On Well-Posed Boundary Conditions for the Linear Non-Homogeneous Moment Equations in Half-Space

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Received: 10 September 2022 / Accepted: 16 October 2023 / Published online: 13 November 2023
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Abstract
We investigate the boundary conditions that ensure the well-posedness of the linear non-homogeneous Grad moment equations in half-space. The Grad moment system is based on a Hermite expansion and regarded as an efficient reduced model of the Boltzmann equation. At a solid wall, the moment equations are commonly equipped with a Maxwell-type boundary condition named the Grad boundary condition. We point out the instability of the Grad boundary condition for non-homogeneous half-space problems. Under reasonable assumptions, we propose several well-posedness criteria, which are applied to prove a class of modified boundary conditions well-posed. The technique to make sure existence and uniqueness mainly includes a well-designed preliminary simultaneous transformation of the coefficient matrices, as well as Kreiss’ procedure for analyzing linear boundary value problems with characteristic boundaries. Stability is established through a weighted estimate. At the same time, we obtain analytical expressions of the solution, which may help solve the half-space problem efficiently.

Keywords Half-space problem · Moment method · Well-posed boundary condition · Non-homogeneous equations

Mathematics Subject Classification 34B40 · 35Q35 · 76P05 · 82B40

1 Introduction

The moment equations proposed by Grad [20] are regarded as an efficient reduced model of the Boltzmann equation. The hydrodynamic equations such as the Navier–Stokes equa-

Communicated by Isabelle Gallagher.

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tions fail to describe rarefied gases due to the breakdown of the continuum assumption. The high-dimensional Boltzmann equation accurately describes the behavior of rarefied gases but solving it requires significant computational resources. Nowadays, the moment approximations of the Boltzmann equation have gained much more attention because of the efficiency [11, 27, 50, 51], the hyperbolicity [10, 15, 29, 33], the entropy and H-theorem [41, 52], the available analytical solutions [23, 28, 40, 49] and other advantages.

Despite the wide range of applications, the well-posedness of the initial-boundary value problem for the moment system is doubtable. The classical Grad boundary condition [20] was proposed for the moment system by testing the Maxwell diffuse-specular model with odd polynomials. However, it was reported in [41] that the Grad boundary condition is not stable. Then [43] identified a null-space condition and provided a provably stable modification in the linear case. More structured derivations of the modified boundary condition are given in [8, 9]. Nevertheless, the well-posed theory in [43] only applies to the initial-boundary value problem.

The paper concerns layer problems of the Grad moment equations. Layer problems of the Boltzmann equation arise from the asymptotic analysis and play a crucial role in understanding the boundary-layer behavior of rarefied gases [44–46]. The relevant study helps prescribe slip boundary conditions for hydrodynamic equations [1, 24, 25, 35] and impose the interface coupling condition between kinetic and hydrodynamic equations [2, 13, 32]. For layer problems of the Boltzmann equation, the well-posedness theory has been well developed; see [3] and the references cited therein.

On the one hand, layer problems for the Grad moment equations could be derived from similar asymptotic analysis [35]. On the other hand, the corresponding moment system may serve as an efficient numerical solver of kinetic layer equations. Some most famous analytical methods to solve layer equations are essentially low-order moment methods, including the Maxwell method [12], Loyalka’s method [36, 37], and the half-range moment method [22]. The arbitrary order moment equations are also widely used to resolve layer problems [16, 23, 48] due to the available analytical solutions.

In this paper, we focus on the linear steady non-homogeneous equations in half-space:

\[
A \frac{dW(y)}{dy} = -QW(y) + h(y), \quad y \in [0, +\infty),
\]

\[
BW(0) = g,
\]

where \( e^{\alpha y} W(y) \in L^2(\mathbb{R}_+; L^2(\mathbb{R}^N)) \) and \( e^{\alpha y} h(y) \in L^2(\mathbb{R}_+; L^2(\mathbb{R}^N)) \) for some constant \( \alpha > 0 \). Here \( A, Q, B \) are \( N \times N \) matrices, and \( g \) is an \( N \times 1 \) vector, all with constant coefficients. For the Grad moment equations, the matrix \( A \) is symmetric while \( Q \) is symmetric positive semi-definite, and they respectively have a special block structure as will be shown later in the article.

This work has two main objects. First, we study the criteria for well-posedness of the non-homogeneous linear Grad moment equations in half-space. Then, we verify that the modified boundary condition with a similar form to that in the initial-boundary value problem is also well-posed for layer problems.

In general, the concept of well-posedness has three aspects [17]. First, the solution exists. Second, the solution is unique. Third, the solution depends continuously on the boundary data and non-homogeneous term. For the initial-boundary value problem of the linear Grad moment equations, [43] analyzed its well-posedness through an energy estimate. This method can not apply to the half-space problem directly. Our method is similar to Kreiss’ procedure [30] for studying linear hyperbolic systems, i.e., finding their analytical solu-
tions and then estimating them. We have studied layer problems for the linear homogeneous moment equations using the same ideas in [34]. However, the non-homogeneous case is not a trivial corollary of the homogeneous situation. We have established conditions on the non-homogeneous term that ensure well-posedness.

Our method is essentially basic linear algebra. Because the matrices $A$ and $Q$ may both have zero eigenvalues, the problem has a characteristic boundary where the characteristic variables have a vanishing speed at the boundary [26]. To simplify the analysis, we perform a simultaneous transformation of the coefficient matrices to consider an equivalent but simpler system. Then following the characteristic analysis of ODEs, we explicitly write the analytical solution to the half-space problem. By analyzing the stability of the solution, we finally achieve well-posedness criteria for the linear non-homogeneous moment system in half-space. We exhibit the instability of the Grad boundary condition through examples. The modified boundary condition is then proven to also be well-posed for layer problems.

A discrete system similar to (1.1) arises from the discrete velocity method (DVM) of the Boltzmann equation, where the matrix $A$ is commonly diagonal. The solvability of these discrete equations has been exhaustively studied by Bernhoff [4–6]. These results can apply to the system (1.1) to obtain the existence and uniqueness of the solution. In comparison, our method leverages the specific structure of the Grad moment equations, which gives a more subtle description of the solution. We also identify an additional stability condition in addition to the solvability condition. The general abstract theory regarding linear boundary value problems can be found in [30, 31, 38, 42].

The paper is arranged as follows: in Sect. 2, we briefly introduce layer problems of the Grad moment equations derived from the linearized Boltzmann equation (LBE). Then we outline the well-posed conditions without including a comprehensive proof. In Sect. 3, we illustrate the instability of the Grad boundary condition by simple examples and discuss its well-posed modification. In Sect. 4, we complete the proof of well-posedness. The paper ends with conclusions.

2 Well-Posedness of Layer Problems

2.1 Basic Equations

For single-species monatomic molecules, we assume that the rarefied gas is close to the Maxwellian:

$$\mathcal{M} = \mathcal{M}(\xi) = \frac{1}{(2\pi)^{3/2}} \exp\left(-\frac{|\xi|^2}{2}\right),$$

where $\xi = (\xi_1, \xi_2, \xi_3)$ is the microscopic velocity. Then the LBE with the linearized Maxwell boundary condition reads as

$$\frac{\partial f}{\partial t} + \sum_{d=1}^{3} \xi_d \frac{\partial f}{\partial x_d} = \mathcal{L}[f], \quad f = f(t, x, \xi), \quad x \in \Omega \subset \mathbb{R}^3, \quad \xi \in \mathbb{R}^3,$$

$$f(t, x, \xi) = \chi f^w(t, x, \xi) + (1 - \chi) f(t, x, \xi^*), \quad x \in \partial \Omega, \quad (\xi - u^w) \cdot n < 0,$$

$$f(0, x, \xi) = f_0(x, \xi), \quad x \in \Omega, \quad \xi \in \mathbb{R}^3,$$
where \( f \) is the perturbed velocity distribution function, \( t \) denoting the time, \( x = (x_1, x_2, x_3) \) the spatial coordinates, \( f_0(x, \xi) \) the initial value. Here \( \mathcal{L} \) is a linear operator depicting the collision between gas molecules. A simplest example is the linearized BGK collision operator [46], where

\[
\mathcal{L}[f] = \mathcal{M}(\xi) \left( \rho + u \cdot \xi + \theta |\xi|^2 - \frac{3}{2} f \right).
\]

The density \( \rho \), velocity \( u = (u_1, u_2, u_3) \) and temperature \( \theta \) are defined by the formulas

\[
\rho = \langle f \rangle, \quad u_i = \langle \xi_i \rangle, \quad \theta = \left( \frac{|\xi|^2}{3} - \frac{3}{2} f \right), \quad \langle \cdot \rangle := \int_{\mathbb{R}^3} \cdot \, d\xi.
\]

(2.2)

It’s not our purposes to discuss all properties of \( \mathcal{L} \). We refer interested readers to [12, Chapter III] and [46, Chapter 1] for more details.

