INTERNATIONAL JOURNAL OF
NUMERICAL ANALYSIS AND MODELING
Volume 20, Number 2, Pages 153–175

doi: 10.4208/ijnam2023-1007

LINEAR MOMENT MODELS TO APPROXIMATE KNUDSEN LAYERS

RUO LI AND YICHEN YANG

Abstract. We propose a well-posed Maxwell-type boundary condition for the linear moment system in half-space. As a reduction model of the Boltzmann equation, the moment equations are available to model Knudsen layers near a solid wall, where proper boundary conditions play a key role. In this paper, we will collect the moment system into the form of a general boundary value problem in half-space. Utilizing an orthogonal decomposition, we separate the part with a damping term from the system and then impose a new class of Maxwell-type boundary conditions on it. Due to the block structure of boundary conditions, we show that the half-space boundary value problem admits a unique solution with explicit expressions. Instantly, the well-posedness of the linear moment system is achieved. We apply the procedure to classical flow problems with the Shakhov collision term, such as the velocity slip and temperature jump problems. The model can capture Knudsen layers with very high accuracy using only a few moments.

Key words. Knudsen layer, half-space moment system, Maxwell-type boundary condition, well-posedness.

1. Introduction

The Knudsen layer is an important rarefaction effect of gas flows near the surface [25], where non-Maxwellian velocity distribution functions must be considered because of the gas-surface interaction. The gas exhibits non-Newtonian behavior in the Knudsen layer, and there is a finite velocity or temperature gap at the surface, known as the velocity slip or temperature jump [21, 37]. A better understanding of the Knudsen layer may help design numerical methods for coupling the Boltzmann and Euler equations [13, 39], avoiding solving the complex multidimensional Boltzmann equation in the whole space.

The linearized Boltzmann equation (LBE) [38] is widely used to depict the Knudsen layer. Half-space problems for the Boltzmann equation are often solved by the direct simulation Monte Carlo (DSMC) method [7] or discrete velocity/ordinates method (DVM/DOM) [8, 32, 5]. Numerical results for various collision models have been reported [26, 27, 32]. In theory, the well-posedness has been exhaustively studied for linear half-space kinetic equations [3, 23, 24] and discrete Boltzmann equations in the DVM [5].

Meanwhile, Grad's moment method [16] has been developed [35, 9, 10] into a popular reduction model of the Boltzmann equation with efficient numerical methods [11, 28, 20]. It is also available [34, 17, 14] to model the Knudsen layer. Compared with kinetic equations, the moment system often gives a formal analytical general solution and leads to empirical formulas describing the gas behavior in the Knudsen layer. These formulas may help simplify the coupling of the Knudsen layer and bulk solutions. However, the Maxwell boundary condition proposed by Grad [16] is shown unstable [30] even in the linearized case. For the linear initial-boundary

Received by the editors on April 12, 2022; accepted on November 2, 2022.
2000 *Mathematics Subject Classification.* 34B40, 34B05, 35Q35, 76P05, 82B40.

value problem (IBVP) of moment equations, [30] has defined stability criteria and constructed the formulation of stable boundary conditions.

To our best knowledge, the well-posedness results are still scattered for half-space problems based on Grad's arbitrary order moment equations with Maxwell-type boundary conditions. In numeric, there are also few universal methods to deal with different flow problems. For example, [14] numerically solves Kramers' problem for the BGK [6] model and proves the well-posedness when the accommodation coefficient is an algebraic number. This paper aims to overcome these two lacks.

One of our main contributions is to propose a new class of Maxwell-type boundary conditions. It makes sure the well-posedness of the linear homogeneous moment system in half-space. The system is derived from Grad's moment equations under some Knudsen layer assumptions and can deal with different specific flow problems with various collision terms. We first collect the system into a general half-space boundary value problem. Then we make an orthogonal decomposition to separate the equations with a damping term from the whole system. With the method of characteristics, we get several well-posedness criteria about boundary conditions. Under these criteria, the solvability of the moment system is ensured. From the constructive proof, we can even write explicit analytical solutions to the moment system. The procedure gives an efficient algorithm to solve half-space problems, which is another contribution of this paper.

Specifically, the construction of boundary conditions mainly follows Grad's idea [16, 11] by imposing the continuity of odd fluxes [2] at the boundary. The obtained Maxwell-type boundary conditions are in a common even-odd parity form [34, 14]. To meet the well-posedness criteria for half-space problems, the linear space determined by Maxwell-type boundary conditions is encouraged to contain the null space of the boundary matrix. This idea has been emphasized in many other problems [22, 29, 30, 40]. We will first get redundant boundary conditions and then combine them linearly to meet the above criteria.

This paper is organized as follows. In Section 2, we summarize the main well-posedness result of linear half-space boundary value problems. In Section 3, we derive the moment system in half-space with Maxwell-type boundary conditions. In Section 4, we apply our model to velocity slip and temperature jump problems with the Shakhov collision term. The paper ends with a conclusion.

2. Solvability Conditions for Half-Space Problems

We consider the boundary layer problem arising in rarefied gas flows when the Knudsen number tends to zero. These equations are often linear [1] regardless of the nonlinear setting of the original equations. Meanwhile, the resulting half-space moment system may have block structures due to the orthogonality and the recursion relation of Hermite polynomials.

Therefore, we consider the linear half-space boundary value problem with constant coefficients

$$
\begin{aligned}
\boldsymbol{A}\frac{\mathrm{d}\boldsymbol{w}(y)}{\mathrm{d}y} &= -\boldsymbol{Q}\boldsymbol{w}(y), \quad y \in [0, +\infty), \\
\boldsymbol{w}(+\infty) &= \boldsymbol{0},
\end{aligned} \tag{1}
$$

where $\boldsymbol{w}(y) \in \mathbb{R}^{m+n}$ with $m \geq n$, and

$$
\boldsymbol{A} = \begin{bmatrix} \boldsymbol{0} & \boldsymbol{M} \\ \boldsymbol{M}^T & \boldsymbol{0} \end{bmatrix}, \qquad \boldsymbol{Q} = \begin{bmatrix} \boldsymbol{Q}_e & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{Q}_o \end{bmatrix}. \tag{2}
$$

We assume that the matrix $\boldsymbol{M} \in \mathbb{R}^{m\times n}$ has a full column rank of n, and the matrices $\boldsymbol{Q}_e \in \mathbb{R}^{m\times m}$ as well as $\boldsymbol{Q}_o \in \mathbb{R}^{n\times n}$ are symmetric positive semi-definite. We also let $\mathrm{Null}(\boldsymbol{A}) \cap \mathrm{Null}(\boldsymbol{Q}) = \{\boldsymbol{0}\}$.

Our main point is to prescribe appropriate boundary conditions at $y = 0$ to ensure the well-posedness of (1). The result is not as straightforward as it appears since the matrices $\boldsymbol{A}$ and $\boldsymbol{Q}$ may both have zero eigenvalues [1].

If $\boldsymbol{Q}$ is invertible, we can consider the eigenvalue decomposition of $\boldsymbol{Q}^{-1}\boldsymbol{A}$ and only prescribe boundary conditions for some "incoming waves" as in the hyperbolic problem. While both the coefficient matrices have zero eigenvalues, we should consider the generalized eigenvalue problem of $\boldsymbol{A}$ and $\boldsymbol{Q}$. We try to reduce the generalized eigenvalue problem by simultaneous reduction. Roughly speaking, we may split the space into several parts and only need to prescribe boundary conditions for the projection of $\boldsymbol{w}$ on some spaces.

We first consider the null space of $\boldsymbol{Q}$. We let $\boldsymbol{G} \in \mathbb{R}^{(m+n)\times p}$ be the orthonormal basis matrix of $\mathrm{Null}(\boldsymbol{Q})$, i.e., $\boldsymbol{Q}\boldsymbol{G} = \boldsymbol{0}$ and $\boldsymbol{G}$ is column orthogonal. It's not enough to consider $\boldsymbol{Q}$ and its orthogonal complement. In fact, multiply (1) left by $\boldsymbol{G}^T$ and we find $\boldsymbol{G}^T\boldsymbol{A}\boldsymbol{w}(y) = 0$ because $\boldsymbol{Q}$ is symmetric and $\boldsymbol{w}(+\infty) = \boldsymbol{0}$. So the projection of $\boldsymbol{w}$ on $\mathrm{span}\{\boldsymbol{A}\boldsymbol{G}\}$ does not need extra boundary conditions. We need to consider the intersection of $\mathrm{span}\{\boldsymbol{G}\}$ and the orthogonal complement of $\mathrm{span}\{\boldsymbol{A}\boldsymbol{G}\}$. Denote $\boldsymbol{V}_1 = \boldsymbol{G}\boldsymbol{X} \in \mathbb{R}^{(m+n)\times r}$ where $\boldsymbol{X} \in \mathbb{R}^{p\times r}$ is the orthonormal basis matrix of $\mathrm{Null}(\boldsymbol{G}^T\boldsymbol{A}\boldsymbol{G})$, i.e., $\boldsymbol{G}^T\boldsymbol{A}\boldsymbol{G}\boldsymbol{X} = \boldsymbol{0}$ and $\boldsymbol{X}$ is column orthogonal. Then $\mathrm{span}\{\boldsymbol{V}_1\}$ is the intersection mentioned above.

To be rigorous, we let $\boldsymbol{U}_1 = \boldsymbol{G}, \boldsymbol{U}_2 = \boldsymbol{A}\boldsymbol{G}\boldsymbol{X}$, and introduce the following lemma, whose proof is put in Appendix A.

Lemma 1. *There exist matrices $\boldsymbol{V}_2 \in \mathbb{R}^{(m+n)\times p}$ and $\boldsymbol{V}_3 \in \mathbb{R}^{(m+n)\times(m+n-p-r)}$ such that*

(1) $\mathrm{span}\{\boldsymbol{V}_2\} = \mathrm{span}\{\boldsymbol{A}\boldsymbol{G}\}$;
(2) $\boldsymbol{V} = [\boldsymbol{V}_1, \boldsymbol{V}_2, \boldsymbol{V}_3]$ *is orthogonal and* $\boldsymbol{U} = [\boldsymbol{U}_1, \boldsymbol{U}_2, \boldsymbol{V}_3]$ *is invertible;*
(3) $\mathrm{rank}(\boldsymbol{U}_2^T\boldsymbol{A}\boldsymbol{V}_1) = r$, $\boldsymbol{V}_3^T\boldsymbol{A}\boldsymbol{V}_1 = \boldsymbol{0}$ *and* $\boldsymbol{V}_3^T\boldsymbol{Q}\boldsymbol{V}_3$ *symmetric positive definite.*

The matrix $\boldsymbol{V}_3$ satisfying Lemma 1 is not unique, which can differ by an orthogonal transformation. However, our proof would not rely on the choices of $\boldsymbol{V}_3$ in this paper. As mentioned before, we may only prescribe additional boundary conditions at $y = 0$ for $\boldsymbol{V}_3^T\boldsymbol{w}(0)$. So we assume the boundary condition

$$\boldsymbol{B}\boldsymbol{V}_3(\boldsymbol{V}_3^T\boldsymbol{w}(0)) = \boldsymbol{g}, \tag{3}$$

where the constant matrix $\boldsymbol{B} \in \mathbb{R}^{n\times(m+n)}$ and the vector $\boldsymbol{g} \in \mathbb{R}^n$.

