}^{(0)}}{b_{200}^{(0)}}\left(\sqrt{2n'+7}\,b_{20n'}^{(0)} - \sqrt{2(n'+1)}\,b_{20,n'+1}^{(0)}\right). \tag{C.2}$$

These results are obtained by asymptotic analysis. The derivation is similar to the steady-state case. Here we omit the details and refer interested readers to Cai *et al.* (2024*b*).

η	m_{11}	m_{12}	m_{13}	m_{14}	m_{15}
5	$2/\sqrt{2\pi}$	$1/2\sqrt{2\pi}$	$8/5\sqrt{2\pi}$	$48/25\sqrt{2\pi}$	0
7	8.2699×10^{-1}	1.7756×10^{-1}	5.9524×10^{-1}	7.7155×10^{-1}	4.0454×10^{-2}
10	8.4706×10^{-1}	1.6277×10^{-1}	5.7153×10^{-1}	7.7914×10^{-1}	6.9432×10^{-2}
17	8.6507×10^{-1}	1.4961×10^{-1}	5.5359×10^{-1}	7.8843×10^{-1}	9.6598×10^{-2}
∞	8.8890×10^{-1}	1.3234×10^{-1}	5.3390×10^{-1}	8.0443×10^{-1}	1.3481×10^{-1}

η	m_{21}	m_{22}	m_{23}	m_{24}	m_{25}
5	–	–	–	–	–
7	4.9821×10^{-3}	1.9210×10^{-2}	3.5585×10^{-3}	4.6126×10^{-3}	2.4185×10^{-4}
10	7.5057×10^{-3}	3.1012×10^{-2}	4.9556×10^{-3}	6.7557×10^{-3}	6.0203×10^{-4}
17	9.2216×10^{-3}	4.0714×10^{-2}	5.6679×10^{-3}	8.0723×10^{-3}	9.8900×10^{-4}
∞	1.0730×10^{-2}	5.2344×10^{-2}	5.9826×10^{-3}	9.0140×10^{-3}	1.5106×10^{-3}

η	m_{26}	m_{27}	m_{28}
5	–	–	–
7	2.9445×10^{-2}	1.1082×10^{-1}	4.5197×10^{-4}
10	5.0347×10^{-2}	1.9074×10^{-1}	9.9954×10^{-4}
17	7.0089×10^{-2}	2.6780×10^{-1}	1.6422×10^{-3}
∞	9.8823×10^{-2}	3.8322×10^{-1}	2.6338×10^{-3}

η	m_{31}	m_{32}	m_{33}	m_{34}	m_{35}
5	$1/\sqrt{2\pi}$	$1/5\sqrt{2\pi}$	0	$2/\sqrt{2\pi}$	0
7	4.0358×10^{-1}	7.2977×10^{-2}	5.8325×10^{-8}	7.8808×10^{-1}	7.6807×10^{-6}
10	4.0655×10^{-1}	6.8340×10^{-2}	2.4645×10^{-7}	7.8723×10^{-1}	2.8477×10^{-5}
17	4.0908×10^{-1}	6.4237×10^{-2}	5.9816×10^{-7}	7.9036×10^{-1}	6.3150×10^{-5}
∞	4.1227×10^{-1}	5.8927×10^{-2}	1.3613×10^{-6}	8.0020×10^{-1}	1.3351×10^{-4}

η	m_{41}	m_{42}	m_{43}	m_{44}	m_{45}
5	$1/\sqrt{2\pi}$	$11/5\sqrt{2\pi}$	0	$2/\sqrt{2\pi}$	0
7	3.4342×10^{-1}	8.5528×10^{-1}	5.6647×10^{-8}	7.6541×10^{-1}	7.4598×10^{-6}
10	3.0441×10^{-1}	8.4194×10^{-1}	2.3349×10^{-7}	7.4584×10^{-1}	2.6980×10^{-5}
17	2.6826×10^{-1}	8.3207×10^{-1}	5.5187×10^{-7}	7.2919×10^{-1}	5.8263×10^{-5}
∞	2.1746×10^{-1}	8.2380×10^{-1}	1.2025×10^{-6}	7.0683×10^{-1}	1.1793×10^{-4}

η	m_{46}	m_{47}	m_{48}
5	0	0	24/5
7	1.2222×10^{-1}	2.4505×10^{-1}	4.7008
10	2.0315×10^{-1}	4.0914×10^{-1}	4.6366
17	2.7309×10^{-1}	5.5322×10^{-1}	4.5779
∞	3.6056×10^{-1}	7.3790×10^{-1}	4.4916

Table 3. Part 1 of the coefficients in boundary conditions (3.9)–(3.17) for some power indices η in the inverse-power-law model.