The Maxwell boundary condition (2.1b) assumes that the reflection at the wall is divided into a sum of \( 1 - \chi \) portion of specular reflection and \( \chi \) portion of diffuse reflection, where \( \chi \in [0, 1] \) is the tangential momentum accommodation coefficient. The boundary is assumed to be an impermeable wall with a unit normal vector \( n \) exiting the region, a given velocity \( u^w \), and a given temperature \( \theta^w \). To avoid cumbersome details about rotation invariance, we assume

\[
\Omega = \{ x \in \mathbb{R}^3 : x_2 \geq 0 \},
\]

with a fixed \( n = (0, -1, 0) \). To consider steady layer equations, we further assume

\[
u^w \cdot n = 0.
\]

Then the velocity from specular reflection is

\[
\xi^* = \xi - 2[ (\xi - u^w) \cdot n ] n = (\xi_1, -\xi_2, \xi_3).
\]

The linearized diffuse distribution [46] is given by

\[
f^w(t, x, \xi) = \mathcal{M}(\xi) \left( \rho^w + u^w \cdot \xi + \theta^w |\xi|^2 - \frac{3}{2} f \right),
\]

(2.3)

where \( \rho^w \) is determined by the subsequent no mass flow condition imposed at the wall:

\[
\int_{\mathbb{R}^3} (\xi - u^w) \cdot n \, f(t, x, \xi) \, d\xi = 0, \quad x \in \partial \Omega.
\]

(2.4)

The Grad moment equations serve as a reduced model of the Boltzmann equation [20]. We assume that the distribution function has a Hermite expansion as

\[
f(t, x, \xi) = \mathcal{M}(\xi) \sum_{|\alpha| \leq M} w_\alpha(t, x) \phi_\alpha(\xi),
\]

(2.5)

where \( M \geq 2 \) is a chosen integer and \( \alpha = (\alpha_1, \alpha_2, \alpha_3) \in \mathbb{N}^3 \) is the multi-index, \( |\alpha| = \alpha_1 + \alpha_2 + \alpha_3 \). The orthonormal Hermite polynomial \( \phi_\alpha = \phi_\alpha(\xi) \) is defined [19] by ensuring

\[
\langle \mathcal{M} \phi_\alpha \phi_\beta \rangle = \delta_{\alpha, \beta}, \quad \phi_0 = 1, \quad \phi_{e_i} = \xi_i,
\]

where \( e_i \in \mathbb{N}^3 \) is a unit vector with the i-th component being one. So the ansatz (2.5) gives

\[
w_\alpha = w_\alpha(t, x) = \langle f \phi_\alpha \rangle.
\]
Substituting the ansatz into the linearized Boltzmann equation and equating the coefficients in front of the basis functions on both sides, we obtain the $M$-th order Grad moment equations

$$\frac{\partial w_\alpha}{\partial t} + \sum_{d=1}^{3} \sum_{|\beta| \leq M} \langle M_{i_d} \phi_\alpha \phi_\beta \rangle \frac{\partial w_\beta}{\partial x_d} = \sum_{|\beta| \leq M} \langle L[M \phi_\beta] \phi_\alpha \rangle w_\beta, \quad |\alpha| \leq M. \quad (2.6)$$

To ensure the correct number of boundary conditions for the hyperbolic system (2.6), Grad [20] suggested testing the Maxwell boundary condition (2.1b) with odd polynomials (about the argument $(\xi - u^w) \cdot n = -\xi_2$) of degree no higher than $M$ to construct moment boundary conditions. The Grad boundary condition has some equivalent formulations [8, 11, 16, 48]. If we extract the factor $\xi_2$ from the odd polynomials [34], testing (2.1b) with odd polynomials yields

$$\int_{\mathbb{R}^2} \int_0^{+\infty} \xi_2 \phi_\alpha f(t, x, \xi) \, d\xi = \chi \int_{\mathbb{R}^2} \int_0^{+\infty} \xi_2 \phi_\alpha f^w(t, x, \xi) \, d\xi + (1 - \chi) \int_{\mathbb{R}^2} \int_0^{+\infty} \xi_2 \phi_\alpha f(t, x, \xi^w) \, d\xi, \quad x \in \partial \Omega, \quad (2.7)$$

where $\alpha_2$ is even and $|\alpha| \leq M - 1$. Plugging the ansatz (2.5) into the above formula and utilizing the even-odd parity of Hermite polynomials, we obtain the Grad boundary condition (in the considered plane geometry):

$$\left(1 - \frac{\chi}{2}\right) \sum_{|\beta| \leq M, \beta_2 \text{ odd}} \langle \xi_2 M \phi_\alpha \phi_\beta \rangle w_\beta = -\frac{\chi}{2} \sum_{|\beta| \leq M, \beta_2 \text{ even}} \langle |\xi_2| M \phi_\alpha \phi_\beta \rangle (w_\beta - b_\beta), \quad x_2 = 0. \quad (2.8)$$

where $\alpha_2$ is even and $|\alpha| \leq M - 1$. The entries $b_0 = \rho^w$, $b_{\alpha_1} = u_i^w$, $b_{2\alpha_1} = \theta^w / \sqrt{2}$ and otherwise $b_\beta = 0$. Here $\rho^w$ is determined by the no mass flow condition (2.4), expressed as $w_{x_2} - u_i^w = 0$ at $x_2 = 0$. That’s to say, if we let $\alpha = 0$ in (2.7), the left-hand side term of (2.7) should be zero because of the no mass flow condition. Then $\rho^w$ can be represented by the moment variables $w_\alpha$.

Layer problems focus on the boundary-layer behavior of rarefied gases; see [3, 7, 32, 46]. To study the boundary layer near $\partial \Omega = \{x_2 = 0\}$, one could separate the moment variables into the bulk flow part and boundary layer corrections. The boundary layer corrections are assumed to be fast variables, which vary dramatically normal to the wall, but vanish outside the boundary layer. According to the asymptotic analysis of (2.6), these fast variables (also denoted as $w_\alpha$ for simplicity) satisfy the linear steady moment equations in half-space:

$$\sum_{|\beta| \leq M} \langle M_{i_2} \phi_\alpha \phi_\beta \rangle \frac{dw_\beta}{dy} = \sum_{|\beta| \leq M} \langle L[M \phi_\beta] \phi_\alpha \rangle w_\beta + h_\alpha, \quad |\alpha| \leq M, \quad (2.9)$$

where the unknowns $w_\beta = w_\beta(y)$, $y \in [0, +\infty)$, with $w_\beta(+\infty) = 0$. The given non-homogeneous term $h_\alpha = h_\alpha(y)$ arises from the other contributions in the boundary layer. Correspondingly, the Grad boundary condition for these fast variables becomes

$$\left(1 - \frac{\chi}{2}\right) \sum_{|\beta| \leq M, \beta_2 \text{ odd}} \langle \xi_2 M \phi_\alpha \phi_\beta \rangle (w_\beta + \bar{w}_\beta) = -\frac{\chi}{2} \sum_{|\beta| \leq M, \beta_2 \text{ even}} \langle |\xi_2| M \phi_\alpha \phi_\beta \rangle (w_\beta + \bar{w}_\beta - b_\beta), \quad y = 0. \quad (2.10)$$
where \( \alpha_2 \) is even with \(|\alpha| \leq M - 1 \), and \( \bar{w}_\beta \) is given by the bulk flow outside the boundary layer. In short, we shall emphasize that in (2.9), the moment variables \( w_\beta \) and the non-homogeneous terms \( h_\alpha \) exhibit a natural decay as \( y \) approaches infinity. A brief derivation from (2.6) to (2.9) is provided in Appendix A; see [34, 35] for more comprehensive discussions.

2.2 Stability Criteria

We now aim to establish a sufficient and necessary condition (under certain assumptions) to ensure the well-posedness of a class of boundary value problems (BVPs). Our starting point is recognizing that the Grad moment equations in half-space (2.9) admit representation in an abstract form:

\[
A \frac{dW(y)}{dy} = -QW(y) + h(y), \quad y \in [0, +\infty),
\]

\[
W(+\infty) := \lim_{y \to +\infty} W(y) = 0,
\]

(2.11)

where \( W = W(y) \in \mathbb{R}^N \) is the solution vector. \( A \in \mathbb{R}^{N \times N} \) and \( Q \in \mathbb{R}^{N \times N} \) are constant coefficient matrices, and \( h = h(y) \in \mathbb{R}^N \) is the given inhomogeneous term. In the specific case of the Grad moment equations, the integer \( N \) and coefficient matrices \( A, Q \) possess well-defined forms [34]. However, in this manuscript, we address general BVPs of the form (2.11) with the following properties:

(M1). \( A = A^T \), i.e., the matrix \( A \) is real symmetric.

(M2). \( Q \geq 0 \), i.e., the matrix \( Q \) is symmetric positive semi-definite.

(M3). The non-singular condition:

\[
\text{Null}(A) \cap \text{Null}(Q) = \{0\},
\]

(2.12)

where \( \text{Null}(A) := \{x \in \mathbb{R}^N, \; Ax = 0\} \) means the null space of the matrix \( A \).

This work will discuss the scenarios where \( h \neq 0 \). For technical reasons, we assume that for some positive constant \( a \),

\[
\|h\|_a := \left( \int_0^{+\infty} e^{2ay} h^T h(y) \, dy \right)^{1/2} < +\infty.
\]

This implies that the inhomogeneous term must decay faster than any polynomials at infinity, a requirement consistent with the condition \( W(+\infty) = 0 \).

The well-posedness of (2.11) intrinsically encompasses three properties [17]: the existence of the solution, uniqueness, and continuous dependence on both prescribed boundary data and the inhomogeneous term. For the BVP specified in (2.11), additional boundary conditions at \( y = 0 \) should typically be imposed to guarantee well-posedness. Our aim herein is to find stability criteria of (2.11) such that the additional boundary conditions satisfying these criteria render the whole system well-posed.

Closely related is the well-posedness of linear initial boundary value problems (IBVPs) for the Grad moment equations, discussed comprehensively in [43] through the classical energy estimate [17, 26]. However, the energy method of [43] cannot be directly applied to the BVP (2.11) as \( Q \) may admit zero eigenvalues. Because the linear Grad moment equations are symmetric hyperbolic, these IBVPs require a number of boundary conditions exactly equal to the number of negative eigenvalues of the boundary matrix; e.g., \(-A\) at \( y = 0 \). In contrast,
the requisite number of boundary conditions for the BVP (2.11) depends also on \(Q\); see [4, 34]. Here, we analyze the well-posedness by first finding the analytical solutions to the system, which involves solving the generalized eigenvalue problem of \((A, Q)\) [53].