We then denote by $\boldsymbol{Q}_{33} = \boldsymbol{V}_3^T\boldsymbol{Q}\boldsymbol{V}_3$ and $\boldsymbol{A}_{33} = \boldsymbol{V}_3^T\boldsymbol{A}\boldsymbol{V}_3$. Let n_+ be the number of positive eigenvalues of $\boldsymbol{Q}_{33}^{-1}\boldsymbol{A}_{33}$. We may show below that there exists $\boldsymbol{T}_+ \in \mathbb{R}^{(m+n-p-r)\times n_+}$ and a positive diagonal matrix $\boldsymbol{\Lambda}_+$ such that

$$\boldsymbol{Q}_{33}^{-1}\boldsymbol{A}_{33}\boldsymbol{T}_+ = \boldsymbol{T}_+\boldsymbol{\Lambda}_+. \tag{4}$$

One has the following well-posedness theorem.

---

[1] For equations like (1), there are some classical results if $\boldsymbol{Q}$ is symmetric positive definite [22] or $\boldsymbol{A}$ does not have zero eigenvalues [19]. Here we consider the situation without such restrictions. Incidentally, the well-posedness for kinetic layer equations is well solved [3].

Theorem 1. *The system* (1) *with the boundary condition* (3) *has a unique solution of* $\boldsymbol{w}(y)$ *if the constant matrix* $\boldsymbol{B}$ *and the vector* $\boldsymbol{g}$ *in* (3) *satisfy that*

$$\operatorname{rank}(\boldsymbol{B}\boldsymbol{V}_3\boldsymbol{T}_+) = n_+, \quad \boldsymbol{g} \in \operatorname{span}\{\boldsymbol{B}\boldsymbol{V}_3\boldsymbol{T}_+\}, \tag{5}$$

where $\boldsymbol{V}_3$ *satisfies Lemma 1 and* $\boldsymbol{T}_+$ *satisfies* (4). *What's more, the analytical solutions to the system are explicitly given by the expressions* (7), (6), *and* (9) *below.*

Proof. The proof is constructive. It is clear that (1) is equivalent to

$$\boldsymbol{U}^T\boldsymbol{A}\boldsymbol{V}\frac{\mathrm{d}(\boldsymbol{V}^T\boldsymbol{w})}{\mathrm{d}y} = -\boldsymbol{U}^T\boldsymbol{Q}\boldsymbol{V}(\boldsymbol{V}^T\boldsymbol{w}), \quad \boldsymbol{w}(+\infty) = \boldsymbol{0}.$$

Since $\boldsymbol{G}^T\boldsymbol{Q} = \boldsymbol{0}$ and $\boldsymbol{Q}\boldsymbol{V}_1 = \boldsymbol{Q}\boldsymbol{G}\boldsymbol{X} = \boldsymbol{0}$, the above system becomes

$$\begin{bmatrix} * & * & * \\ \boldsymbol{A}_{21} & * & * \\ \boldsymbol{A}_{31} & * & \boldsymbol{A}_{33} \end{bmatrix} \frac{\mathrm{d}}{\mathrm{d}y} \begin{bmatrix} \boldsymbol{V}_1^T\boldsymbol{w} \\ \boldsymbol{V}_2^T\boldsymbol{w} \\ \boldsymbol{V}_3^T\boldsymbol{w} \end{bmatrix} = - \begin{bmatrix} \boldsymbol{0} & \boldsymbol{0} & \boldsymbol{0} \\ \boldsymbol{0} & * & * \\ \boldsymbol{0} & * & \boldsymbol{Q}_{33} \end{bmatrix} \begin{bmatrix} \boldsymbol{V}_1^T\boldsymbol{w} \\ \boldsymbol{V}_2^T\boldsymbol{w} \\ \boldsymbol{V}_3^T\boldsymbol{w} \end{bmatrix}, \quad \boldsymbol{w}(+\infty) = \boldsymbol{0},$$

where $\boldsymbol{A}_{21} = \boldsymbol{U}_2^T\boldsymbol{A}\boldsymbol{V}_1$, $\boldsymbol{A}_{31} = \boldsymbol{V}_3^T\boldsymbol{A}\boldsymbol{V}_1$, $\boldsymbol{A}_{33} = \boldsymbol{V}_3^T\boldsymbol{A}\boldsymbol{V}_3$, $\boldsymbol{Q}_{33} = \boldsymbol{V}_3^T\boldsymbol{Q}\boldsymbol{V}_3$.

With the condition $\boldsymbol{w}(+\infty) = \boldsymbol{0}$, the first p equations would give

$$\boldsymbol{G}^T\boldsymbol{A}\boldsymbol{w}(y) = \boldsymbol{0} \quad \Rightarrow \quad \boldsymbol{V}_2^T\boldsymbol{w}(y) = \boldsymbol{0}. \tag{6}$$

By Lemma 1, we have $\operatorname{rank}(\boldsymbol{A}_{21}) = r$, $\boldsymbol{A}_{31} = \boldsymbol{0}$ and $\boldsymbol{Q}_{33} > 0$. So we can directly solve $\boldsymbol{V}_1^T\boldsymbol{w}$ from the next r equations, if $\boldsymbol{V}_3^T\boldsymbol{w}(y)$ is known, to be

$$\boldsymbol{V}_1^T\boldsymbol{w}(y) = -\boldsymbol{A}_{21}^{-1}\boldsymbol{U}_2^T\boldsymbol{A}\boldsymbol{V}_3(\boldsymbol{V}_3^T\boldsymbol{w}(y)) + \int_y^{+\infty} \boldsymbol{A}_{21}^{-1}\boldsymbol{U}_2^T\boldsymbol{Q}\boldsymbol{V}_3(\boldsymbol{V}_3^T\boldsymbol{w}(s))\,\mathrm{d}s. \tag{7}$$

Noting that $\boldsymbol{A}_{31} = \boldsymbol{0}$, the last $m + n - p - r$ equations are separated alone as

$$\boldsymbol{A}_{33}\frac{\mathrm{d}}{\mathrm{d}y}(\boldsymbol{V}_3^T\boldsymbol{w}) = -\boldsymbol{Q}_{33}(\boldsymbol{V}_3^T\boldsymbol{w}), \;\; \boldsymbol{V}_3^T\boldsymbol{w}(+\infty) = \boldsymbol{0}.$$

Since $\boldsymbol{Q}_{33} > 0$, we apply the Cholesky decomposition to have $\boldsymbol{Q}_{33} = \boldsymbol{L}\boldsymbol{L}^T$. Then for the symmetric matrix $\boldsymbol{A}_{33}$, due to Sylvester's law of inertia and the symmetry, there exists an orthogonal diagonalization $\boldsymbol{L}^{-1}\boldsymbol{A}_{33}\boldsymbol{L}^{-T}\boldsymbol{R}_+ = \boldsymbol{R}_+\boldsymbol{\Lambda}_+$ with $\boldsymbol{R}_+^T\boldsymbol{R}_+ = \boldsymbol{I}_{n_+}$ where $\boldsymbol{\Lambda}_+$ is a positive diagonal matrix. One possible choice of $\boldsymbol{T}_+$ is

$$\boldsymbol{T}_+ = \boldsymbol{L}^{-T}\boldsymbol{R}_+, \tag{8}$$

then we have $\boldsymbol{Q}_{33}^{-1}\boldsymbol{A}_{33}\boldsymbol{T}_+ = \boldsymbol{T}_+\boldsymbol{\Lambda}_+$.

Since $\boldsymbol{V}_3^T\boldsymbol{w}(+\infty) = 0$, characteristic variables corresponding to non-positive eigenvalues of $\boldsymbol{Q}_{33}^{-1}\boldsymbol{A}_{33}$ have to be zero. Therefore, there exists $\boldsymbol{z} \in \mathbb{R}^{n_+}$ such that $\boldsymbol{V}_3^T\boldsymbol{w} = \boldsymbol{T}_+\boldsymbol{z}$. Under the condition (3)(5), the linear algebraic system

$$\boldsymbol{B}\boldsymbol{V}_3(\boldsymbol{T}_+\boldsymbol{z}(0)) = \boldsymbol{g}$$

has a unique solution of $\boldsymbol{z}(0)$. Consequently, we can uniquely solve

$$\boldsymbol{V}_3^T\boldsymbol{w}(y) = \boldsymbol{T}_+\exp\left(-\boldsymbol{\Lambda}_+^{-1}y\right)\boldsymbol{z}(0). \tag{9}$$

Until now, we show that the unique solution of $\boldsymbol{w}$ is determined by explicit expressions (7), (6), and (9). □

Theorem 1 has clarified the conditions to ensure the existence of a unique solution for the system (1). Due to the explicit expressions (9), we can see that the solution $\boldsymbol{w}$ continuously relies on $\boldsymbol{z}(0)$, where $\boldsymbol{z}(0)$ is solved by a linear algebraic system with the boundary data $\boldsymbol{g}$. Since all matrices have constant coefficients, the solution must change continuously with the boundary data and Theorem 1 ensures the well-posedness of the system (1).

With the block structure in (2), we can say more about the value of n_+. The key point lies in the following lemma.

Lemma 2. *Let $\boldsymbol{D} \in \mathbb{R}^{\alpha\times\beta}$ and $\operatorname{rank}(\boldsymbol{D}) = \gamma$. Then $\begin{bmatrix} \boldsymbol{0} & \boldsymbol{D} \\ \boldsymbol{D}^T & \boldsymbol{0} \end{bmatrix}$ has $\alpha+\beta-2\gamma$ zero eigenvalues, γ positive eigenvalues and γ negative eigenvalues.*

Proof. The symmetric matrix $\tilde{\boldsymbol{D}} := \begin{bmatrix} \boldsymbol{0} & \boldsymbol{D} \\ \boldsymbol{D}^T & \boldsymbol{0} \end{bmatrix}$ must have $\alpha + \beta$ real eigenvalues. Assume $\lambda \in \mathbb{R}$ is an eigenvalue, then there exists $\boldsymbol{x}_e \in \mathbb{R}^\alpha$ and $\boldsymbol{x}_o \in \mathbb{R}^\beta$ such that

$$\begin{bmatrix} \boldsymbol{0} & \boldsymbol{D} \\ \boldsymbol{D}^T & \boldsymbol{0} \end{bmatrix} \begin{bmatrix} \boldsymbol{x}_e \\ \boldsymbol{x}_o \end{bmatrix} = \lambda \begin{bmatrix} \boldsymbol{x}_e \\ \boldsymbol{x}_o \end{bmatrix} \quad \Rightarrow \quad \begin{bmatrix} \boldsymbol{0} & \boldsymbol{D} \\ \boldsymbol{D}^T & \boldsymbol{0} \end{bmatrix} \begin{bmatrix} \boldsymbol{x}_e \\ -\boldsymbol{x}_o \end{bmatrix} = -\lambda \begin{bmatrix} \boldsymbol{x}_e \\ -\boldsymbol{x}_o \end{bmatrix}.$$