Appendix D. Computation of the coefficients $c_k^{\ell,n}$

The expressions of $c_1^{1,n}$ and $c_2^{0,n}$ have been introduced in (4.20) and (4.22). In this appendix we focus on the coefficients appearing in (4.29).

The coefficients $c_0^{2,n}$ must be chosen such that $\langle \phi^2, \psi^n - d_{02}^n \psi^2 \rangle = 0$ for all $n \geqslant 3$. This leads to

$$c_0^{2,n} = d_{02}^n c_0^{2,2}, \qquad \text{for all } n \geqslant 3. \tag{D.1}$$

η	m_{51}	m_{52}	m_{53}	m_{54}	m_{55}
5	–	–	–	–	–
7	3.4282×10^{-2}	8.5377×10^{-2}	5.6547×10^{-9}	7.6406×10^{-2}	7.4466×10^{-7}
10	5.2206×10^{-2}	1.4439×10^{-1}	4.0044×10^{-8}	1.2791×10^{-1}	4.6270×10^{-6}
17	6.4303×10^{-2}	1.9945×10^{-1}	1.3228×10^{-7}	1.7479×10^{-1}	1.3966×10^{-5}
∞	7.3794×10^{-2}	2.7955×10^{-1}	4.0806×10^{-7}	2.3986×10^{-1}	4.0020×10^{-5}

η	m_{56}	m_{57}	m_{58}
5	–	–	–
7	2.7746×10^{-2}	5.5632×10^{-2}	4.7964×10^{-1}
10	6.0867×10^{-2}	1.2259×10^{-1}	8.1033×10^{-1}
17	1.0110×10^{-1}	2.0482×10^{-1}	1.1154
∞	1.7187×10^{-1}	3.5174×10^{-1}	1.5445

η	m_{61}	m_{62}	m_{63}	m_{64}	m_{65}
5	$2/5\sqrt{2\pi}$	$7/5\sqrt{2\pi}$	$8/25\sqrt{2\pi}$	$48/125\sqrt{2\pi}$	0
7	1.5598×10^{-1}	6.0144×10^{-1}	1.1141×10^{-1}	1.4441×10^{-1}	7.5718×10^{-3}
10	1.5101×10^{-1}	6.2395×10^{-1}	9.9703×10^{-2}	1.3592×10^{-1}	1.2112×10^{-2}
17	1.4747×10^{-1}	6.5107×10^{-1}	9.0636×10^{-2}	1.2909×10^{-1}	1.5815×10^{-2}
∞	1.4418×10^{-1}	7.0335×10^{-1}	8.0389×10^{-2}	1.2112×10^{-1}	2.0298×10^{-2}

η	m_{66}	m_{67}	m_{68}	m_{69}
5	0	2	0	0
7	2.1284×10^{-7}	2.0460	9.0196×10^{-8}	3.5825×10^{-7}
10	1.6606×10^{-6}	2.0707	3.0801×10^{-7}	2.8135×10^{-6}
17	5.1333×10^{-6}	2.1281	6.3694×10^{-7}	8.7714×10^{-6}
∞	1.5172×10^{-5}	2.2756	1.2781×10^{-6}	2.6311×10^{-5}

η	m_{71}	m_{81}
5	$1/2\sqrt{2\pi}$	$1/2\sqrt{2\pi}$
7	2.0678×10^{-1}	2.0678×10^{-1}
10	2.0996×10^{-1}	2.0996×10^{-1}
17	2.1152×10^{-1}	2.1152×10^{-1}
∞	2.1169×10^{-1}	2.1169×10^{-1}

Table 4. Part 2 of the coefficients in boundary conditions (3.9)–(3.17) for some power indices η in the inverse-power-law model.

We choose the coefficient $c_0^{2,2}$ such that $c_0^{2,2} > 0$ and

$$\sum_{n=2}^{+\infty} |c_0^{2,n}|^2 = 1. \tag{D.2}$$

In our implementation, we truncate this infinite series up to $n = 20$.