The backgrounds of the generalized eigenvalue problem can be found in [18, 39, 53]. To illustrate the basic ideas, we assume that there exist \(\lambda_i \in \mathbb{R} \cup \{\infty\}\) and \(x_i \in \mathbb{R}^N\) such that

\[
Ax_i = \lambda_i Qx_i. \tag{2.13}
\]

Then since \(A\) and \(Q\) are symmetric, we have \(x_i^T A = \lambda_i x_i^T Q\). Let \(v_i(y) = x_i^T QW(y)\) and \(h_i(y) = x_i^T h(y)\). Multiplying (2.11) left by \(x_i^T\) gives the characteristic equations

\[
\lambda_i \frac{dv_i(y)}{dy} = -v_i(y) + h_i(y), \quad y \in [0, +\infty), \quad v_i(+\infty) = 0.
\]

If \(\lambda_i = 0\), we have \(v_i(y) = h_i(y)\) and \(v_i(0) = h_i(0)\). If \(\lambda_i \neq 0\), we formally have

\[
v_i(y) = e^{-\lambda_i^{-1}y} v_i(0) + \lambda_i^{-1} \int_0^y e^{-\lambda_i^{-1}(y-s)} h_i(s)\, ds.
\]

So to make sure \(v_i(+\infty) = 0\), when \(\lambda_i < 0\), there must be

\[
v_i(0) = -\lambda_i^{-1} \int_0^{+\infty} e^{\lambda_i^{-1}s} h_i(s)\, ds.
\]

If \(\lambda_i > 0\), we can see above that \(v_i(0)\) can be arbitrarily given when

\[
\lim_{y \to +\infty} \int_0^y e^{-\lambda_i^{-1}(y-s)} h_i(s)\, ds = 0.
\]

Finally, if \(\lambda_i = \infty\), the system should be understood as

\[
\frac{dv_i(y)}{dy} = \lambda_i^{-1}(-v_i + h_i) = 0, \quad v_i(+\infty) = 0.
\]

Therefore, \(v_i(y)\) should be a constant and must be zero. This coarse example implies that we only need to prescribe extra boundary conditions at \(y = 0\) for \(\lambda_i > 0\).

Note that the above illustrations only provide a rough explanation. Strictly speaking, we will directly solve the system (2.11) and find its analytical solutions. Although the procedure can be adapted to solve the generalized eigenvalue problem of \((A, Q)\), we avoid these unnecessary details for conciseness. Due to the structure of the coefficient matrices as in (M1)–(M3), we can construct an interpretable simultaneous transformation with the bases \((U, V)\) to get an equivalent but simpler system:

\[
U^T A V \frac{d(V^T W)}{dy} = -U^T Q V (V^T W) + U^T h, \quad V^T W(+\infty) = 0. \tag{2.14}
\]

Here \(V\) is an orthogonal matrix and \(U\) is invertible, satisfying the properties in Lemma 2.1. Thanks to the above transformation, we seek to decompose the null space of \(Q\) such that solving a common eigenvalue problem yields the analytical solutions to the ODEs. We note that a similar transformation appears in [4, 6] expressed in the language of projection operators. Henceforth, we will denote a matrix by square brackets, using commas to emphasize its partition; see [14].

**Lemma 2.1** Assume \(A\) and \(Q\) satisfy (M1)–(M3). Suppose \(p = \dim \text{Null}(Q)\) and \(G \in \mathbb{R}^{N \times p}\) is column orthogonal with \(\text{Range}(G) := \{y \in \mathbb{R}^N : y = Gx \text{ for some } x \in \mathbb{R}^p\} = \text{Null}(Q)\). Suppose \(r = \dim \text{Null}(G^T A G)\) and \(X \in \mathbb{R}^{p \times r}\) is column orthogonal with \(\text{Range}(X) = \)
Null($G^TAG$). Then there exist an orthogonal matrix $V = [V_1, V_2, V_3] \in \mathbb{R}^{N \times N}$ and an invertible matrix $U = [U_1, U_2, U_3] \in \mathbb{R}^{N \times N}$ such that:

- $V_1 = GX \in \mathbb{R}^{N \times r}$.
- $V_2 \in \mathbb{R}^{N \times p}$ and $\text{Range}(V_2) = \text{Range}(AG)$.
- $U_1 = G \in \mathbb{R}^{N \times p}$, $U_2 = AGX \in \mathbb{R}^{N \times r}$, $U_3 = V_3$.

If we let $A_{ij} := U_i^TAV_j$ and $Q_{ij} := U_i^TQV_j$, then

- $Q_{1j} = 0$, $Q_{1i} = 0$, $Q_{33} > 0$, for $i, j = 1, 2, 3$.
- $A_{31} = 0$, $A_{33}^{T} = A_{33}$ and $\text{rank}(A_{21}) = \text{rank}(U_2)$.

**Proof**

Note that $V_1$ and $U$ are defined directly. Since $\text{Null}(A) \cap \text{Null}(Q) = \{0\}$, we have $\text{rank}(AG) = \text{rank}(G) = p$. Thus, a column orthogonal $V_2$ can be constructed by applying Gram-Schmidt orthogonalization to the columns in $AG$; see [18, Thm. 5.2.3]. Then $V_2^TV_1 = 0$ since $\text{Range}(X) = \text{Null}(G^TAG)$. Because $[V_1, V_2]$ is column orthogonal, there must exist $V_3 \in \mathbb{R}^{N \times (N-p-r)}$ such that $V = [V_1, V_2, V_3]$ is orthogonal.

We claim that the above $U$ is invertible. Since $V_2^TV_2 = 0$, we have $U_3^TU_2 = 0$. Noting that $U_3^TU_1 = 0$, it suffices to show that

$$\text{Range}(U_1) \cap \text{Range}(U_3) = \text{Range}(V_3) \cap \text{Range}(G) = \{0\}. \quad (2.15)$$

In fact, if $Gc_1 = V_3c_2$ for some $c_1 \in \mathbb{R}^p$ and $c_2 \in \mathbb{R}^{(N-p-r)}$, then $(Gc_1)^TAG = 0$ since $V_2^TV_1 = 0$. So $c_1 \in \text{Range}(X)$ and $V_3c_2 \in \text{Range}(GX) = \text{Range}(V_1)$. Thus, from $V_3^TV_1 = 0$ we have $c_2 = 0$, which implies (2.15).

By definition, $A_{33}$ is symmetric. Since $QG = 0$, we have $Q_{1j} = 0$ and $Q_{1i} = 0$. From (2.15), we have $Q_{33} > 0$. We have $\text{rank}(A_{21}) = \text{rank}(U_3^TU_2) = \text{rank}(U_2)$ and $A_{31} = U_3^TU_1 = 0$. \hfill $\square$

The choices of $U$ and $V$ are not unique, but they do not affect the results if they satisfy the properties in Lemma 2.1. If $U$ and $V$ satisfy these properties, the system (2.14) becomes

$$\begin{bmatrix}
A_{21} & * & * \\
* & * & A_{33}
\end{bmatrix} \begin{bmatrix}
\frac{d}{dy}V_1^TW \\
\frac{d}{dy}V_2^TW \\
\frac{d}{dy}V_3^TW
\end{bmatrix} = -\begin{bmatrix}
0 & 0 & 0 \\
0 & * & * \\
0 & * & Q_{33}
\end{bmatrix} \begin{bmatrix}
V_1^TW \\
V_2^TW \\
V_3^TW
\end{bmatrix} + U^Th, \quad V^T(+\infty) = 0.$$

As will be demonstrated in the proof of Lemma 4.1, from the first $p$ lines of (2.14) we can solve for $U_1^TAW(y)$, which coincidently determines $V_2^TW(y)$. When $V_2^TW(y)$ is given, the last $N - p - r$ lines of (2.14) would give

$$A_{33} \frac{d}{dy}(V_3^TW) = -Q_{33}(V_3^TW) + V_3^Th - Q_{32}V_2^TW - A_{32} \frac{dV_2^TW}{dy},$$

where $Q_{33}$ is symmetric positive definite. Since $V_1^TW(y)$ can be determined by the middle $r$ lines of (2.14) when $V_2^TW(y)$ and $V_3^TW(y)$ are known, the general solutions of (2.14) shall be expressed using the eigenvalue decomposition of $Q_{33}^{-1}A_{33}$. In this way, the transformation allows one to reduce the full generalized eigenvalue problem to the one on $(A_{33}, Q_{33})$.

Since $A_{33}$ is symmetric and $Q_{33}$ is symmetric positive definite, $Q_{33}^{-1}A_{33}$ should have the same number of positive, negative and zero eigenvalues as $A_{33}$ according to Sylvester’s law of inertia. The real symmetric matrix $A_{33}$ must have $N - p - r$ real eigenvalues. We assume $A_{33}$ has $n_+$ positive eigenvalues, $n_-$ negative eigenvalues and $n_0$ zero eigenvalues. Then we
can always find an invertible matrix $T = [T_+, T_0, T_-]$ such that
\[
Q^{-1}_{33} A_{33} [T_+, T_0, T_-] = [T_+, T_0, T_-] \begin{bmatrix} \Lambda_+ & 0 \\ 0 & \Lambda_- \end{bmatrix}.
\] (2.16)

Here $T_+$, $T_0$ and $T_-$ respectively have $n_+$, $n_0$ and $n_-$ columns. $\Lambda_+ \in \mathbb{R}^{n_+ \times n_+}$ is diagonal with positive diagonal entries and $\Lambda_- \in \mathbb{R}^{n_- \times n_-}$ is diagonal with negative diagonal entries.

Now we have the following well-posed theorem:

**Theorem 2.1** Given $0 < a < 1/\lambda_{\text{max}}$, where $\lambda_{\text{max}}$ is the maximal eigenvalue of $Q^{-1}_{33} A_{33}$. Assume (M1)–(M3) hold and the system (2.11) has the boundary condition
\[
BV^T W(0) = g,
\] (2.17)
where $B \in \mathbb{R}^{n_+ \times (n_+ + n_0 + n_-)}$ and $g \in \mathbb{R}^{n_+}$ are given, with constant coefficients. Then for any $\|h\|_a < +\infty$ and $\|g\| := \sqrt{g^T g} < +\infty$, the system (2.11) has a unique solution $W(y)$, and there exists a positive constant $C_{a,M}$ independent of the non-homogeneous term $h$ such that the following estimate holds:
\[
\|W\|_a \leq C_{a,M} (\|h\|_a + \|g\|),
\] (2.18)
if and only if the boundary condition satisfies the following conditions

1. $\text{rank}(BT_+) = n_+$.
2. $BT_0 = 0$.

Here $T_+$ and $T_0$ are arbitrary matrices satisfying (2.16). The analytical expressions for the solution are given by (4.2), (4.1) and (4.4).