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

By some direct but lengthy manipulations, we can write all matrices in Theorem 1 as a block form. Let $p_1, p_2 \in \mathbb{N}$ that $p_1 = \dim(\operatorname{Null}(\boldsymbol{Q}_e))$ and $p_2 = \dim(\operatorname{Null}(\boldsymbol{Q}_o))$. Then it's direct to verify that $p = p_1 + p_2$ and the matrices $\boldsymbol{G}$ as well as $\boldsymbol{X}$ can be chosen as

$$\boldsymbol{G} = \begin{bmatrix} \boldsymbol{G}_e & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{G}_o \end{bmatrix}, \qquad \boldsymbol{X} = \begin{bmatrix} \boldsymbol{X}_e & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{X}_o \end{bmatrix}, \tag{10}$$

where $\boldsymbol{G}_e \in \mathbb{R}^{m\times p_1}$, $\boldsymbol{G}_o \in \mathbb{R}^{n\times p_2}$, $\boldsymbol{X}_e \in \mathbb{R}^{p_1\times r_1}$, and $\boldsymbol{X}_o \in \mathbb{R}^{p_2\times r_2}$. Here we let $c = \operatorname{rank}(\boldsymbol{G}_e^T \boldsymbol{M} \boldsymbol{G}_o)$ and $r_1 = p_1 - c$, $r_2 = p_2 - c$. By Lemma 2, we have $r_1 + r_2 = r$ and consequently

$$r_1 + p_2 = (p_1 - c) + p_2 = (p_2 - c) + p_1 = r_2 + p_1 = (r + p)/2.$$

Denote by $\boldsymbol{Y}_1 = \boldsymbol{G}_e \boldsymbol{X}_e$ and $\boldsymbol{Z}_1 = \boldsymbol{G}_o \boldsymbol{X}_o$. According to the proof of Lemma 1, we can construct the matrices $\boldsymbol{V}_2$ and $\boldsymbol{V}_3$ as

$$\boldsymbol{V}_2 = \begin{bmatrix} \boldsymbol{Y}_2 & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{Z}_2 \end{bmatrix}, \quad \boldsymbol{V}_3 = \begin{bmatrix} \boldsymbol{Y}_3 & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{Z}_3 \end{bmatrix}, \tag{11}$$

where $\boldsymbol{Y}_2 \in \mathbb{R}^{m\times p_2}$ and $\boldsymbol{Z}_2 \in \mathbb{R}^{n\times p_1}$ that $\operatorname{span}\{\boldsymbol{Y}_2\} = \operatorname{span}\{\boldsymbol{M}\boldsymbol{G}_o\}$, $\operatorname{span}\{\boldsymbol{Z}_2\} = \operatorname{span}\{\boldsymbol{M}^T\boldsymbol{G}_e\}$. $\boldsymbol{Y}_3 \in \mathbb{R}^{m\times(m-r_1-p_2)}$ and $\boldsymbol{Z}_3 \in \mathbb{R}^{n\times(n-r_2-p_1)}$ are chosen to let $[\boldsymbol{Y}_1, \boldsymbol{Y}_2, \boldsymbol{Y}_3]$ and $[\boldsymbol{Z}_1, \boldsymbol{Z}_2, \boldsymbol{Z}_3]$ both be orthogonal. With these structures in mind, we note the following lemma:

Lemma 3. *The matrix $\boldsymbol{Y}_3^T \boldsymbol{M} \boldsymbol{Z}_3$ is of full column rank.*

The proof of this lemma is put in Appendix A. With the help of this lemma,

Corollary 1. *The value of n_+ is $n_+ = n - (p + r)/2$.*

Proof. According to (11), we have $\boldsymbol{A}_{33} = \begin{bmatrix} \boldsymbol{0} & \boldsymbol{Y}_3^T \boldsymbol{M} \boldsymbol{Z}_3 \\ \boldsymbol{Z}_3^T \boldsymbol{M}^T \boldsymbol{Y}_3 & \boldsymbol{0} \end{bmatrix}$. Since $\boldsymbol{Y}_3^T \boldsymbol{M} \boldsymbol{Z}_3$ is of full column rank, the matrix $\boldsymbol{A}_{33}$ should have $n-(p+r)/2$ positive eigenvalues by Lemma 2. □

3. Half-Space Moment System

3.1. Knudsen Layer Equations. We focus on Grad's arbitrary order moment equations [16] which are about moments of the velocity distribution function. Besides low-order moments such as the density, the macroscopic velocity, the temperature, etc., Grad tested the Boltzmann equation by multidimensional Hermite polynomials to get equations of higher-order moments. For single-species monatomic gas without external forces, the linear homogeneous half-space problem for Grad's moment equations (cf. Appendix B) can write as

$$\begin{aligned} \boldsymbol{A}_2 \frac{\mathrm{d}\boldsymbol{h}(y)}{\mathrm{d}y} &= -\boldsymbol{J}\boldsymbol{h}(y), \quad y \in [0, +\infty), \\ \boldsymbol{h}(+\infty) &= \boldsymbol{0}, \end{aligned} \tag{12}$$

where $\boldsymbol{h} = \boldsymbol{h}(y) \in \mathbb{R}^N$ and $N = \#\mathbb{I}_M$ with $\mathbb{I}_M = \{\boldsymbol{\alpha} \in \mathbb{N}^D : \ |\boldsymbol{\alpha}| \leq M\}$. Here $\boldsymbol{\alpha} = (\alpha_1, ..., \alpha_D) \in \mathbb{N}^D$ is a multi-index with $|\boldsymbol{\alpha}| = \sum \alpha_i$, and M is often called the moment order.

For economy of words, we use $\boldsymbol{h}[\boldsymbol{\alpha}]$ to represent its $\mathcal{N}(\boldsymbol{\alpha})$-th component, analogously for other vectors and matrices, where the one to one mapping $\mathcal{N} : \ \mathbb{I}_M \to \{1, 2, ..., N\}$ is defined as follows.

Definition 1. *For $\boldsymbol{\alpha}, \boldsymbol{\beta} \in \mathbb{I}_M$,*

1. *If α_2 is even and β_2 is odd, then $\mathcal{N}(\boldsymbol{\alpha}) < \mathcal{N}(\boldsymbol{\beta})$.*
2. *If α_2 and β_2 have the same parity, but $|\boldsymbol{\alpha}| < |\boldsymbol{\beta}|$, then $\mathcal{N}(\boldsymbol{\alpha}) < \mathcal{N}(\boldsymbol{\beta})$.*
3. *If α_2 and β_2 have the same parity and $|\boldsymbol{\alpha}| = |\boldsymbol{\beta}|$, but there exists a smallest $1 \leq i \leq D$ such that $\alpha_i \neq \beta_i$. Then $\mathcal{N}(\boldsymbol{\alpha}) < \mathcal{N}(\boldsymbol{\beta})$ when $\alpha_i > \beta_i$. Otherwise $\mathcal{N}(\boldsymbol{\alpha}) > \mathcal{N}(\boldsymbol{\beta})$.*

In the indexing provided by Defintion 3.1, the indices with even second components are always ordered before the ones with odd second components, e.g. $(a_1, 0, a_3)$ is before $(b_1, 1, b_3)$. Then the indices are sorted by the multi-index norm and finally by the anti-lexicographic order. For example, indices from $\{\boldsymbol{\alpha} \in \mathbb{N}^3, \ |\boldsymbol{\alpha}| \leq 2\}$ are sorted as $(0,0,0)$,$(1,0,0)$,$(0,0,1)$,$(2,0,0)$,$(1,0,1)$,$(0,2,0)$, $(0,0,2)$, $(0,1,0)$,$(1,1,0)$,$(0,1,1)$.

Now the coefficient matrices in (12) have the following explicit expressions:

$$\boldsymbol{A}_2[\boldsymbol{\alpha}, \boldsymbol{\beta}] = \langle \xi_2 \omega \phi_{\boldsymbol{\alpha}} \phi_{\boldsymbol{\beta}} \rangle = \sqrt{\alpha_2}\delta_{\boldsymbol{\beta}, \boldsymbol{\alpha}-\boldsymbol{e}_2} + \sqrt{\alpha_2+1}\delta_{\boldsymbol{\beta}, \boldsymbol{\alpha}+\boldsymbol{e}_2}, \tag{13}$$

$$\boldsymbol{J}[\boldsymbol{\alpha}, \boldsymbol{\beta}] = -\langle \mathcal{L}[\omega \phi_{\boldsymbol{\beta}}] \phi_{\boldsymbol{\alpha}} \rangle, \tag{14}$$

where $\delta_{\boldsymbol{\alpha}, \boldsymbol{\beta}}$ equals one when $\boldsymbol{\alpha} = \boldsymbol{\beta}$ and otherwise zero. Here $\boldsymbol{e}_2 \in \mathbb{N}^D$ is a unit vector with only the second component being one.

Definition 2. *In the above expressions, we denote the integral on the whole velocity space by*

$$\langle \cdot \rangle = \int_{\mathbb{R}^D} \cdot \, \mathrm{d}\boldsymbol{\xi}.$$

The isotropic weight function ω and the orthonormal Hermite polynomial $\phi_{\boldsymbol{\alpha}}$ are defined as

$$\begin{aligned} \omega = \omega(\boldsymbol{\xi}) &= (2\pi)^{-D/2} \exp\left(-|\boldsymbol{\xi}|^2/2\right), \\ \phi_{\boldsymbol{\alpha}} = \phi_{\boldsymbol{\alpha}}(\boldsymbol{\xi}) &= \frac{(-1)^{|\boldsymbol{\alpha}|}}{\sqrt{\boldsymbol{\alpha}!}} \frac{\partial^{|\boldsymbol{\alpha}|}\omega}{\partial \boldsymbol{\xi}^{\boldsymbol{\alpha}}} \omega^{-1}, \end{aligned}$$

where $\boldsymbol{\xi} = (\xi_1, ..., \xi_D) \in \mathbb{R}^D$, $\boldsymbol{\xi}^{\boldsymbol{\alpha}} = \prod \xi_i^{\alpha_i}$, $\boldsymbol{\alpha}! = \prod \alpha_i!$. *According to* [9, 15], *we have*

- *Recursion relation.*

$$\xi_d \phi_{\boldsymbol{\alpha}} = \sqrt{\alpha_d}\phi_{\boldsymbol{\alpha}-\boldsymbol{e}_d} + \sqrt{\alpha_d+1}\phi_{\boldsymbol{\alpha}+\boldsymbol{e}_d}, \quad d = 1, 2, ..., D.$$

- *Orthogonal relation.*

$$\langle \omega \phi_{\boldsymbol{\alpha}} \phi_{\boldsymbol{\beta}} \rangle = \delta_{\boldsymbol{\alpha},\boldsymbol{\beta}}.$$

The linearized Boltzmann operator $\mathcal{L}[f](\boldsymbol{\xi})$ *is defined as*

$$\mathcal{L}[f](\boldsymbol{\xi}) = \int_{\mathbb{R}^D}\int_{\mathbb{S}^{D-1}} \mathcal{K}[f/\omega]\omega(\boldsymbol{\xi})\omega(\boldsymbol{\xi}_1) B(|\boldsymbol{\xi}-\boldsymbol{\xi}_1|, \Theta)\,\mathrm{d}\Theta \mathrm{d}\boldsymbol{\xi}_1,$$

where $B(|\boldsymbol{\xi}-\boldsymbol{\xi}_1|, \Theta)$ *is a collision kernel. The operator* $\mathcal{K}$ *is defined as*

$$\mathcal{K}[g](\boldsymbol{\xi}, \boldsymbol{\xi}_1, \Theta) = g(\boldsymbol{\xi}') + g(\boldsymbol{\xi}_1') - g(\boldsymbol{\xi}) - g(\boldsymbol{\xi}_1),$$

where the post-collisional velocities $\boldsymbol{\xi}'$ *and* $\boldsymbol{\xi}_1'$ *are determined by* $\boldsymbol{\xi}$, $\boldsymbol{\xi}_1$ *as well as* Θ.