The coefficients $c_1^{2,n}$ and $c_1^{3,n}$ must be chosen such that, for all $n \geqslant 4$, $\langle \phi_i^2, \varphi_1^n \rangle = \langle \phi_i^3, \varphi_1^n \rangle = 0$,

$$\varphi_1^n = \left(\psi_i^n - \frac{\beta_1^{(1),n}}{\beta_1^{(1),1}} \psi_i^1 \right) - d_{12}^n \left(\psi_i^2 - \frac{\beta_1^{(1),2}}{\beta_1^{(1),1}} \psi_i^1 \right) - d_{13}^n \left(\psi_i^3 - \frac{\beta_1^{(1),3}}{\beta_1^{(1),1}} \psi_i^1 \right). \tag{D.3}$$

Therefore, the coefficients $c_1^{2,n}$ and $c_1^{3,n}$ must satisfy

$$c_1^{2,n} - d_{12}^n c_1^{2,2} - d_{13}^n c_1^{2,3} + \left(\frac{\beta_1^{(1),n}}{\beta_1^{(1),1}} - \frac{\beta_1^{(1),2}}{\beta_1^{(1),1}} d_{12}^n - \frac{\beta_1^{(1),3}}{\beta_1^{(1),1}} d_{13}^n \right) \sum_{n'=2}^{+\infty} \frac{\beta_1^{(1),n'}}{\beta_1^{(1),1}} c_1^{2,n'} = 0,$$

$$c_1^{3,n} - d_{12}^n c_1^{3,2} - d_{13}^n c_1^{3,3} + \left(\frac{\beta_1^{(1),n}}{\beta_1^{(1),1}} - \frac{\beta_1^{(1),2}}{\beta_1^{(1),1}} d_{12}^n - \frac{\beta_1^{(1),3}}{\beta_1^{(1),1}} d_{13}^n \right) \sum_{n'=2}^{+\infty} \frac{\beta_1^{(1),n'}}{\beta_1^{(1),1}} c_1^{3,n'} = 0 \quad \text{(D.4)}$$

for all $n \geq 4$. The linear systems for $c_1^{2,n}$ and $c_1^{3,n}$ are actually the same, and we just need to find linearly independent solutions for them. Note that we need to find all coefficients $c_1^{2,n}$ and $c_1^{3,n}$ for $n \geq 2$, while the linear equations (D.4) are defined only for $n \geq 4$, the solutions are expected to form a two-dimensional linear space. Then $c_1^{2,n}$ and $c_1^{3,n}$ should form a basis of the space. In our implementation, we choose $c_1^{2,n}$ and $c_1^{3,n}$ such that:

  i. the norms of ϕ_i^2 and ϕ_i^3 are equal to 1;
 ii. $\langle \phi_i^2, \phi_i^3 \rangle = 0$;
iii. $c_1^{2,2} > 0$, $c_1^{2,3} = 0$ and $c_1^{3,3} > 0$.

The last condition is to guarantee that when the collision model tends to Maxwell molecules, we have $\phi_i^2 \to \psi_i^2$ and $\phi_i^3 \to \psi_i^3$. To solve (D.4), the system is again truncated up to $n = 20$.

The determination of $c_2^{1,n}$ and $c_2^{2,n}$ is similar to that of $c_1^{2,n}$ and $c_1^{3,n}$. The equations that $c_2^{1,n}$ and $c_2^{2,n}$ satisfy are

$$c_2^{1,n} - d_{21}^n c_2^{1,1} - d_{22}^n c_2^{1,2} + \left(\frac{\beta_2^{(1),n}}{\beta_2^{(1),0}} - \frac{\beta_2^{(1),1}}{\beta_2^{(1),0}} d_{21}^n - \frac{\beta_2^{(1),2}}{\beta_2^{(1),0}} d_{22}^n \right) \sum_{n'=1}^{+\infty} \frac{\beta_2^{(1),n'}}{\beta_2^{(1),0}} c_2^{1,n'} = 0,$$

$$c_2^{2,n} - d_{21}^n c_2^{2,1} - d_{22}^n c_2^{2,2} + \left(\frac{\beta_2^{(1),n}}{\beta_2^{(1),0}} - \frac{\beta_2^{(1),1}}{\beta_2^{(1),0}} d_{21}^n - \frac{\beta_2^{(1),2}}{\beta_2^{(1),0}} d_{22}^n \right) \sum_{n'=1}^{+\infty} \frac{\beta_2^{(1),n'}}{\beta_2^{(1),0}} c_2^{2,n'} = 0.$$

$$\text{(D.5)}$$

To determine these coefficients, we require that:

  i. the norms of ϕ_{ij}^1 and ϕ_{ij}^2 are equal to 1;
 ii. $\langle \phi_{ij}^1, \phi_{ij}^2 \rangle = 0$;
iii. $c_2^{1,1} > 0$, $c_2^{1,2} = 0$ and $c_2^{2,2} > 0$.