**Proof** See Sect. 4. \qed

According to the proof in Sect. 4, the first condition in Theorem 2.1 makes sure the unique solvability of the solution. A similar condition has been proposed for the BVPs arising from discrete velocity methods (DVMs); see e.g., [4]. The second condition in Theorem 2.1 ensures the stability of the solution. Precisely speaking, this condition guarantees the estimate (2.18). In the homogeneous case, i.e., $h \equiv 0$, there is no need to consider this condition; see [34]. In the case where $n_0 = 0$, the second condition in Theorem 2.1 always holds since $T_0 = 0$, and therefore can be ignored. For the $M$-th order Grad moment system, $n_0$ often depends on the parity of $M$. For instance, in the example of Sect. 3.1 related to Kramers’ problem, $n_0$ equals zero when $M$ is an even number but possesses a non-zero value otherwise. However, for the DVMs, choosing non-zero discrete velocity points guarantees that $n_0 = 0$.

**Remark 2.1** For ease of exposition, we restrict the shape of the coefficient matrix $B$ to be $n_+ \times (n_+ + n_0 + n_-)$ in Theorem 2.1. The well-posed conditions would be more complicated if we impose more than $n_+$ boundary conditions. For example, the Grad boundary condition (2.10) does not have the same shape as $B$. The general boundary condition may be
\[
B_3 V_3^T W(0) = \tilde{g},
\]
where $B_3 \in \mathbb{R}^{\tilde{n} \times (n_+ + n_- + n_0)}$ and $\tilde{n} > n_+$. Now we may have restrictions on $\tilde{g}$ to ensure the well-posedness. We will discuss this case in Sect. 3, where we aim to find a matrix $C \in \mathbb{R}^{\tilde{n} \times n_+}$ such that $C^T B_3 T_+$ is invertible and $C^T B_3 T_0 = 0$. Then Theorem 2.1 helps to give the estimate.
It is also valuable to compare Theorem 2.1 with the results for initial-boundary value problems of the linear Grad moment equations presented in [43]. In our opinion, Condition 1 and Condition 3 in [43] are similar to the first condition in Theorem 2.1. Condition 2 in [43] corresponds to the second condition in Theorem 2.1. Condition 4 in [43] is similar to a restriction on $\tilde{g}$, which is omitted here due to the assumption regarding the shape of $B$. Although the forms of the well-posed conditions are analogous, their precise interpretations differ between the half-space problem in the present work and the initial-boundary value problem studied in [43]. This will be shown clearly in Sect. 3.

3 Modified Boundary Conditions

3.1 Instability of the Grad Boundary Condition

In this subsection, we first discuss the relationship between the Grad boundary condition (2.10) and the proposed boundary condition (2.17) in Theorem 2.1. Then, we use simple examples to demonstrate the instability of the Grad boundary condition.

For the $M$-th order moment equations, we assume

$$I_e = \{ \alpha \in \mathbb{N}^3 : \alpha_2 \text{ even}, |\alpha| \leq M \}, \quad I_o = \{ \alpha \in \mathbb{N}^3 : \alpha_2 \text{ odd}, |\alpha| \leq M \}.$$  

Suppose $I_e$ has $m$ elements and $I_o$ has $n$ elements. Therefore, we have $N = m + n$ and $m \geq n$. Suppose the multi-indices with even second components are always ordered before those with odd second components, e.g., $(a_1, 0, a_3)$ is ordered before $(b_1, 1, b_3)$ for any $a_1, a_3, b_1, b_3$. Then, we can write the Grad boundary condition (2.10) as

$$EM(W_o + \bar{W}_o) + \hat{\chi} ES(W_e + \bar{W}_e - b_e) = 0, \quad y = 0,$$

where $\hat{\chi} = \frac{2\chi}{2 - \chi \sqrt{2 \pi}}$. The matrix $M \in \mathbb{R}^{m \times n}$ has entries $\langle M | \xi_2 | \phi_{\alpha} \phi_{\beta} \rangle$ for $\alpha \in I_e$ and $\beta \in I_o$. The matrix $S \in \mathbb{R}^{m \times m}$ has entries $\langle M | \eta_2 | \phi_{\alpha} \phi_{\beta} \rangle$ for $\alpha, \beta \in I_e$. Every row of $E \in \mathbb{R}^{n \times m}$ is a unit vector with only one component being one, such that the entries of $EM$ are $\langle M | \xi_2 | \phi_{\alpha} \phi_{\beta} \rangle$ for $\alpha \in I_e, |\alpha| \leq M - 1$, and $\beta \in I_o$. According to the aforementioned ordering, we have divided the variables as

$$W = \begin{bmatrix} W_e & W_o \end{bmatrix}, \quad W_e \in \mathbb{R}^m, \quad W_o \in \mathbb{R}^n,$$

where the elements of $W_e$ are $w_{\alpha}, \alpha \in I_e$, and the elements of $W_o$ are $w_{\alpha}, \alpha \in I_o$. The vectors $\bar{W}_e, \bar{W}_o$ and $b_e$ carry analogous meanings. In a word, the boundary condition (3.1) is equivalent to the Grad boundary condition (2.10), expressed in matrix form.

Remark 3.1 Due to the recursion relation and orthogonality of Hermite polynomials [10], we can structure the coefficient matrices as

$$A = \begin{bmatrix} 0 & M \\ M^T & 0 \end{bmatrix}, \quad Q = \begin{bmatrix} Q_e & 0 \\ 0 & Q_o \end{bmatrix},$$

where $Q_e \in \mathbb{R}^{m \times m}$ and $Q_o \in \mathbb{R}^{n \times n}$. By definition, we also know that $M$ is of full column rank and $S$ is symmetric positive definite [34]. A matrix with the same structure as $A^T$ is referred to as Onsager compatible in [43]. More structured discussions regarding the derivation of $A$ can be found in [8, 9].
We can see that the boundary condition (3.1) provides \( n \) boundary conditions but, as shown in Theorem 2.1, the moment system in half-space requires \( n_+ \) boundary conditions. Note that for initial-boundary value problems of the linear Grad moment system, the number \( n \) corresponds precisely to the number of negative eigenvalues (counting the multiplicity) of the boundary matrix [20, 21], which is the requisite number [26]. It was only recently that [43] highlighted that the linear Grad boundary condition is unstable for initial-boundary value problems. The reason lies in the existence of some vector in the null space of the boundary matrix that does not satisfy the homogeneous boundary conditions [38]. The situation differs in the half-space case. In general, the boundary condition (3.1) can be divided into \( n + n_+ \) boundary conditions in the form of (2.17) with a specific coefficient matrix \( B \) and \( n - n_+ \) conditions on \( \bar{W}_e, \bar{W}_o \) and \( b_e \). Thus, we consider the moment boundary conditions (3.1) to be stable if both the solution \( W(y) \) and \( n - n_+ \) additional conditions depend continuously on the input data, as strictly stated in Theorem 3.1.

As the first example, we consider Kramers’ problem with the BGK collision term [16] for the case where \( M = 3 \). Now the moment system is

\[
\begin{align*}
\frac{d\sigma_{12}}{dy} &= 0, \\
\frac{du_1}{dy} + \sqrt{2} \frac{df_3}{dy} &= -v\sigma_{12}, \\
\sqrt{2} \frac{d\sigma_{12}}{dy} &= -vf_3 + h_3, \\
\end{align*}
\]

(3.3)

where \( v > 0 \) is a constant and \( h_3 = h_3(y) \) is the given non-homogeneous term. The Grad boundary condition is

\[
\bar{\sigma} + \sigma_{12}(0) + \hat{\chi} \left( u_1(0) + \bar{u} + \frac{\sqrt{2}}{2} f_3(0) \right) = 0.
\]

(3.4)

Since the moment variables vanish when \( y = +\infty \), we can write the analytical solution to the system (3.3) as

\[
W = \begin{bmatrix} u_1 \\ f_3 \\ \sigma_{12} \end{bmatrix} = \begin{bmatrix} \frac{-\sqrt{2}h_3/v}{2} \\ h_3/v \\ 0 \end{bmatrix},
\]

(3.5)

with the additional condition

\[
\tilde{u} = -\frac{1}{c\hat{\chi}} \bar{\sigma} + \frac{\sqrt{2}}{v} h_3(0).
\]

(3.6)

Only when \( \tilde{u} \) and \( \bar{\sigma} \) satisfy the relation (3.6) can the half-space problem have a unique solution. However, \( \|\tilde{u}\| \) cannot be controlled by the weighted \( L^2 \) norm \( \|h_3\|_a \) since \( h_3(0) \) cannot be controlled by \( \|h_3\|_a \). This exhibits the instability of the Grad boundary condition in this example.

To overcome this drawback, one may modify (3.4) as

\[
c(\bar{\sigma} + \sigma_{12}(0)) + \hat{\chi} \left( u_1(0) + \bar{u} + \frac{\sqrt{2}}{2} f_3(0) \right) = 0
\]

to obtain the relation

\[
\tilde{u} = -\frac{1}{c\hat{\chi}} \bar{\sigma},
\]
where \( c > 0 \) is an arbitrary positive constant. Hence, the modified boundary condition is stable in this example. However, it remains unclear which value of \( c \) would be optimal. The authors of [43] suggest choosing \( c = 1 \), such that the modified boundary condition only differs from the Grad boundary condition with respect to the coefficients in front of the highest-order moment variables, i.e., \( f_3 \) in this example.

**Remark 3.2** This concrete example can also help illustrate the notations used in Theorem 2.1. Here we have \( m = 2 \), \( n = 1 \), and

\[
A = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & \sqrt{2} \\ 1 & \sqrt{2} & 0 \end{bmatrix}, \quad Q = \begin{bmatrix} 0 \\ v \\ h_3 \end{bmatrix}, \quad h = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix}, \quad W = \begin{bmatrix} u_1 \\ f_3 \\ \sigma_{12} \end{bmatrix}.
\]

According to Lemma 2.1, we can construct

\[
V_1 = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}, \quad V_2 = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}, \quad V_3 = \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} \Rightarrow U = V = \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \\ 1 \end{bmatrix}.
\]

We have \( p = 1 \) and \( r = 1 \),

\[
U^T A V = \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & \sqrt{2} \\ 0 & \sqrt{2} & 0 \end{bmatrix}, \quad U^T Q V = \begin{bmatrix} 0 & 0 & 0 \\ 0 & v & 0 \\ 0 & 0 & v \end{bmatrix}, \quad U^T h = \begin{bmatrix} 0 \\ 0 \\ h_3 \end{bmatrix}.
\]

Therefore, we have \( A_{33} = 0 \in \mathbb{R}^{1 \times 1} \), \( n_+ = n_- = 0 \) and \( n_0 = 1 \), which means that \( A_{33} \) only has one zero eigenvalue.