Calculations of $\boldsymbol{J}$ can refer to [36]. We also consider the (linearized) Shakhov model [31], which aims to approximate the original (linearized) Boltzmann equation. It's defined by setting $\boldsymbol{J} = \boldsymbol{J}_{Sh}$ in (12), where nonzero entries of $\boldsymbol{J}_{Sh}$ (cf. [11]) are

$$\begin{aligned}
\boldsymbol{J}_{Sh}[2\boldsymbol{e}_i, 2\boldsymbol{e}_j] &= \delta_{ij} - \frac{1}{D}, \ i,j = 1,2,...,D; \\
\boldsymbol{J}_{Sh}[\boldsymbol{e}_i + 2\boldsymbol{e}_j, \boldsymbol{e}_i + 2\boldsymbol{e}_k] &= \delta_{jk} - \frac{1-\mathrm{Pr}}{5}\sqrt{1+2\delta_{ij}}\sqrt{1+2\delta_{ik}}, \ i,j,k = 1,2,...,D; \\
\boldsymbol{J}_{Sh}[\boldsymbol{\alpha}, \boldsymbol{\alpha}] &= 1, \ |\boldsymbol{\alpha}| \geq 2 \text{ and } \boldsymbol{\alpha} \neq 2\boldsymbol{e}_i, \ \boldsymbol{e}_i + 2\boldsymbol{e}_j.
\end{aligned} \tag{15}$$

When the Prandtl number $\mathrm{Pr} = 1$, the Shakhov model reduces to the celebrated BGK model.

Considering the computational efficiency, (12) is unsatisfactory to solve half-space problems since the size of (12) reaches

$$N = \#\{\boldsymbol{\alpha} \in \mathbb{N}^D : \ |\boldsymbol{\alpha}| \leq M\} = \binom{M+D}{D} = \frac{(M+D)\cdots(M+1)}{D!} = O(M^D),$$

but very few quantities are cared about in physics. We can formally write the density ρ_K, the macroscopic velocity $u_{i,K}$, the temperature θ_K and the stress tensor $\sigma_{ij,K}$ as

$$\rho_K = \boldsymbol{h}[\boldsymbol{0}], \ u_{i,K} = \boldsymbol{h}[\boldsymbol{e}_i], \ \frac{\sigma_{ij,K} + \delta_{ij}\theta_K}{\sqrt{1+\delta_{ij}}} = \boldsymbol{h}[\boldsymbol{e}_i + \boldsymbol{e}_j], \tag{16}$$

where we assume $\sum \sigma_{ii,K} = 0$ and the subscript K is attached to discriminate the Knudsen layer solutions. Then, for example, in Kramers' problem, we consider the tangential velocity $u_{1,K}$, where a gas flow passes by an infinite plate. We assume the gas velocity is parallel to the plate, and the only driven force is from the tangential stress. Due to the symmetry, Kramers' problem is essentially a one-dimensional problem rather than the D-dimensional problem. For the BGK model, the moment system (12) for Kramers' problem [14] can reduce to

$$\begin{aligned}
\frac{\mathrm{d}\sigma_{12,K}}{\mathrm{d}y} =&0,\\
\frac{\mathrm{d}u_{1,K}}{\mathrm{d}y}+\sqrt{2}\frac{\mathrm{d}\boldsymbol{h}[\boldsymbol{e}_1+2\boldsymbol{e}_2]}{\mathrm{d}y} =&-\sigma_{12,K},\\
\sqrt{2}\frac{\mathrm{d}\sigma_{12,K}}{\mathrm{d}y}+\sqrt{3}\frac{\mathrm{d}\boldsymbol{h}[\boldsymbol{e}_1+3\boldsymbol{e}_2]}{\mathrm{d}y} =&-\boldsymbol{h}[\boldsymbol{e}_1+2\boldsymbol{e}_2],\\
&\cdots\\
\sqrt{k}\frac{\mathrm{d}\boldsymbol{h}[\boldsymbol{e}_1+(k-1)\boldsymbol{e}_2]}{\mathrm{d}y}&+(1-\delta_{k,M-1})\sqrt{k+1}\frac{\mathrm{d}\boldsymbol{h}[\boldsymbol{e}_1+(k+1)\boldsymbol{e}_2]}{\mathrm{d}y}\\
=&-\boldsymbol{h}[\boldsymbol{e}_1+k\boldsymbol{e}_2], \quad k\le M-1.
\end{aligned}$$

When $M=4$, the small moment system is

$$\begin{aligned}
\frac{\mathrm{d}\sigma_{12,K}}{\mathrm{d}y} &= 0,\\
\frac{\mathrm{d}u_{1,K}}{\mathrm{d}y}+\sqrt{2}\frac{\mathrm{d}\boldsymbol{h}[\boldsymbol{e}_1+2\boldsymbol{e}_2]}{\mathrm{d}y} &= -\sigma_{12,K},\\
\sqrt{2}\frac{\mathrm{d}\sigma_{12,K}}{\mathrm{d}y}+\sqrt{3}\frac{\mathrm{d}\boldsymbol{h}[\boldsymbol{e}_1+3\boldsymbol{e}_2]}{\mathrm{d}y} &= -\boldsymbol{h}[\boldsymbol{e}_1+2\boldsymbol{e}_2],\\
\sqrt{3}\frac{\mathrm{d}\boldsymbol{h}[\boldsymbol{e}_1+2\boldsymbol{e}_2]}{\mathrm{d}y} &= -\boldsymbol{h}[\boldsymbol{e}_1+3\boldsymbol{e}_2].
\end{aligned}$$

This inspires us to reduce (12) for specific flow problems. We introduce a projection matrix $\boldsymbol{P}_{\mathbb{I}}\in\mathbb{R}^{N\times(m+n)}$ relying on an index set $\mathbb{I}\subset\mathbb{I}_M$, and the reduced system would be

$$(17)\quad \boldsymbol{A}\frac{\mathrm{d}\boldsymbol{w}}{\mathrm{d}y}=-\boldsymbol{Q}\boldsymbol{w},\ \boldsymbol{w}(+\infty)=\boldsymbol{0};\quad \boldsymbol{w}=\boldsymbol{P}_{\mathbb{I}}^T\boldsymbol{h},\ \boldsymbol{A}=\boldsymbol{P}_{\mathbb{I}}^T\boldsymbol{A}_2\boldsymbol{P}_{\mathbb{I}},\ \boldsymbol{Q}=\boldsymbol{P}_{\mathbb{I}}^T\boldsymbol{J}\boldsymbol{P}_{\mathbb{I}}.$$

Now (17) consists of $m+n$ equations, and we expect to reduce the system without compromising the accuracy of the concerned physical quantities. Assume $\boldsymbol{P}_{\mathbb{I}}$ is column orthogonal. We suggest choosing $\boldsymbol{P}_{\mathbb{I}}$ such that it spans an invariant space of $\boldsymbol{A}_2$ and $\boldsymbol{J}$, i.e., $\boldsymbol{A}_2\boldsymbol{P}_{\mathbb{I}}=\boldsymbol{P}_{\mathbb{I}}\boldsymbol{C}_1,\ \boldsymbol{J}\boldsymbol{P}_{\mathbb{I}}=\boldsymbol{P}_{\mathbb{I}}\boldsymbol{C}_2$ for some matrices $\boldsymbol{C}_1,\boldsymbol{C}_2$. If so, the system (17) can be obtained by multiplying (12) left by $\boldsymbol{P}_{\mathbb{I}}^T$.

In this paper, we let $\boldsymbol{P}_{\mathbb{I}}$ be the selection matrix with $\boldsymbol{P}_{\mathbb{I}}[\boldsymbol{\alpha},\boldsymbol{\beta}]=\delta_{\boldsymbol{\alpha},\boldsymbol{\beta}}$, where $\boldsymbol{\alpha}\in\mathbb{I}_M$ and $\boldsymbol{\beta}\in\mathbb{I}$. Thus (17) can be viewed as selecting some row equations of (12) and then dropping out extra unknowns to close the system. Here $\boldsymbol{P}_{\mathbb{I}}[\boldsymbol{\alpha},\boldsymbol{\beta}]$ means the entry in the $\mathcal{N}(\boldsymbol{\alpha})$-th row and $\mathcal{N}_1(\boldsymbol{\beta})$-th column where $\mathcal{N}$ is defined in Definition 1 and $\mathcal{N}_1:\ \mathbb{I}\to\{1,2,...,m+n\}$ gives an indexing of $\mathbb{I}$. We define $\mathcal{N}_1$ by retaining the order in $\mathbb{I}_M$, i.e.,

$$\mathcal{N}_1(\boldsymbol{\alpha})<\mathcal{N}_1(\boldsymbol{\beta})\ \Leftrightarrow\ \mathcal{N}(\boldsymbol{\alpha})<\mathcal{N}(\boldsymbol{\beta}),\quad \boldsymbol{\alpha},\boldsymbol{\beta}\in\mathbb{I}\subset\mathbb{I}_M.$$

Hence, if we assume

$$\mathbb{I}_e=\{\boldsymbol{\alpha}\in\mathbb{I},\ \alpha_2\text{ even}\},\quad \mathbb{I}_o=\{\boldsymbol{\alpha}\in\mathbb{I},\ \alpha_2\text{ odd}\},\quad m=\#\mathbb{I}_e,\ n=\#\mathbb{I}_o,$$

then $\boldsymbol{\alpha}\in\mathbb{I}_e$ is always ordered in front of $\boldsymbol{\beta}\in\mathbb{I}_o$.

Due to the special sparsity pattern (13) of $\boldsymbol{A}_2$, it can be checked that $\boldsymbol{P}_{\mathbb{I}}$ with the following choice of $\mathbb{I}$ spans an invariant space of $\boldsymbol{A}_2$:

(C1). If $\boldsymbol{\gamma}=(\gamma_i)\in\mathbb{I},$ then $\boldsymbol{\gamma}-\gamma_2\boldsymbol{e}_2+\alpha_2\boldsymbol{e}_2\in\mathbb{I},\ 0\le\alpha_2\le M-|\boldsymbol{\gamma}|+\gamma_2.$

Intuitively, this condition says that all indices differing only by the second component should either belong to or not belong to $\mathbb{I}$. For example, if $(1,0,0) \in \mathbb{I}$, then $(1,1,0)$,$(1,2,0)$,...,$(1,M-1,0)$ should all belong to $\mathbb{I}$. Under this choice, every $\boldsymbol{\alpha} \in \mathbb{I}_o$ implies $\boldsymbol{\alpha} - \boldsymbol{e}_2 \in \mathbb{I}_e$, which leads to $m \geq n$. Thus, from (13), we immediately know that $\boldsymbol{A}$ has the block structure

$$\boldsymbol{A} = \begin{bmatrix} \boldsymbol{0} & \boldsymbol{M} \\ \boldsymbol{M}^T & \boldsymbol{0} \end{bmatrix}, \quad \boldsymbol{M}[\boldsymbol{\alpha},\boldsymbol{\beta}] = \langle \xi_2 \omega \phi_{\boldsymbol{\beta}} \phi_{\boldsymbol{\alpha}} \rangle, \quad \boldsymbol{\alpha} \in \mathbb{I}_e,\ \boldsymbol{\beta} \in \mathbb{I}_o. \tag{18}$$

As proved in Appendix A, the equations (17) in fact satisfy the following lemma:

Lemma 4. *Assume $\mathbb{I}$ satisfies* **(C1)** *and the multi-indices are ordered by Definition 1. Then, Knudsen layer equations* (17) *satisfy conditions in* (1)*, i.e.,*

(1) *The matrix $\boldsymbol{A}$ has a block structure as* (18)*, where* $\operatorname{rank}(\boldsymbol{M}) = n$.
(2) *The matrix $\boldsymbol{Q}$ has a block structure as* (2)*, and is symmetric positive semi-definite.*
(3) $\operatorname{Null}(\boldsymbol{A}) \cap \operatorname{Null}(\boldsymbol{Q}) = \{\boldsymbol{0}\}$.