When the collision model tends to Maxwell molecules, we have $\phi_{ij}^1 \to \psi_{ij}^1$ and $\phi_{ij}^2 \to \psi_{ij}^2$.

The determination of $c_3^{0,n}$ is similar to that of $c_0^{2,n}$. The solution is

$$c_3^{0,n} = d_{30} c_3^{0,0}, \quad \text{(D.6)}$$

where $c_3^{0,0}$ is selected to be positive and satisfies

$$\sum_{n=0}^{+\infty} |c_3^{0,n}|^2 = 1. \quad \text{(D.7)}$$

Appendix E. Expressions of A_{ij}

The expressions of A_{ij} explicitly depends on the coefficients $c_k^{\ell,n}$, which are given as follows:

$$A_{45} = 3 \sum_{n=1}^{+\infty} c_1^{1,n} \left(\sqrt{2n+5} c_2^{0,n} - \sqrt{2n} c_2^{0,n-1} \right), \tag{E.1}$$

$$A_{46} = \sum_{n=1}^{+\infty} c_1^{1,n} \left(\sqrt{2n+3} c_0^{2,n} - \sqrt{2(n+1)} c_0^{2,n+1} \right), \tag{E.2}$$

$$A_{49} = 3 \sum_{n=1}^{+\infty} c_1^{1,n} \left(\sqrt{2n+5} c_2^{1,n} - \sqrt{2n} c_2^{1,n-1} \right), \tag{E.3}$$

$$A_{4,10} = 3 \sum_{n=1}^{+\infty} c_1^{1,n} \left(\sqrt{2n+5} c_2^{2,n} - \sqrt{2n} c_2^{2,n-1} \right), \tag{E.4}$$

$$A_{57} = 3 \sum_{n=0}^{+\infty} c_2^{0,n} \left(\sqrt{2n+5} c_1^{2,n} - \sqrt{2(n+1)} c_1^{2,n+1} \right), \tag{E.5}$$

$$A_{58} = 3 \sum_{n=0}^{+\infty} c_2^{0,n} \left(\sqrt{2n+5} c_1^{3,n} - \sqrt{2(n+1)} c_1^{3,n+1} \right), \tag{E.6}$$

$$A_{5,11} = \frac{15}{2} \sum_{n=0}^{+\infty} c_2^{0,n} \left(\sqrt{2n+7} c_3^{0,n} - \sqrt{2n} c_3^{0,n-1} \right), \tag{E.7}$$

$$A_{67} = \sum_{n=2}^{+\infty} c_0^{2,n} \left(\sqrt{2n+3} c_1^{2,n} - \sqrt{2n} c_1^{2,n-1} \right), \tag{E.8}$$

$$A_{68} = \sum_{n=2}^{+\infty} c_0^{2,n} \left(\sqrt{2n+3} c_1^{3,n} - \sqrt{2n} c_1^{3,n-1} \right), \tag{E.9}$$

$$A_{79} = 3 \sum_{n=1}^{+\infty} c_1^{2,n} \left(\sqrt{2n+5} c_2^{1,n} - \sqrt{2n} c_2^{1,n-1} \right), \tag{E.10}$$

$$A_{7,10} = 3 \sum_{n=1}^{+\infty} c_1^{2,n} \left(\sqrt{2n+5} c_2^{2,n} - \sqrt{2n} c_2^{2,n-1} \right), \tag{E.11}$$

$$A_{89} = 3 \sum_{n=1}^{+\infty} c_1^{3,n} \left(\sqrt{2n+5} c_2^{1,n} - \sqrt{2n} c_2^{1,n-1} \right), \tag{E.12}$$

$$A_{8,10} = 3 \sum_{n=1}^{+\infty} c_1^{3,n} \left(\sqrt{2n+5} c_2^{2,n} - \sqrt{2n} c_2^{2,n-1} \right), \tag{E.13}$$

$$A_{9,11} = \frac{15}{2} \sum_{n=0}^{+\infty} c_2^{1,n} \left(\sqrt{2n+7} c_3^{0,n} - \sqrt{2n} c_3^{0,n-1} \right), \tag{E.14}$$

$$A_{10,11} = \frac{15}{2} \sum_{n=0}^{+\infty} c_2^{2,n} \left(\sqrt{2n+7} c_3^{0,n} - \sqrt{2n} c_3^{0,n-1} \right). \tag{E.15}$$

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