In the second example, we verify that the Grad boundary condition does not satisfy \( B T_0 = 0 \) for the case where \( M = 5 \). Hence, according to Theorem 2.1, the solution vector \( W(y) \) can not be controlled by \( \|h\|_a \), demonstrating the instability of the Grad boundary condition in this example.

**Remark 3.3** The detailed calculation proceeds as follows. When \( M = 5 \), the moment system for Kramers’ problem with the BGK collision term gives

\[
A = \begin{bmatrix} 0 & M^T \\ M & 0 \end{bmatrix}, \quad M = \begin{bmatrix} 1 \\ \sqrt{2} \\ \sqrt{3} \\ 2 \end{bmatrix}, \quad Q = \begin{bmatrix} 0 \\ vI_4 \end{bmatrix}.
\]

Here \( I_4 \) is the 4 \( \times \) 4 identity matrix and we may assume without loss of generality that \( v = 1 \). We have \( p = 1 \) and \( r = 1 \). We can construct

\[
V_3 = \begin{bmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} \Rightarrow A_{33} = \begin{bmatrix} 0 & 0 & \sqrt{3} \\ 0 & 0 & 2 \\ \sqrt{3} & 2 & 0 \end{bmatrix}, \quad Q_{33} = \begin{bmatrix} 1 \\ 1 \end{bmatrix} \Rightarrow T_0 = \begin{bmatrix} 2 \\ -\sqrt{3} \\ 0 \end{bmatrix}.
\]

Here \( n_+ = n_- = n_0 = 1 \). The Grad boundary condition (3.1) is transformed to get

\[
[\tilde{\chi} E S, \quad E M] V (V^T (W + \tilde{W} - b)) = 0, \quad y = 0, \quad \tilde{W} = \begin{bmatrix} \tilde{W}_e \\ \tilde{W}_o \end{bmatrix}, \quad b = \begin{bmatrix} b_e \\ 0 \end{bmatrix}.
\]
Thus, we have
\[
[\hat{\chi} E_S, EM]V_3 = \begin{bmatrix}
\sqrt{3} \hat{\chi} & -1 & -2 \sqrt{6} \hat{\chi} & 0 \\
-2 & \frac{5}{2} \hat{\chi} & \frac{7}{4} & \frac{5}{2} \hat{\chi} \\
\frac{7}{4} & \frac{5}{2} \hat{\chi} & \frac{7}{4} & \sqrt{3} \\
\end{bmatrix}.
\]

As will be demonstrated in the proof of Theorem 3.1, to separate \( V_1^T W \) from the coupled conditions containing \( V_1^T W \), one must multiply the above matrix left by \( Z_3^T \in \mathbb{R}^{n_+ \times n} \) to get \( B \). Here \( Z_3^T = [0, 1] \) and \( B = \begin{bmatrix} \frac{5}{2} \hat{\chi}, \frac{7}{4} \hat{\chi}, \sqrt{3} \end{bmatrix} \). Hence, we have \( BT_0 \neq 0 \).

### 3.2 Modified Boundary Conditions

This subsection systematically introduces a class of modified boundary conditions and proves their well-posedness. For half-space problems, the modified boundary condition [43] can write as
\[
H(W_o + \hat{W}_o) + \hat{\chi} M^T (W_e + \hat{W}_e - b_e) = 0,
\]
where \( H \in \mathbb{R}^{n \times n} \) is an arbitrary symmetric positive definite matrix. The outline of the proof is as follows. We can first find a matrix \( C \in \mathbb{R}^{n \times n_+} \) and multiply (3.7) left by \( C^T \) to utilize Theorem 2.1. Then, we solve the remaining part of (3.7) to obtain relationships between the vectors \( \hat{W}_o, b_e \) and \( \hat{W}_e \). Following this way, we first derive an expression for \( n_+ \) under the assumption that \( A \) and \( Q \) satisfy conditions (M1)–(M3) and have the same structure as in (3.2).

**Lemma 3.1** Suppose \( p_1 = \dim \text{Null}(Q_e) \) and \( G_e \in \mathbb{R}^{m \times p_1} \) is column orthogonal with \( \text{Range}(G_e) = \text{Null}(Q_e) \). Suppose \( p_2 = \dim \text{Null}(Q_o) \) and \( G_o \in \mathbb{R}^{n \times p_2} \) is column orthogonal with \( \text{Range}(G_o) = \text{Null}(G_o) \). Suppose \( r_1 = \dim \text{Null}(G_o^T M^T G_e) \) and \( X_e \in \mathbb{R}^{p_1 \times r_1} \) is column orthogonal with \( \text{Range}(X_e) = \text{Null}(G_o^T M^T G_e) \). Suppose \( r_2 = \dim \text{Null}(G_e^T M G_o) \) and \( X_o \in \mathbb{R}^{p_2 \times r_2} \) is column orthogonal with \( \text{Range}(X_o) = \text{Null}(G_e^T M G_o) \). Then we have
\[
n_+ = n - r_2 - p_1.
\]

**Proof** Due to the block structure in (3.2), without loss of generality we can write
\[
G = \begin{bmatrix}
G_e & G_o
\end{bmatrix}, \quad X = \begin{bmatrix}
X_e \\
X_o
\end{bmatrix}.
\]

Accordingly, we can construct \( V = [V_1, V_2, V_3] \) with the following block structures:
\[
V_1 = \begin{bmatrix} Y_1 \\ Z_1 \end{bmatrix}, \quad V_2 = \begin{bmatrix} Y_2 \\ Z_2 \end{bmatrix}, \quad V_3 = \begin{bmatrix} Y_3 \\ Z_3 \end{bmatrix},
\]

where \( Y_1 = G_e X_e, Z_1 = G_o X_o, \)

\[
\text{Range}(Y_2) = \text{Range}(M G_o), \quad \text{Range}(Z_2) = \text{Range}(M^T G_e), \quad Y_3 \in \mathbb{R}^{m \times (m - r_1 - p_2)} \text{ and } Z_3 \in \mathbb{R}^{n \times (n - r_2 - p_1)}.
\]

Note that \( n_+ \) is the number of positive eigenvalues of \( A_{33} = V_3^T A V_3 \), i.e.,
\[
A_{33} = \begin{bmatrix}
0 & Y_3^T M Z_3 \\
Z_3^T M^T Y_3 & 0
\end{bmatrix}.
\]
We will show that $Y_3^TMZ_3$ is of full column rank, and the eigenvalues of $A_{33}$ occur in pairs of opposites, with a positive eigenvalue accompanied by a negative eigenvalue of the same magnitude. These facts will lead to $n_+ = n - r_2 - p_1$.

Suppose $Y_3^TMZ_3x = 0$ for some $x \in \mathbb{R}^{n - r_2 - p_1}$. Since $\{Y_1, Y_2, Y_3\}$ is orthogonal, there exists $x_1 \in \mathbb{R}^n$ and $x_2 \in \mathbb{R}^{p_2}$ such that

$$MZ_3x = Y_1x_1 + Y_2x_2. \quad (3.8)$$

Since $Z_3^TM^TY_1 = 0$ and $Y_2^TY_1 = 0$, we have $x_1 = 0$. The relation (2.15) implies that

$$\text{Range}(Z_3) \cap \text{Range}(G_o) = \{0\}.$$

Since both matrices $M$ and $Z_3$ have full column rank, there must be $x = 0$. This shows that $Y_3^TMZ_3$ is of full column rank.

We present a general conclusion regarding the eigenvalues and eigenvectors of symmetric matrices. Let $D \in \mathbb{R}^{\alpha \times \beta}$ and rank($D$) = $\gamma$. Then

$$\tilde{D} := \begin{bmatrix} 0 & D \\ D^T & 0 \end{bmatrix}$$

has $\alpha + \beta - 2\gamma$ zero eigenvalues, $\gamma$ positive eigenvalues and $\gamma$ negative eigenvalues. In fact, the symmetric matrix $\tilde{D}$ must have $\alpha + \beta$ real eigenvalues. Assume $\lambda \in \mathbb{R}$ is an eigenvalue, then there exist $x \in \mathbb{R}^\alpha$ and $y \in \mathbb{R}^\beta$ such that

$$\begin{bmatrix} 0 & D \\ D^T & 0 \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = \lambda \begin{bmatrix} x \\ y \end{bmatrix} \Rightarrow \begin{bmatrix} 0 & D \\ D^T & 0 \end{bmatrix} \begin{bmatrix} x \\ -y \end{bmatrix} = -\lambda \begin{bmatrix} x \\ -y \end{bmatrix}.$$

So $-\lambda$ is also an eigenvalue, which implies that $\tilde{D}$ has the same number of positive and negative eigenvalues. Since rank($D$) = rank($D^T$) = $\gamma$, there must be $\alpha + \beta - 2\gamma$ zero eigenvalues.

As an application of the above result, we have $r_1 + p_2 = r_2 + p_1$ considering the structure of $G^TAG$. For the matrix $A_{33}$, we then have $n_+ = n - r_2 - p_1$. \hfill $\Box$

The following lemma illustrates an attribute of the modified boundary condition (3.7).

**Lemma 3.2.** Under the assumptions of Lemma 3.1, let $B_3 = [\hat{\chi}^T, H]V_3 \in \mathbb{R}^{n \times (n_+ + n - n_0)}$ and $C = Z_3 \in \mathbb{R}^{n \times n_+}$. Then, when $\chi \in [0, 1]$,

i. $CT_3T_+^2$ is invertible.

ii. $CT_3T_0 = 0$.