The lemma also holds for the Shakhov model, i.e. $\boldsymbol{J} = \boldsymbol{J}_{Sh}$ in (17).

Remark 1. *From another point of view,* (17) *can be viewed as directly testing the kinetic layer equations by linear combinations of Hermite polynomials, and then truncating the collision term to obtain a closed system. It's clearly shown in the expressions* (13)(14).

Remark 2. *The rigorous error analysis between* (17) *and kinetic layer equations is beyond this paper's scope. We notice that if $\boldsymbol{J}$ shares a sparsity pattern, then $\boldsymbol{P}_{\mathbb{I}}$ can be chosen to span an invariant space of $\boldsymbol{J}$ easily. For example, if we consider the Shakhov model and focus on the tangential velocity $\boldsymbol{h}[\boldsymbol{e}_1]$, we can choose*

$$\mathbb{I} = \{\boldsymbol{e}_1 + 2\boldsymbol{e}_j + \alpha_2 \boldsymbol{e}_2,\ j \neq 2,\ 0 \leq \alpha_2 \leq M-3\} \cup \{\boldsymbol{e}_1 + \alpha_2 \boldsymbol{e}_2,\ 0 \leq \alpha_2 \leq M-1\}.$$

When $D = 3$, the above $\mathbb{I}$ consists of all indices in the form of $(1,\alpha_2,0)$, $(3,\alpha_2,0)$ and $(1,\alpha_2,2)$. So $\#\mathbb{I} = 3M-4$ and the scale is reduced from $O(M^D)$ to $O(M)$. It's direct to check that $\boldsymbol{J}_{Sh}\boldsymbol{P}_{\mathbb{I}} = \boldsymbol{P}_{\mathbb{I}}\boldsymbol{C}$ for some matrix $\boldsymbol{C}$.

3.2. Maxwell-Type Boundary Conditions. Maxwell's boundary condition describes the diffuse-specular process between the gas and solid wall, i.e., the reflected distribution of particles is divided into a sum of χ portion of diffuse reflection and $(1-\chi)$ portion of specular reflection:

$$f(\boldsymbol{\xi}) = \chi \mathcal{M}^w(\boldsymbol{\xi}) + (1-\chi) f(\boldsymbol{\xi}^*), \quad (\boldsymbol{\xi} - \boldsymbol{u}^w) \cdot \boldsymbol{n} < 0, \tag{19}$$

where $\chi \in [0,1]$ is the accommodation coefficient. The wall is assumed impermeable and can not deform. We assume the reflected distribution caused by the diffuse reflection is the Maxwellian

$$\mathcal{M}^w(\boldsymbol{\xi}) = \frac{\rho^w}{(2\pi\theta^w)^{D/2}} \exp\left(-\frac{|\boldsymbol{\xi} - \boldsymbol{u}^w|^2}{2\theta^w}\right), \tag{20}$$

where $\boldsymbol{u}^w$ and θ^w are given, with ρ^w determined by the no mass flow condition $(\boldsymbol{u} - \boldsymbol{u}^w) \cdot \boldsymbol{n} = 0$. Here $\boldsymbol{n}$ is the outward unit normal vector at the boundary and $\boldsymbol{\xi}^* = \boldsymbol{\xi} - 2\boldsymbol{n}(\boldsymbol{\xi} \cdot \boldsymbol{n})$. In Knudsen layer problems, we further assume $\boldsymbol{n} = (0,-1,0,...,0)$ and $\boldsymbol{u}^w \cdot \boldsymbol{n} = 0$.

Following Grad's idea [16], we test (19) by polynomials which are odd about the direction normal to the boundary. Rather than directly choosing [11, 30] the Hermite polynomials, we let the test polynomials be

$$p_{\boldsymbol{\alpha}}(\boldsymbol{\xi}) = \xi_2 \phi_{\boldsymbol{\alpha}}(\boldsymbol{\xi}),\ \boldsymbol{\alpha} \in \mathbb{I}_e,$$

which may simplify the analysis. Then under some Knudsen layer assumptions, when χ is not a small quantity, we would (cf. Appendix C) have m boundary conditions in an abstract form:

$$\boldsymbol{M}(\boldsymbol{w}_o(0)+\boldsymbol{f}_o) = -b(\chi)\boldsymbol{S}(\boldsymbol{w}_e(0)+\boldsymbol{f}_e), \ \boldsymbol{w} = \begin{bmatrix}\boldsymbol{w}_e \\ \boldsymbol{w}_o\end{bmatrix}, \ \boldsymbol{w}_e \in \mathbb{R}^m, \ \boldsymbol{w}_o \in \mathbb{R}^n, \tag{21}$$

where $b(\chi) = \frac{2\chi}{2-\chi}\left(\sqrt{2\pi}\right)^{-1}$ and $\boldsymbol{f}_o \in \mathbb{R}^n, \ \boldsymbol{f}_e \in \mathbb{R}^m$. Here $\boldsymbol{w}$ is the unknown in (17) and $\boldsymbol{M}$ is given in (18). Entries of $\boldsymbol{S} \in \mathbb{R}^{m\times m}$ are

$$\boldsymbol{S}[\boldsymbol{\alpha},\boldsymbol{\beta}] = \frac{\sqrt{2\pi}}{2}\left\langle |\xi_2|\omega\phi_{\boldsymbol{\alpha}}\phi_{\boldsymbol{\beta}}\right\rangle, \quad \boldsymbol{\alpha},\boldsymbol{\beta} \in \mathbb{I}_e, \tag{22}$$

which are explicitly calculated in Appendix D. What's more, Appendix A will show that

Lemma 5. *The matrix $\boldsymbol{S}$ defined in* (22) *is symmetric positive definite.*

Remark 3. *Grad's boundary condition can be regarded as*

$$\boldsymbol{E}\boldsymbol{M}(\boldsymbol{w}_o(0)+\boldsymbol{f}_o) = -b(\chi)\boldsymbol{E}\boldsymbol{S}(\boldsymbol{w}_e(0)+\boldsymbol{f}_e), \tag{23}$$

where $\boldsymbol{E} = [\boldsymbol{I}_n, \boldsymbol{0}]$ with $\boldsymbol{E} \in \mathbb{R}^{n\times m}$. In the IBVP for moment equations, this gives a correct number [16, 29] *of boundary conditions for the linear hyperbolic system. But the well-posedness of* (23) *has never been proved. In fact,* [30] *shows that* (23) *is unstable in the IBVP. A similar problem arises in the half-space problem, where it's difficult to prove the well-posedness of Grad's boundary condition in the general case.*

By Lemma 4, the Knudsen layer equations (17) satisfy all conditions in Theorem 1. Recalling Sylvester's rank inequality of the product of two matrices and its condition of the equality, we are inspired to multiply (21) left by $\boldsymbol{M}^T\boldsymbol{S}^{-1}$ to get n boundary conditions

$$\boldsymbol{M}^T\boldsymbol{S}^{-1}\boldsymbol{M}(\boldsymbol{w}_o(0)+\boldsymbol{f}_o) = -b(\chi)\boldsymbol{M}^T(\boldsymbol{w}_e(0)+\boldsymbol{f}_e), \tag{24}$$

which satisfy the following well-posedness theorem:

Theorem 2. *Suppose $\chi \in (0,1]$ and $r_2 = 0$ in* (10)*. Then there exists a unique $\boldsymbol{G}_e^T\boldsymbol{f}_e$ such that the system* (17) *with Maxwell-type boundary conditions* (24) *has a unique solution of $\boldsymbol{w}(y)$.*

Proof. Denote by $\boldsymbol{H} = \boldsymbol{M}^T\boldsymbol{S}^{-1}\boldsymbol{M}$ and $\boldsymbol{B} = [b(\chi)\boldsymbol{M}^T, \boldsymbol{H}] \in \mathbb{R}^{n\times(m+n)}$. By Theorem 1, we substitute $\boldsymbol{V}_2^T\boldsymbol{w} = \boldsymbol{0}$ and $\boldsymbol{V}_3^T\boldsymbol{w} = \boldsymbol{T}_+\boldsymbol{z}$ into (24). Due to the block structure (10)(11), we write $\boldsymbol{f}_e = \boldsymbol{G}_e\boldsymbol{G}_e^T\boldsymbol{f}_e + (\boldsymbol{I}_m - \boldsymbol{G}_e\boldsymbol{G}_e^T)\boldsymbol{f}_e$. Then the boundary condition (24) becomes

$$\begin{aligned} & b(\chi)\boldsymbol{M}^T\boldsymbol{G}_e(\boldsymbol{X}_e\boldsymbol{X}_e^T\boldsymbol{G}_e^T\boldsymbol{w}_e(0) + \boldsymbol{G}_e^T\boldsymbol{f}_e) + \boldsymbol{B}\boldsymbol{V}_3(\boldsymbol{T}_+\boldsymbol{z}(0)) \\ = \ & -\boldsymbol{H}\boldsymbol{f}_o - b(\chi)\boldsymbol{M}^T(\boldsymbol{I}_m - \boldsymbol{G}_e\boldsymbol{G}_e^T)\boldsymbol{f}_e. \end{aligned} \tag{25}$$

We only need to claim that $\operatorname{rank}(\boldsymbol{B}\boldsymbol{V}_3\boldsymbol{T}_+) = \operatorname{rank}(\boldsymbol{T}_+)$ and $\operatorname{rank}([\boldsymbol{M}^T\boldsymbol{G}_e, \boldsymbol{B}\boldsymbol{V}_3\boldsymbol{T}_+]) = n$.

In fact, if the two claims are right, when $b(\chi) = 0$, we can solve a unique $\boldsymbol{z}(0)$ if $\boldsymbol{H}\boldsymbol{f}_o \in \operatorname{span}\{\boldsymbol{B}\boldsymbol{V}_3\boldsymbol{T}_+\}$. When $b(\chi) > 0$, we can uniquely solve $\boldsymbol{G}_e^T\boldsymbol{f}_e$ and $\boldsymbol{z}(0)$ for arbitrary given $\boldsymbol{f}_o$ and $(\boldsymbol{I}_m - \boldsymbol{G}_e\boldsymbol{G}_e^T)\boldsymbol{f}_e$, since $\boldsymbol{Y}_1^T\boldsymbol{w}_e$ is determined (7) by $\boldsymbol{z}$ and $\boldsymbol{G}_e^T\boldsymbol{G}_e = \boldsymbol{I}_{p_1}$.