**Proof**  It is readily apparent that we need only prove the properties in the lemma for particular matrices $T_+$ and $T_0$ satisfying (2.16). Assume the Cholesky decomposition $Q_{33} = LL^T$ where $L$ is lower triangular and has the block structure

$$L = \begin{bmatrix} L_e \\ L_o \end{bmatrix}, \quad L_e \in \mathbb{R}^{(m - r_1 - p_2) \times (m - r_1 - p_2)}, \quad L_o \in \mathbb{R}^{n_+ \times n_+}.$$

Then, the matrix $L^{-1}A_{33}L^{-T}$ is symmetric. There must exists an orthogonal eigenvalue decomposition

$$L^{-1}A_{33}L^{-T}R = RA,$$
where $\mathbf{R} = [\mathbf{R}_+, \mathbf{R}_0, \mathbf{R}_-]$ is assumed orthogonal. The column counts of $\mathbf{R}_+$, $\mathbf{R}_0$ and $\mathbf{R}_-$ are $n_+, n_0$ and $n_-$, respectively. The matrix $\mathbf{A}$ is diagonal with the same structure in (2.16), i.e.,

$$
\mathbf{A} = \begin{bmatrix}
\Lambda_+ & 0 \\
0 & \Lambda_-
\end{bmatrix}.
$$

According to the proof of Lemma 3.1, we have $n_+ = n_-$ and can assume

$$
\mathbf{R}_+ = \begin{bmatrix} \mathbf{R}_e \\ \mathbf{R}_o \end{bmatrix}, \quad \mathbf{R}_- = \begin{bmatrix} \mathbf{R}_e \\ -\mathbf{R}_o \end{bmatrix}, \quad \mathbf{R}_e \in \mathbb{R}^{(m-r_1-p_2) \times n_+}, \quad \mathbf{R}_o \in \mathbb{R}^{n_+ \times n_+},
$$

where $\mathbf{R}_e^T \mathbf{R}_e = \mathbf{R}_o^T \mathbf{R}_o = \frac{1}{2} \mathbf{I}_{n_+}$ with $\mathbf{I}_{n_+}$ the $n_+ \times n_+$ identity matrix. Now $\mathbf{T} = \mathbf{L}^{-T} \mathbf{R}$ satisfies the condition (2.16), where

$$
\mathbf{T}_+ = \mathbf{L}^{-T} \mathbf{R}_+, \quad \mathbf{T}_0 = \mathbf{L}^{-T} \mathbf{R}_0.
$$

Using the condition (2.16), we have

$$
\mathbf{Z}_3^T \mathbf{B}_3 \mathbf{T}_+ = \hat{\chi} \mathbf{Z}_3^T \hat{\mathbf{M}}^T \mathbf{Y}_3 \mathbf{L}_o^{-T} \mathbf{R}_e + \mathbf{Z}_3^T \mathbf{H} \mathbf{Z}_3 \mathbf{L}_o^{-T} \mathbf{R}_o = \hat{\chi} \mathbf{L}_o \mathbf{R}_o \mathbf{A}_+ + \mathbf{Z}_3^T \mathbf{H} \mathbf{Z}_3 \mathbf{L}_o^{-T} \mathbf{R}_o.
$$

Since $\hat{\chi} \geq 0$ when $\chi \in [0, 1]$, for any $x \in \mathbb{R}^{n_+}$, we have

$$
x^T \mathbf{R}_o^T \mathbf{L}_o^{-1} \mathbf{Z}_3^T \mathbf{B}_3 \mathbf{T}_+ x = \frac{1}{2} \hat{\chi} x^T \mathbf{A}_+ x + x^T \mathbf{R}_o^T \mathbf{L}_o^{-1} \mathbf{Z}_3^T \mathbf{H} \mathbf{Z}_3 \mathbf{L}_o^{-T} \mathbf{R}_o x \\
\geq x^T \mathbf{R}_o^T \mathbf{L}_o^{-1} \mathbf{Z}_3^T \mathbf{H} \mathbf{Z}_3 \mathbf{L}_o^{-T} \mathbf{R}_o x \geq 0. \quad (3.9)
$$

The equality holds if and only if $x = 0$. This shows that $\mathbf{R}_o^T \mathbf{L}_o^{-1} \mathbf{Z}_3^T \mathbf{B}_3 \mathbf{T}_+$ is symmetric positive definite. Therefore, the matrix $\mathbf{Z}_3^T \mathbf{B}_3 \mathbf{T}_+$ is invertible.

On the other hand, the condition $\mathbf{Q}_{33}^{-1} \mathbf{A}_{33} \mathbf{T}_0 = \mathbf{0}$ shows that $\mathbf{A}_{33} \mathbf{T}_0 = \mathbf{0}$. Since $\mathbf{Y}_3^T \mathbf{M} \mathbf{Z}_3$ is of full column rank, we can express the matrix $\mathbf{T}_0$ as

$$
\mathbf{T}_0 = \begin{bmatrix} \mathbf{T}_0^* \\ \mathbf{0} \end{bmatrix}, \quad \mathbf{T}_0^* \in \mathbb{R}^{(m-r_1-p_2) \times n_0},
$$

where $\mathbf{Z}_3^T \mathbf{M}^T \mathbf{Y}_3 \mathbf{T}_0^* = \mathbf{0}$. Hence,

$$
\mathbf{Z}_3^T \mathbf{B}_3 \mathbf{T}_0 = \hat{\chi} \mathbf{Z}_3^T \mathbf{M}^T \mathbf{Y}_3 \mathbf{T}_0^* = \mathbf{0},
$$

which completes the proof. \hfill \square

With the aid of the aforementioned lemmas, we present the ensuing well-posedness theorem:

**Theorem 3.1** Assume $\mathbf{A}$ and $\mathbf{Q}$ satisfy conditions (M1)–(M3) and have the same structure as in (3.2). Suppose $\hat{\chi} > 0$ and $r_2 = 0$. Let $\mathbf{g}_1 = \hat{\mathbf{W}}_o$ and $\mathbf{g}_2 = (\mathbf{I}_m - \mathbf{G}_e \mathbf{T}_e) (\hat{\mathbf{W}}_e - b_e)$. Then, for any $\|h\|_a < +\infty$, $\|\mathbf{g}_1\| < +\infty$ and $\|\mathbf{g}_2\| < +\infty$, the moment system (2.11) with the boundary condition (3.7) has a unique solution of $W$ and $\mathbf{G}_e^T (\hat{\mathbf{W}}_e - b_e)$, satisfying the estimates

$$
\|\mathbf{W}\|_a \lesssim \|h\|_a + \|\mathbf{g}_1\| + \|\mathbf{g}_2\|,
\|\mathbf{G}_e^T (\hat{\mathbf{W}}_e - b_e)\| \lesssim \|h\|_a + \|\mathbf{g}_1\| + \|\mathbf{g}_2\|,
$$

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where $a \lesssim b$ represents that there exists a constant $c > 0$ such that $a \leq cb$.

**Proof** The matrices $X_o$ and $Z_1$ vanish when $r_2 = 0$, thereby simplifying the proof. Plugging $VV^T$ before the variables $W_e$ and $W_o$ in (3.7), and decomposing $\tilde{W}_e - b_e$ as

$$\tilde{W}_e - b_e = G_eG_e^T(\tilde{W}_e - b_e) + (I_m - G_eG_e^T)(\tilde{W}_e - b_e),$$

the boundary condition can be expressed as

$$\hat{\chi}M^T \left( Y_1Y_1^TW_e(0) + G_eG_e^T(\tilde{W}_e - b_e) \right) + B_3V_3^TW(0)$$

$$= -H\tilde{W}_o - \hat{\chi}M^T(I_m - G_eG_e^T)(\tilde{W}_e - b_e) - [\hat{\chi}M^T, H]V_2V_2^TW(0), \quad (3.10)$$

where $B_3 = [\hat{\chi}M^T, H]V_3$.

Let $\tilde{U} = [G_o, M^TG_eX_e, Z_3] \in \mathbb{R}^{n \times n}$. Then $\tilde{U}$ is invertible since it is the lower block of $U$ and $U$ is invertible. Multiplying (3.10) left by $\tilde{U}^T$ divides the boundary condition into three parts. The first part corresponds to multiply (3.10) left by $Z_3^T$. Since Range($M^TG_e$) = Range($Z_2$), $Y_1 = G_eX_e$, and $Z_3^TZ_2 = 0$, we have

$$Z_3^TM^TY_1 = Z_3^TM^TG_e = 0.$$ 

Now the boundary condition gives

$$Z_3^TB_3V_3^TW(0) = -Z_3^HHg_1 - \hat{\chi}Z_3^TM^Tg_2 - Z_3^T[\hat{\chi}M^T, H]V_2V_2^TW(0), \quad (3.11)$$

which satisfies the well-posedness conditions in Theorem 2.1 due to Lemma 3.2. From the proof of Theorem 2.1, we know

$$\|V_2^TW(0)\| \lesssim \|h\|_a.$$ 

So from Theorem 2.1, the half-space system (2.11) with the boundary condition (3.11) has a unique solution of $W$ and

$$\|W\|_a \lesssim \|h\|_a + \|g_1\| + \|g_2\|.$$ 

Let $U_0 = [G_o, M^TG_eX_e] \in \mathbb{R}^{n \times p_1}$. Then the remaining part of the boundary condition (3.7) corresponds to multiply (3.10) left by $U_0^T$. We claim that

$$\text{rank}(U_0^TM^TG_e) = p_1.$$ 

Otherwise, there exists $x \in \mathbb{R}^{p_1}$ such that $x \in \text{Range}(U_0)$ and $x^TM^TG_e = 0$. Since $Z_1$ vanishes and $[Z_2, Z_3]$ is orthogonal, we have $x \in \text{Range}(Z_3)$. But $[U_0, Z_3]$ is invertible. So $x = 0$ and $\text{rank}(U_0^TM^TG_e) = p_1$. Thus, when $W$ is known, we can solve for a unique $G_e^T(\tilde{W}_e - b_e)$ from the boundary condition. From (4.2), the term $A_{21}V_1^TW(0) + A_{23}V_3^TW(0)$ does not contain $z_0(0)$ and can be controlled by $\|h\|_a$. Therefore, we have the estimate

$$\|G_e^T(\tilde{W}_e - b_e)\| \lesssim \|g_1\| + \|g_2\| + \|h\|_a.$$ 

This completes the proof. \hfill $\Box$

In summary, we have proven the well-posedness of the modified boundary condition for the non-homogeneous linear Grad moment equations in half-space. The modified boundary condition has a similar form to that in the initial-boundary value problem [8, 9, 43]. However, only when the variables given by the external flow, e.g., $\tilde{W}_e$, $b_e$ and $\tilde{W}_o$, satisfy certain relations can the half-space problem have a unique solution.
To modify the Grad moment boundary, a convenient choice of $H$ is $H = M^T S^{-1} M$. The construction means imposing alternative continuity of fluxes at the boundary within Grad’s framework. To see this, we first test the Maxwell boundary condition with $\xi_2 \phi_\alpha, \alpha \in \mathbb{I}_{e}$ to get

$$M(W_\alpha + \bar{W}_\alpha) + \hat{\chi} S(W_e + \bar{W}_e - b_e) = 0.$$  

(3.12)