We first show $\operatorname{rank}(\boldsymbol{B}\boldsymbol{V}_3\boldsymbol{T}_+) = \operatorname{rank}(\boldsymbol{T}_+)$. Let $\tilde{m} = m - r_1 - p_2$. By (8), we assume $\boldsymbol{T}_+ = \boldsymbol{L}^{-T}\boldsymbol{R}_+$ with $\boldsymbol{L}^{-1}\boldsymbol{A}_{33}\boldsymbol{L}^{-T}\boldsymbol{R}_+ = \boldsymbol{R}_+\boldsymbol{\Lambda}_+$ and $\boldsymbol{R}_+^T\boldsymbol{R}_+ = \boldsymbol{I}_{n_+}$. Due to the block structure of $\boldsymbol{Q}_{33} = \boldsymbol{L}\boldsymbol{L}^T$, we assume $\boldsymbol{L} = \operatorname{diag}(\boldsymbol{L}_e, \boldsymbol{L}_o)$ with $\boldsymbol{L}_e \in \mathbb{R}^{\tilde{m}\times\tilde{m}}$ and $\boldsymbol{L}_o \in \mathbb{R}^{n_+\times n_+}$. Since $\boldsymbol{L}^{-1}\boldsymbol{A}_{33}\boldsymbol{L}^{-T}$ has a block structure, its positive and negative eigenvalues always appear in pair and have a special relation (cf. proof of Lemma 2). So if we write $\boldsymbol{R}_+ = \begin{bmatrix}\boldsymbol{R}_e\\ \boldsymbol{R}_o\end{bmatrix}$ where $\boldsymbol{R}_e \in \mathbb{R}^{\tilde{m}\times n_+}$ and $\boldsymbol{R}_o \in \mathbb{R}^{n_+\times n_+}$, we can assume $\boldsymbol{R}_e^T\boldsymbol{R}_e = \boldsymbol{R}_o^T\boldsymbol{R}_o = \frac{1}{2}\boldsymbol{I}_{n_+}$. Since $\boldsymbol{S} > 0$ and $\operatorname{rank}(\boldsymbol{M}) = n$, we have $\boldsymbol{H} > 0$. Now we have

$$\begin{aligned}\boldsymbol{Z}_3^T\boldsymbol{B}\boldsymbol{V}_3\boldsymbol{T}_+ &= b(\chi)\boldsymbol{Z}_3^T\boldsymbol{M}^T\boldsymbol{Y}_3\boldsymbol{L}_e^{-T}\boldsymbol{R}_e + \boldsymbol{Z}_3^T\boldsymbol{H}\boldsymbol{Z}_3\boldsymbol{L}_o^{-T}\boldsymbol{R}_o\\ &= b(\chi)\boldsymbol{L}_o\boldsymbol{R}_o\boldsymbol{\Lambda}_+ + \boldsymbol{Z}_3^T\boldsymbol{H}\boldsymbol{Z}_3\boldsymbol{L}_o^{-T}\boldsymbol{R}_o.\end{aligned}$$

For any $\boldsymbol{x} \in \mathbb{R}^{n_+}$, since $\boldsymbol{\Lambda}_+ > 0$ and $b(\chi) \geq 0$ when $\chi \in [0,1]$, we have

$$\begin{aligned}\boldsymbol{x}^T\boldsymbol{R}_o^T\boldsymbol{L}_o^{-1}\boldsymbol{Z}_3^T\boldsymbol{B}\boldsymbol{V}_3\boldsymbol{T}_+\boldsymbol{x} &= \frac{1}{2}b(\chi)\boldsymbol{x}^T\boldsymbol{\Lambda}_+\boldsymbol{x} + \boldsymbol{x}^T\boldsymbol{R}_o^T\boldsymbol{L}_o^{-1}\boldsymbol{Z}_3^T\boldsymbol{H}\boldsymbol{Z}_3\boldsymbol{L}_o^{-T}\boldsymbol{R}_o\boldsymbol{x}\\ &\geq \boldsymbol{x}^T\boldsymbol{R}_o^T\boldsymbol{L}_o^{-1}\boldsymbol{Z}_3^T\boldsymbol{H}\boldsymbol{Z}_3\boldsymbol{L}_o^{-T}\boldsymbol{R}_o\boldsymbol{x} \geq 0.\end{aligned} \tag{26}$$

The equality holds if and only if $\boldsymbol{x} = \boldsymbol{0}$ since $\boldsymbol{Z}_3$ is also of full column rank. Hence,

$$n_+ = \operatorname{rank}(\boldsymbol{R}_o^T\boldsymbol{L}_o^{-1}\boldsymbol{Z}_3^T\boldsymbol{B}\boldsymbol{V}_3\boldsymbol{T}_+) \leq \operatorname{rank}(\boldsymbol{B}\boldsymbol{V}_3\boldsymbol{T}_+) \leq n_+ \quad\Rightarrow\quad \operatorname{rank}(\boldsymbol{B}\boldsymbol{V}_3\boldsymbol{T}_+) = n_+.$$

Then we show that $\operatorname{rank}([\boldsymbol{B}\boldsymbol{V}_3\boldsymbol{T}_+, \boldsymbol{M}^T\boldsymbol{G}_e]) = n$. Since $r_2 = 0$ and $\operatorname{rank}(\boldsymbol{M}^T\boldsymbol{G}_e) = p_1$, it's enough to show that

$$\operatorname{span}\{\boldsymbol{B}\boldsymbol{V}_3\boldsymbol{T}_+\} \cap \operatorname{span}\{\boldsymbol{M}^T\boldsymbol{G}_e\} = \{\boldsymbol{0}\}.$$

If $\boldsymbol{x} \in \operatorname{span}\{\boldsymbol{M}^T\boldsymbol{G}_e\} = \operatorname{span}\{\boldsymbol{Z}_2\}$, then we have $\boldsymbol{Z}_3^T\boldsymbol{x} = \boldsymbol{0}$ since $\boldsymbol{Z}_3^T\boldsymbol{Z}_2 = \boldsymbol{0}$. But from (26), if this $\boldsymbol{x}$ also belongs to $\operatorname{span}\{\boldsymbol{B}\boldsymbol{V}_3\boldsymbol{T}_+\}$, then $\boldsymbol{x} = \boldsymbol{0}$. This completes the proof. ☐

Remark 4. *The modification of* (23) *is not unique. From the above proof, we know that for any symmetric positive definite matrix $\boldsymbol{H} \in \mathbb{R}^{n\times n}$, the boundary condition*

$$\boldsymbol{H}(\boldsymbol{w}_o(0) + \boldsymbol{f}_o) = -b(\chi)\boldsymbol{M}^T(\boldsymbol{w}_e(0) + \boldsymbol{f}_e)$$

would satisfy a theorem similarly as Theorem 2. We leave the comparison of different modifications elsewhere. We note that the solvable Maxwell-type boundary condition with an even-odd parity form appears commonly in literature for many other problems [5, 24, 30].

Note that $\boldsymbol{M}$ is invertible when $m = n$. So the new boundary condition (24) *is equivalent to Grad's boundary condition* (23) *when $m = n$. This is also an advantage of the modification.*

4. Applications

4.1. Kramers' Problem. *Kramers' problem* [21] concerns the tangential velocity of a gas flow when passing by an infinite plate, with the only driven force from the tangential stress. For the Shakhov model, when $D = 3$, we can choose the index set $\mathbb{I}$ as

$$\mathbb{I} = \{\boldsymbol{e}_1 + 2\boldsymbol{e}_j + \alpha_2\boldsymbol{e}_2,\ j = 1,3,\ 0 \leq \alpha_2 \leq M-3\} \cup \{\boldsymbol{e}_1 + \alpha_2\boldsymbol{e}_2,\ 0 \leq \alpha_2 \leq M-1\}.$$

This choice gives $p_1 = 1,\ p_2 = 0,\ p = 1$ and $r_1 = 1,\ r_2 = 0,\ r = 1$. By Theorem 1, we can solve $p + r = 2$ variables by (7) and (6):

$$\sigma_{12,K}(y) = 0, \tag{27}$$

$$u_{1,K}(y) = -\sqrt{2}\boldsymbol{w}[\boldsymbol{e}_1 + 2\boldsymbol{e}_2](y). \tag{28}$$

In (24), we suppose the wall is motionless. Let non zero entries of $\boldsymbol{f}_e$ and $\boldsymbol{f}_o$ be $\boldsymbol{f}_e[\boldsymbol{e}_1] = u_{1,B}$ and $\boldsymbol{f}_o[\boldsymbol{e}_1+\boldsymbol{e}_2] = \sigma_{12,B}$, where $\sigma_{12,B}$ is given. Now $\boldsymbol{G}_e^T\boldsymbol{f}_e = \boldsymbol{f}_e[\boldsymbol{e}_1] = u_{1,B}$. By Theorem 2, when $0 < \chi \leq 1$, we can solve constants $\boldsymbol{z} \in \mathbb{R}^{n-1}$ and $c_0 \in \mathbb{R}$ depending on $\sigma_{12,B}$ that

$$u_{1,K}(y) = \boldsymbol{c}_1^T \exp\left(-\boldsymbol{\Lambda}_+^{-1}y\right)\boldsymbol{z}; \qquad u_{1,B} = c_0,$$

where $\boldsymbol{c}_1$ and $\boldsymbol{\Lambda}_+$ are determined by the proof process of Theorem 1.

Remark 5. *Under the above settings, we can formally establish the relationship between the moment system and kinetic equations for Kramers' problem* [32]*. The details can refer to* [14]*.*

Now we define the viscous slip coefficient η as

$$\eta = -\mu u_{1,B}/\sigma_{12,B}, \tag{29}$$

where μ is the viscosity coefficient determined by the collision term. For the Shakhov model with different Pr, the value of μ should be same (cf. [27, 18]). We let $\mu = \sqrt{2}/2$ to follow Siewert's results [32]. Below we use the Shakhov model to refer to the case Pr $= 2/3$ especially. We also consider the normalized velocity profile in the Knudsen layer, i.e., the velocity defect

$$u_d(y) = \mu u_{1,K}(y)/\sigma_{12,B}. \tag{30}$$

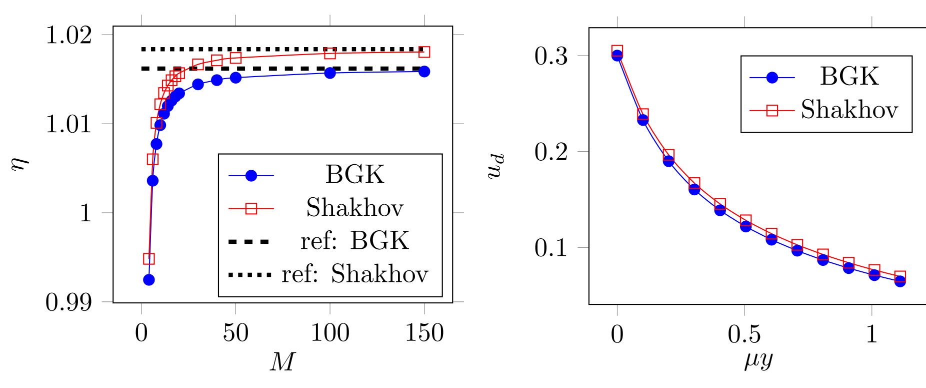

Figure 1. *Left*: Slip coefficients of different even M for various models when $\chi = 1$. *Right*: The normalized velocity profile when $\chi = 1$ and $M = 80$.