Note that the test functions of the Grad boundary condition are $\xi_2 \phi_\alpha, \alpha \in \mathbb{I}_{e}, |\alpha| \leq M - 1$. Combining the test functions of (3.12) linearly, or more precisely, multiplying on the left by $M^T S^{-1}$, yields

$$M^T S^{-1} M(W_\alpha + \bar{W}_\alpha - b_\alpha) + \hat{\chi} M^T (W_e + \bar{W}_e - b_e) = 0.$$  

Therefore, the modified boundary condition with $H = M^T S^{-1} M$ can be regarded as a modification of the Grad boundary condition.

Incidentally, the specific modified boundary condition appearing in [8, 43] corresponds to $H = (E M)^T (E S E^T)^{-1} (E M)$. This modified boundary condition only differs from the Grad boundary condition with respect to the coefficients in front of the highest-order moment variables. Therefore, it is expected to provide a good approximation to the Grad boundary condition. Nevertheless, to the best of our knowledge, this modification can not be justified within Grad’s framework, i.e., derived by testing the Maxwell boundary condition with some odd polynomials.

4 Proof of Theorem 2.1

This section aims to provide the missing details in the proof of Theorem 2.1. The proof primarily involves two steps: first explicitly writing the analytical solution of (2.11), then estimating it.

Lemma 4.1 Under the assumptions of Theorem 2.1, the system (2.11) has a unique solution $W(y)$ given by (4.2), (4.1) and (4.4) if and only if

$$\text{rank}(B T_+) = n_+.$$  

Proof According to Lemma 2.1, we can find orthogonal matrix $V = [V_1, V_2, V_3]$ and invertible matrix $U = [U_1, U_2, U_3]$ such that $U_i$, $V_j$ and $A_{ij} := U_i^T A V_j$, $Q_{ij} := U_i^T Q V_j$ satisfy the properties in Lemma 2.1. The system (2.11) is equivalent to

$$U^T A V \frac{d(V^T W)}{dy} = -U^T Q V (V^T W) + U^T h, \quad V^T W(+\infty) = 0.$$  

Since $Q_{1j} = 0$, the first $p$ lines of the above system would give

$$G^T A W(y) = -\int_y^{+\infty} G^T h(s) ds.$$  

(4.1)

Since Range($V_2$) = Range($AG$), the formula (4.1) can uniquely determine the value of $V_2^T W$. 

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Since \( \text{rank}(A_{21}) = \text{rank}(U_2) = r \), the matrix \( A_{21} \) is invertible and the next \( r \) lines of the system give
\[
V_1^TW(y) = -A_{21}^{-1} \left( A_{22}(V_2^TW(y)) + A_{23}(V_3^TW(y)) \right) + \int_y^{+\infty} A_{21}^{-1} \left( Q_{22}(V_2^TW(s)) + Q_{23}(V_3^TW(s)) - U_2^T h(s) \right) ds.
\]
(4.2)
The formula (4.2) uniquely determines \( V_1^TW \) if \( V_2^TW \) and \( V_3^TW \) are known.

The last \( N - p - r \) equations are separated as
\[
A_{33} \frac{d}{dy}(V_3^TW) = -Q_{33}(V_3^TW) + V_3^TH - Q_{32}V_2^TW - A_{32} \frac{dV_2^TW}{dy},
\]
where \( V_2^TW \) is given by (4.1) and \( Q_{33} > 0 \). Multiplying the above equations left by \( Q_{33}^{-1} \) gives
\[
Q_{33}^{-1} A_{33} \frac{dV_3^TW}{dy} = -V_3^TW + h_3,
\]
(4.3)
where \( h_3 \) is a given vector relying on \( h \):
\[
h_3 = Q_{33}^{-1} \left( V_3^TH - Q_{32}V_2^TW - A_{32} \frac{dV_2^TW}{dy} \right).
\]

From the eigenvalue decomposition (2.16) of \( Q_{33}^{-1} A_{33} \), we can solve the equations (4.3).

Since \( T \) is invertible, we can find the unique \( z_+ = z_+(y) \in \mathbb{R}^{n_+} \), \( z_0 = z_0(y) \in \mathbb{R}^{n_0} \) and \( z_- = z_-(y) \in \mathbb{R}^{n_-} \) such that
\[
V_3^TW = T_+ z_+ + T_0 z_0 + T_- z_-.
\]
(4.4)
Assume \( T^{-1} h_3 = [h_+^T, h_0^T, h_-^T]^T \), where \( h_+ = h_+(y) \in \mathbb{R}^{n_+} \), \( h_0 = h_0(y) \in \mathbb{R}^{n_0} \) and \( h_- = h_- (y) \in \mathbb{R}^{n_-} \). Then the characteristic equations of (4.3) give the solution
\[
z_0 = h_0(y),
\]
(4.5)
\[
z_- = -A_-^{-1} \int_y^{+\infty} \exp(A_-^{-1}(s - y)) h_-(s) ds,
\]
(4.6)
and
\[
z_+ = \exp(-A_+^{-1}y) z_+(0) + A_+^{-1} \int_0^y \exp(A_+^{-1}(s - y)) h_+(s) ds,
\]
(4.7)
where only \( z_+(0) \in \mathbb{R}^{n_+} \) should be determined by additional boundary conditions.

The boundary condition (2.17) leads to
\[
BT_+ z_+(0) = g - B(T_0 z_0(0) + T_- z_-(0)).
\]
(4.8)
According to unique solvability of the linear algebraic system, we can solve a unique \( z_+(0) \) from (4.8) if and only if the first condition in Theorem 2.1 holds, i.e., \( \text{rank}(BT_+) = n_+ \).

In a word, when the system is given, \( V_1^TW \) is determined. Then \( V_3^TW \) is uniquely solvable if and only if \( \text{rank}(BT_+) = n_+ \). Finally, \( V_2^TW \) can be determined. \( \Box \)
To estimate the formal solutions in (4.2), (4.1) and (4.4), we introduce some Poincare-type inequalities. For any \( h \) with \( \|h\|_a < +\infty \), we define
\[
    r(y) = -\int_y^{+\infty} h(s) \, ds. \tag{4.9}
\]
Then we have \( r'(y) = h(y) \) and for any component \( r_i \) of \( r \),
\[
    |r_i(y)|^2 \leq \int_y^{+\infty} e^{-2as} \, ds \int_y^{+\infty} e^{2as} h^T h \, ds < +\infty.
\]

**Lemma 4.2** There exists a constant \( c_0 > 0 \) such that the Poincare inequality holds
\[
    \|r\|_a \leq c_0 \|r'\|_a = c_0 \|h\|_a, \tag{4.10}
\]
and the trace inequality holds
\[
    \|r(0)\| \leq c_0 \|h\|_a. \tag{4.11}
\]

**Proof** By definition, we have
\[
    e^{2ay} r^T(y) r(y) = -\int_y^{+\infty} \partial_s (e^{2as} r^T(r(s)) \, ds
    = -2a \int_y^{+\infty} e^{2as} r^T(r(s)) \, ds - 2 \int_y^{+\infty} e^{2as} (r')^T r(s) \, ds.
\]
Let \( y = 0 \) and use the Cauchy–Schwarz inequality, then we have
\[
    r^T(0) r(0) + 2a \|r\|^2_a \leq 2 \|r\|_a \|h\|_a.
\]
Since \( r^T(0) r(0) \geq 0 \), we have
\[
    \|r\|_a \leq \frac{1}{a} \|h\|_a.
\]
Analogously, we can ignore the term \( \|r\|^2_a \) to get
\[
    \sqrt{r^T(0) r(0)} \leq \sqrt{\frac{2}{a}} \|h\|_a.
\]
This completes the proof. \( \square \)

For convenience, we use \( a \lesssim b \) to mean there exists a constant \( c > 0 \) such that \( a \leq cb \). Since all matrices considered here are finite-dimensional with constant coefficients, they must have a uniform upper bound on some given matrix norm.

**Lemma 4.3** Under the assumptions of Theorem 2.1, we suppose \( \text{rank}(B T_+) = n_+ \). Then the estimate (2.18) holds if and only if \( B T_0 = 0 \).