Fig.1 exhibits the viscous slip coefficient and the normalized velocity profile calculated by our method when $\chi = 1$ and M is an even number. The reference values are $\eta_{BGK} = 1.01619$ and $\eta_{Sh} = 1.01837$ (cf. [32, 18]). From Fig.1, we see a converging trend when M increases, and the relative error compared with the reference value would be lower than 1% when $M > 10$. We also find that the Shakhov model has a Knudsen layer thicker than the BGK model.

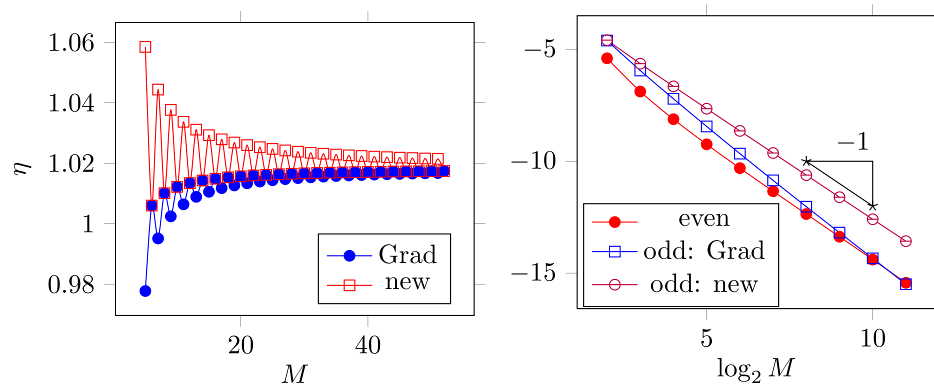

FIGURE 2. *Left*: Slip coefficients η for the BGK model when M ranges from 5 to 52. *Right*: Log-log error diagram of the slip coefficients for the BGK model. y axis: a_k or b_k. ($\chi = 1$).

In Kramers' problem, we have $m = n$ when M is an even number. So as shown in Remark 4, the new boundary condition (24) is equivalent to Grad's boundary condition (23) when M is even. Fig.2 compares the slip coefficients obtained by different boundary conditions for the BGK model. Denoting by η_M the slip coefficient for a given M, we calculate $a_{k-1} = \log_2 |\eta_{BGK} - \eta_{2^k}|$ and $b_{k-1} = \log_2 |\eta_{BGK} - \eta_{2^k+1}|$ for $k = 2, 3, .., 11$. From Fig.2, we see that when M is an odd number, the new boundary condition (24) brings a totally different picture as in the even case. Regardless of the choices, we always observe the first-order convergence of η_M when M increases. The convergence rate may be affected by the discontinuity of the velocity distribution function at the wall.

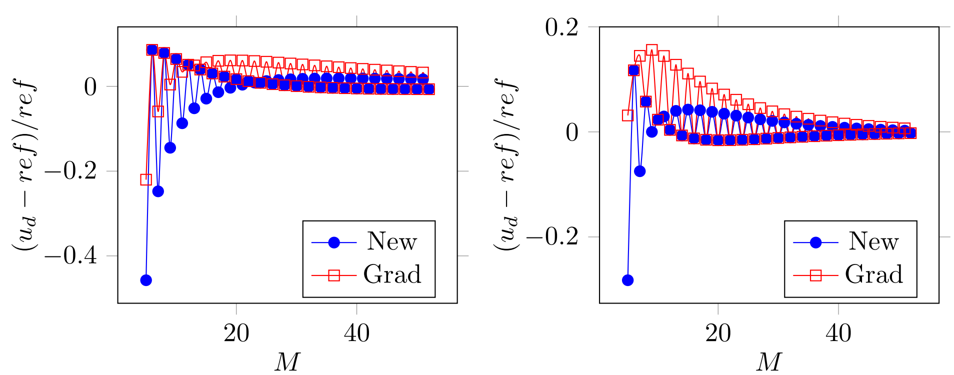

FIGURE 3. Relative errors of the velocity defect for the BGK model when $\chi = 0.1$ and M ranges from 5 to 52. *Left*: At $\mu y = 0.5$. *Right*: At $\mu y = 1.0$.

From Fig.2, we may conclude that the new boundary condition gives a relatively large error in the slip coefficient, compared to the Grad's one when M is odd. But we find that it also gives a better approximation to the velocity defect $u_d(y)$ when y is away from zero. This is shown in Fig.3, where the relative errors of $u_d(y)$ at

$y = 0.5\mu^{-1}$ and $y = \mu^{-1}$ are calculated for the BGK model with different M when $\chi = 0.1$. The reference values are from [32].

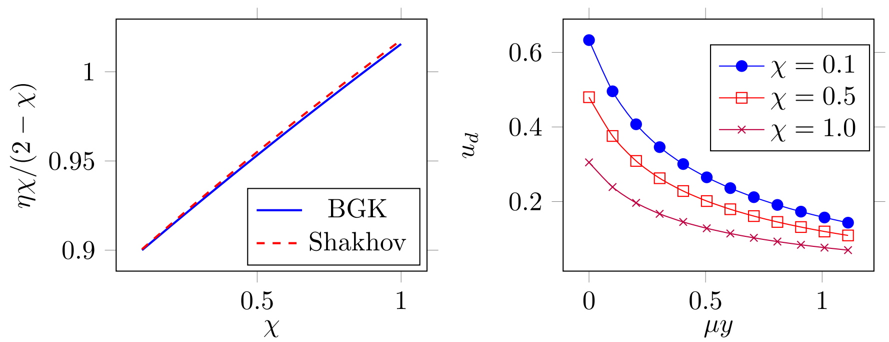

FIGURE 4. *Left*: $\eta\chi/(2-\chi)$. *Right*: Velocity profile of the Shakhov model when χ varies. ($M = 80$).

Fig.4 shows the velocity profile and slip coefficient when the accommodation coefficient χ varies and $M = 80$. We see that η goes larger and the Knudsen layer becomes thicker when χ goes smaller. This observation coincides with the classical qualitative results.

4.2. Thermal Slip Problem. We consider the tangential velocity of the flow caused by a temperature gradient in a direction parallel to the wall, which is called [38] the *thermal slip problem*. For the Shakhov model, when $D = 3$, we choose the same $\mathbb{I}$ as in Kramers' problem:

$$\mathbb{I} = \{\boldsymbol{e}_1 + 2\boldsymbol{e}_j + \alpha_2\boldsymbol{e}_2,\ j = 1, 3,\ 0 \le \alpha_2 \le M - 3\} \cup \{\boldsymbol{e}_1 + \alpha_2\boldsymbol{e}_2,\ 0 \le \alpha_2 \le M - 1\}.$$

The difference lies in the boundary condition (24). We let $\boldsymbol{f}_o$ be zero and non zero entries of $\boldsymbol{f}_e$ be $\boldsymbol{f}_e[\boldsymbol{e}_1] = u_{1,B},\ \boldsymbol{f}_e[3\boldsymbol{e}_1] = \sqrt{3}q_{1,B}$, and $\boldsymbol{f}_e[\boldsymbol{e}_1 + 2\boldsymbol{e}_i] = q_{1,B},\ i \ne 1$, where $q_{1,B}$ is a given constant. By Theorem 2, when $0 < \chi \le 1$, we can solve constants $\boldsymbol{z} \in \mathbb{R}^{n-1}$ and $c_0 \in \mathbb{R}$ depending on $q_{1,B}$ that

$$u_{1,K}(y) = \boldsymbol{c}_1^T \exp\left(-\boldsymbol{\Lambda}_+^{-1} y\right) \boldsymbol{z}, \qquad u_{1,B} = c_0,$$

where $\boldsymbol{c}_1$ and $\boldsymbol{\Lambda}_+$ are determined by the proof process of Theorem 1.

Then we can define the thermal slip coefficient as

$$\eta_t = -\frac{1}{2}\lambda u_{1,B}/q_{1,B}, \tag{31}$$

where λ is the thermal conductivity coefficient determined by the collision term. To agree with [33]'s results about kinetic equations, we let $\lambda = \mathrm{Pr}^{-1}\sqrt{2}/2$ and represent the value of $\mathrm{Pr}\,\eta_t$.

Table.1 compares our results with [33], where the letter S means the Shakhov model with $\mathrm{Pr} = 2/3$. We see that our method already gives high accuracy results when $M = 12$. Fig.5 shows the converging trend when M goes to infinity with $\chi = 1$. We can see the influence of different boundary conditions again from Fig.5.

TABLE 1. The thermal slip coefficient $\mathrm{Pr}\,\eta_t$ compared with [33].

χ	BGK-[33]	S-[33]	BGK$-M=12$	S$-M=12$	BGK$-M=84$	S$-M=84$
0.1	0.264178	0.266064	0.263578	0.265470	0.264101	0.265989
0.2	0.278151	0.281655	0.277030	0.280570	0.278009	0.281521
0.3	0.291924	0.296794	0.290360	0.295311	0.291728	0.296615
0.4	0.305502	0.311501	0.303568	0.309703	0.305263	0.311287
0.5	0.318891	0.325791	0.316657	0.323758	0.318619	0.325554
0.6	0.332095	0.339683	0.329630	0.337485	0.331799	0.339431
0.7	0.345120	0.353193	0.342487	0.350894	0.344808	0.352935
0.8	0.357969	0.366335	0.355231	0.363994	0.357650	0.366077
0.9	0.370648	0.379125	0.367863	0.376794	0.370328	0.378873
1.0	0.383161	0.391575	0.380287	0.389303	0.382847	0.391335

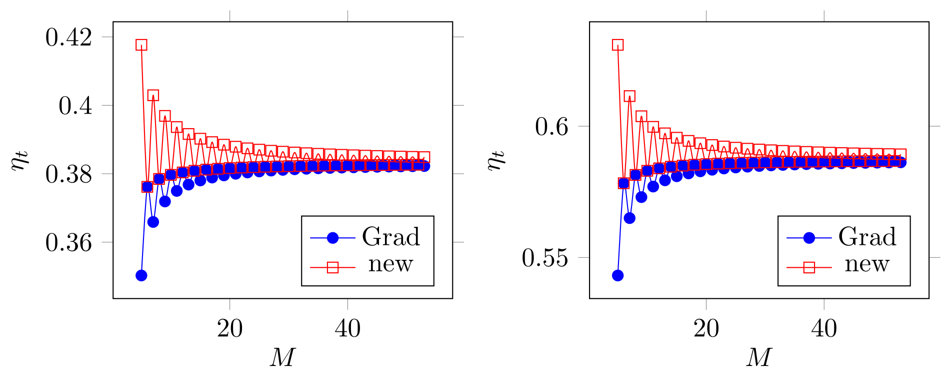

FIGURE 5. The thermal slip coefficient when M range from 5 to 53 and $\chi = 1$. *Left*: The BGK model. *Right*: The Shakhov model with $\mathrm{Pr} = 2/3$.