**Proof** Utilizing the boundedness of the matrices and Poincare inequality, from (4.1), we have
\[
    \|V_2^T W\|_a \lesssim \|G^T A W\|_a \lesssim \|G^T h\|_a \lesssim \|h\|_a.
\]
Analogously, the formula (4.2) gives
\[
    \|V_1^T W\|_a \lesssim \|V_2^T W\|_a + \|V_3^T W\|_a + \|h\|_a \lesssim \|h\|_a + \|V_3^T W\|_a.
\]
The formula (4.4) gives
\[ \| V_T^3 W_a \| \lesssim \| z_0 \|_a + \| z_- \|_a + \| z_+ \|_a. \]

Here \( z_0 \) is given by (4.5),
\[ \| z_0 \|_a \lesssim \| h_3 \|_a \lesssim \| h \|_a. \]

From (4.6), we have
\[ \| z_- \|_a \lesssim \| h_3 \|_a \lesssim \| h \|_a. \]

Due to the condition \( a < 1/\lambda_{\text{max}} \), the term \( \| \exp \left( -\Lambda^+_1 y \right) \|_a \) is bounded and we have
\[ \lim_{y \to +\infty} \Lambda^+_1 \int_0^y \exp(\Lambda^+_1(s - y)) h_+(s) \, ds = 0. \]

So from (4.7), we have
\[ \| z_+ \|_a \lesssim \| z_+(0) \| \| \exp \left( -\Lambda^+_1 y \right) \|_a + \| h \|_a \lesssim \| z_+(0) \| + \| h \|_a. \]

Now the key point lies in estimating \( \| z_+(0) \| \). Since \( \text{rank}(B_T^+) = n_+ \), we can solve for \( z_+(0) \) as
\[ z_+(0) = (B_T^+)^{-1} \left( g - B_T^0 z_0(0) - B_T^- z_-(0) \right). \tag{4.12} \]

If \( B_T^0 = 0 \), then
\[ z_+(0) = (B_T^+)^{-1} \left( g - B_T^- z_-(0) \right). \]

We have
\[ \| z_+(0) \| \lesssim \| g \| + \| z_- \|_a. \]

Due to the trace inequality, we can see from (4.6) that \( \| z_- \|_a \lesssim \| h \|_a. \) Thus, the estimate (2.18) holds.

On the other hand, if \( B_T^0 \neq 0 \), we can always find some \( h \) such that \( \| h \|_a < +\infty \) but the estimate (2.18) does not hold. We assume
\[ h = U^{-T} \begin{bmatrix} 0 \\ Q_{33} T \begin{bmatrix} 0 \\ c_0 \\ 0 \end{bmatrix} \end{bmatrix}, \]
where \( c_0 \in \mathbb{R}^{n_0} \) and the zero vector above \( c_0 \) belongs to \( \mathbb{R}^{n_+} \). Direct calculation gives
\[ V_T^2 W = 0, \quad h_+ = 0, \quad h_- = 0, \quad z_0 = h_0 = c_0. \]

So \( \| z_0(0) \| \) cannot be controlled by \( \| h \|_a \), i.e., for any \( M_0 > 0 \), there exists \( c_0 \) such that \( \| h \|_a = 1 \) but \( \| z_0(0) \| = \| c_0(0) \| > M_0 \). From (4.12), since \( g \) and \( z_-(0) \) are bounded, we can always find \( c_0 \) such that \( \| h \|_a = 1 \) but \( \| z_+(0) \| > M_0 \). So the estimate (2.18) does not hold when \( B_T^0 \neq 0 \). \( \square \)

Theorem 2.1 is a direct combination of Lemma 4.1 and Lemma 4.3.
Remark 4.1 The proof of Lemma 4.3 shows that $\|V_T^3 W(0)\|$ and $\|V_T^1 W(0)\|$ generally can not be controlled by $\|h\|_a$ due to the contribution of $z_0(0)$. But from (4.2), we have
$$\|A_{21} V_T^1 W(0) + A_{23} V_T^3 W(0)\| \lesssim \|h\|_a$$
because of the Poincaré inequality.

5 Conclusions

We focused on the theory of well-posedness for the non-homogeneous linear Grad moment system arising from boundary layer problems. On one front, we proposed criteria ensuring well-posedness for a general class of boundary value problems by deriving their analytical solutions. The deduction reduced the ordinary differential equations to a canonical form via a suitable simultaneous transformation. Due to the system’s inhomogeneity and long-range decay, stability in half-space necessitated additional constraints on the boundary conditions. On the other front, we examined the stability of moment boundary conditions derived from the Maxwell accommodation model. The classical Grad boundary condition was generally shown to be unstable, and a class of modified boundary conditions was proven well-posed. The non-negativity of the boundary conditions guaranteed the well-posedness of the moment system.

Acknowledgements This work is financially supported by the National Key R&D Program of China, Project Number 2020YFA0712000.

Data Availability Statement This theoretical work uses no external dataset.

Appendix A Derivation of Layer Problems

For illustrative reasons, we consider the steady flow confined between two parallel plates, whose governing equations are the linear dimensionless moment equations
$$\sum_{d=1}^3 A_d \frac{\partial W}{\partial x_d} = -\frac{1}{\varepsilon} Q W, \quad W = W(x_1, x_2, x_3) \in \mathbb{R}^N. \quad (A.1)$$
Here $x_2 \in [0, 1]$ and $\varepsilon$ is a small parameter representing the Knudsen number. One may propose boundary conditions at $x_2 = 0$ and $x_2 = 1$ for the system (A.1).

Now we focus on the boundary-layer behavior of the solution around $x_2 = 0$, and introduce the ansatz
$$W(x_1, x_2, x_3) = \bar{W}(x_1, x_2, x_3) + \hat{W} \left( x_1, \frac{x_2}{\varepsilon}, x_3 \right).$$
Here $\bar{W}$ means the bulk flow and $\hat{W}$ is regarded as a boundary-layer correction. We assume the boundary layer around $x_2 = 0$ vanishes far away from $x_2 = 0$. So $\hat{W}(x_1, +\infty, x_3) = 0$. Let $y = x_2/\varepsilon$ and expand these variables in a series with respect to $\varepsilon$, e.g.,
$$\hat{W} = \hat{W}^0 + \varepsilon \hat{W}^1 + \cdots.$$
Substituting the ansatz into (A.1) and matching coefficients in powers of $\varepsilon$, one would get moment equations about $\hat{W}^j$. The moment system about $\hat{W}^j$ is exactly the half-space problem (2.9) considered in this manuscript, where $\hat{W}^j(x_1, +\infty, x_3) = 0$ naturally.
Although (A.1) is homogeneous, the derived half-space problems can exhibit inhomogeneity. For example, it’s not difficult to derive that $\hat{W}^0$ satisfies
\[
A_2 \frac{\partial \hat{W}^0}{\partial y} = -Q \hat{W}^0,
\]
which is a homogeneous system. Then $\hat{W}^1$ satisfies
\[
A_2 \frac{\partial \hat{W}^1}{\partial y} = -Q \hat{W}^1 - \sum_{d \neq 2} A_d \frac{\partial \hat{W}^0}{\partial x_d}, \tag{A.2}
\]
which is generally a non-homogeneous system. Since $\hat{W}^0$ is a boundary-layer correction vanishing when $y \to +\infty$, the non-homogeneous term in (A.2) is also expected to decay for $y \to +\infty$.

The above asymptotic theory was first proposed by Sone in 1960s for the steady Boltzmann equation [44, 45]. We have systematically applied this theory to the Grad moment equations; see [35]. Due to the introduction of the variable $y = x_2/\varepsilon$, the asymptotic analysis above differs slightly from the classical asymptotic analysis of the moment equations, e.g., see [47, 48].

References

1. Aoki, K., Baranger, C., Hattori, M., Kosuge, S., Martalò, G., Julien, M., Mieussens, L.: Slip boundary conditions for the compressible Navier–Stokes equations. J. Stat. Phys. 169, 744–781 (2017)
2. Arnold, A., Giering, U.: An analysis of the Marshak conditions for matching Boltzmann and Euler equations. Math. Models Methods Appl. Sci. 07(04), 557–577 (1997)
3. Bardos, C., Golse, F., Sone, Y.: Half-space problems for the Boltzmann equation: A survey. J. Stat. Phys. 124, 275–300 (2006)
4. Bernhoff, N.: On half-space problems for the linearized discrete Boltzmann equation. Riv. Mat. Univ. Parma 9, 73–124 (2008)
5. Bernhoff, N.: On half-space problems for the discrete Boltzmann equation. Il Nuovo Cimento C 33(1), 47–54 (2010)
6. Bernhoff, N.: On half-space problems for the weakly non-linear discrete Boltzmann equation. Kinet. Relat. Models 3, 195–222 (2010)
7. Bernhoff, N., Golse, F.: On the boundary layer equations with phase transition in the kinetic theory of gases. Arch. Ration. Mech. Anal. 240, 51–98 (2021)
8. Bünger, J., Christhuraj, E., Hanke, A., Torrilhon, M.: Structured derivation of moment equations and stable boundary conditions with an introduction to symmetric, trace-free tensors. Kinet. Relat. Models 16(3), 458–494 (2023)
9. Bünger, J., Sama, N., Torrilhon, M.: Stable boundary conditions and discretization for $p_n$ equations. J. Comput. Math. 40(6), 977–1003 (2022)
10. Cai, Z., Fan, Y., Li, R.: Globally hyperbolic regularization of Grad’s moment system. Commun. Pure Appl. Math. 67(3), 464–518 (2014)
11. Cai, Z., Li, R., Qiao, Z.: NRxx simulation of microflows with Shakhov model. SIAM J. Sci. Comput. 34(1), 339–369 (2011)
12. Cercignani, C.: The Boltzmann Equation and Its Applications. Springer, New York (1988)
13. Chen, H., Li, Q., Lu, J.: A numerical method for coupling the BGK model and Euler equations through the linearized Knudsen layer. J. Comput. Phys. 398, 108893 (2019)
14. Demmel, J.: Applied Numerical Linear Algebra. Society for Industrial and Applied Mathematics, Philadelphia (1997)
15. Fan, Y., Koellermeier, J., Li, J., Li, R., Torrilhon, M.: Model reduction of kinetic equations by operator projection. J. Stat. Phys. 162(2), 457–486 (2016)
16. Fan, Y., Li, J., Li, R., Qiao, Z.: Resolving Knudsen layer by high order moment expansion. Contin. Mech. Thermodyn. 31(5), 1313–1337 (2019)
50. Theisen, L., Torrilhon, M.: FEniCSR13: A tensorial mixed finite element solver for the linear R13 equations using the FEniCS computing platform. ACM Trans. Math. Softw. 47, 1–29 (2021)
51. Torrilhon, M.: Special issues on moment methods in kinetic gas theory. Contin. Mech. Thermodyn. 21(5), 341–343 (2009)
52. Torrilhon, Manuel: H-theorem for nonlinear regularized 13-moment equations in kinetic gas theory. Kinet. Relat. Models 5(1), 185–201 (2012)
53. Wilkinson, J.: Kronecker’s canonical form and the QZ algorithm. Linear Algebra Appl. 28, 285–303 (1979)

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