4.3. Temperature Jump Problem. The *temperature jump problem* [37] concerns the gas temperature near the wall when the flow passes over an infinite plate, with the only driven force from a normal temperature gradient. For the Shakhov model, when $D = 3$, the index set could be

$$\mathbb{I} = \{2\boldsymbol{e}_j + \alpha_2\boldsymbol{e}_2,\ j = 1, 3,\ 0 \le \alpha_2 \le M-2\} \cup \{\alpha_2\boldsymbol{e}_2,\ 0 \le \alpha_2 \le M\}, \tag{32}$$

which gives $p_1 = 2,\ p_2 = 1$ and $r_1 = 1,\ r_2 = 0$. Three variables are solved by (6):

$$u_{2,K}(y) = 0, \tag{33}$$

$$\rho_K(y) + \sqrt{2}\boldsymbol{w}[2\boldsymbol{e}_2](y) = 0, \tag{34}$$

$$5q_{2,K}(y) := \sqrt{3}\boldsymbol{w}[3\boldsymbol{e}_2] + \boldsymbol{w}[\boldsymbol{e}_2 + 2\boldsymbol{e}_1] + \boldsymbol{w}[\boldsymbol{e}_2 + 2\boldsymbol{e}_3] = 0. \tag{35}$$

One variable $\sqrt{2}\rho_K(y) - \sum_i \boldsymbol{w}[2\boldsymbol{e}_i](y)$ is solved by (7), where $\sqrt{2}\sum_i \boldsymbol{w}[2\boldsymbol{e}_i] = 3\theta_K$ according to (16). In (24), we suppose the wall temperature do not change. We let $\boldsymbol{f}_e = \boldsymbol{G}_e\boldsymbol{G}_e^T\boldsymbol{f}_e$ in (25) with $\boldsymbol{f}_e[2\boldsymbol{e}_i] = \theta_B/\sqrt{2}$. Then we let non zero entries of $\boldsymbol{f}_o$ be $\boldsymbol{f}_o[\boldsymbol{e}_2 + 2\boldsymbol{e}_i] = q_{2,B},\ i \ne 2$, and $\boldsymbol{f}_o[3\boldsymbol{e}_2] = \sqrt{3}q_{2,B}$, where $q_{2,B}$ is given. By Theorem 2, when $0 < \chi \le 1$, we can solve $\boldsymbol{z} \in \mathbb{R}^{n-2}$ and $c_1 \in \mathbb{R}$ depending on $q_{2,B}$ that

$$\theta_K(y) = \boldsymbol{c}_1^T \exp\left(-\boldsymbol{\Lambda}_+^{-1} y\right)\boldsymbol{z}, \qquad \theta_B = c_1,$$

where $\boldsymbol{c}_1$ and $\boldsymbol{\Lambda}_+$ can be determined by the proof process of Theorem 1.

Analogously, we define the temperature jump coefficient ζ as

$$\zeta = -\frac{1}{\sqrt{2}}\lambda\theta_B/q_{2,B}, \tag{36}$$

where λ is the thermal conductivity coefficient determined by the collision term. Due to the conversion rule [18], we let $\lambda = \mathrm{Pr}^{-1}\sqrt{2}/2$. Under the choice of (32), Knudsen layer equations (17) in the Shakhov case are the same as in the BGK case. Thus, we immediately have

$$\zeta(\mathrm{Pr}) = \mathrm{Pr}^{-1}\zeta(1), \tag{37}$$

where ζ is viewed as a function of Pr in the Shakhov case. This result coincides with [18] and leads us to only consider the jump coefficient in the BGK case. The normalized temperature profile in the Knudsen layer, or called the temperature defect, is defined as

$$\theta_d(y) = \frac{\lambda}{\sqrt{2}}\theta_K(y)/q_{2,B}. \tag{38}$$

Now $m = n$ when M is an odd number, where the boundary condition (24) is equivalent to Grad's (23). So we first consider the odd case. Table.2 compares our results of the jump coefficient with the kinetic results [4]. We see that the jump coefficient goes larger when χ goes smaller. Our solutions seem to agree with reference solutions well with not too many moments. In fact, when $M = 13$, the relative error is less than 1% in most cases.

Table 2. The temperature jump coefficient compared with Barichello and Siewert's results [4].

χ	[4]	$M=3$	$M=5$	$M=7$	$M=9$	$M=11$	$M=13$
0.1	21.4501	21.0856	21.3565	21.3957	21.4119	21.4208	21.4263
0.3	6.63051	6.31159	6.55416	6.58698	6.60028	6.60742	6.61185
0.5	3.62913	3.35382	3.56804	3.59507	3.60574	3.61139	3.61487
0.6	2.86762	2.61342	2.81345	2.83779	2.84726	2.85224	2.85529
0.7	2.31753	2.08401	2.26984	2.29162	2.29997	2.30432	2.30698
0.9	1.57036	1.37681	1.53420	1.55126	1.55758	1.56081	1.56276
1.0	1.30272	1.12868	1.27183	1.28673	1.29213	1.29488	1.29652

Fig.6 presents the results of different boundary conditions, where the reference solution is from [4]. From the left picture, we again see that when M is an even number, the jump coefficient corresponding to the new boundary condition displays a decreasing converging trend. From the right picture, we see that despite a relatively larger gap at $y = 0$, the temperature defect of the new boundary condition approaches faster to the reference solution than in the Grad's case.

4.4. Remarks. We remark three points which are observed from the numerical results:

(1) We may only need a moderate number of moments, e.g., $10 < M < 20$, to depict the Knudsen layer quite accurately. This empirical choice of M may benefit the practical usage.

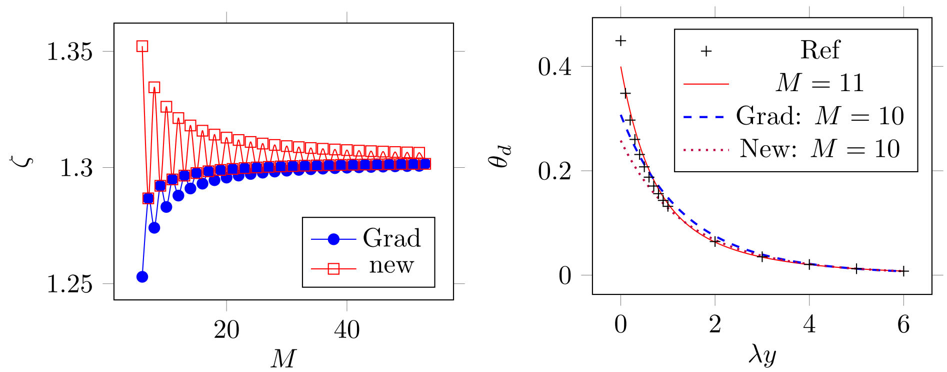

FIGURE 6. *Left*:The temperature jump coefficient ζ when M ranges from 6 to 53. *Right*: The temperature defect $\theta_d(y)$ for different boundary conditions. $(\chi = 1)$.

(2) If $m > n$, the different boundary conditions would affect the results. When y is near zero, the new boundary conditions may provide relatively greater errors about the slip/jump coefficients or the profile of Knudsen layer solutions. When y goes far away from zero, the new boundary condition provides a better approximation, as shown in Fig. 3 and Fig. 6 with $y > 1$.
(3) There is always a converging trend when M goes to infinity. A possible analysis of the convergence and accuracy is beyond the scope of this paper.

5. Conclusions

We imposed a type of Maxwell boundary conditions on the linear half-space moment systems. The proposed boundary condition is derived from the classical diffuse-specular model and proved to satisfy some well-posedness criteria of half-space boundary value problems. The procedure has been applied to flow problems with the Shakhov collision term. In this way, the model with new boundary condition was validated that it can capture viscous and thermal Knudsen layers well with only a few moments. It is straightforward to apply our model to other Knudsen layer problems with various collision terms.

Acknowledgment

This work is financially supported by the National Key R&D Program of China, Project Number 2020YFA0712000. We thank Dr.Jun Li and Dr.Yizhou Zhou for their enthusiastic discussions with us.

References

[1] K. Aoki, C. Baranger, M. Hattori, S. Kosuge, G. Martalò, M. Julien, and L. Mieussens. Slip boundary conditions for the compressible Navier-Stokes equations. J. Stat. Phys., 169:744–781, 2017.
[2] A. Arnold and U. Giering. An analysis of the Marshak conditions for matching Boltzmann and Euler equations. Math. Models Methods Appl. Sci., 07(04):557–577, 1997.
[3] C. Bardos, F. Golse, and Y. Sone. Half-space problems for the Boltzmann equation: A survey. J. Stat. Phys., 124:275–300, 2006.
[4] L. Barichello and C. Siewert. The temperature-jump problem in rarefied-gas dynamics. Eur. J. Appl. Math., 11(4):353–364, 2000.

[5] N. Bernhoff. On half-space problems for the discrete Boltzmann equation. Il Nuovo Cimento C, 33(1):47–54, 2010.
[6] P. Bhatnagar, E. Gross, and M. Krook. A model for collision processes in gases. I. small amplitude processes in charged and neutral one-component systems. Phys. Rev., 94(3):511–525, 1954.
[7] G. Bird. Molecular Gas Dynamics and the Direct Simulation of Gas Flows. Oxford: Clarendon Press, 1994.
[8] J. Broadwell. Study of rarefied shear flow by the discrete velocity method. J. Fluid Mech., 19(3):401–414, 1964.
[9] Z. Cai, Y. Fan, and R. Li. Globally hyperbolic regularization of Grad's moment system. Comm. Pure Appl. Math., 67(3):464–518, 2014.
[10] Z. Cai, Y. Fan, and R. Li. A framework on moment model reduction for kinetic equation. SIAM J. Appl. Math., 75(5):2001–2023, 2015.
[11] Z. Cai, R. Li, and Z. Qiao. NRxx simulation of microflows with Shakhov model. SIAM J. Sci. Comput., 34(1):339–369, 2011.
[12] C. Cercignani. Mathematical Methods in Kinetic Theory. Springer US, New York, 1969.
[13] H. Chen, Q. Li, and J. Lu. A numerical method for coupling the BGK model and Euler equations through the linearized Knudsen layer. J. Comput. Phys., 398:108893, 2019.
[14] Y. Fan, J. Li, R. Li, and Z. Qiao. Resolving Knudsen layer by high order moment expansion. Contin. Mech. Thermodyn., 31(5):1313–1337, 2019.
[15] H. Grad. Note on N-dimensional Hermite polynomials. Comm. Pure Appl. Math., 2(4):325–330, 1949.
[16] H. Grad. On the kinetic theory of rarefied gases. Comm. Pure Appl. Math., 2(4):331–407, 1949.
[17] X. Gu and D. Emerson. Linearized-moment analysis of the temperature jump and temperature defect in the Knudsen layer of a rarefied gas. Phys. Rev. E, 89(6):063020, 2014.
[18] M. Hattori and S. Takata. Slip/jump coefficients and Knudsen-layer corrections for the Shakhov model occurring in the generalized slip-flow theory. AIP Conference Proceedings, 2132(1):130012, 2019.
[19] D. Hilditch. An introduction to well-posedness and free-evolution. Int. J. Mod. Phys. A, 28(22n23):1340015, 2013.
[20] Z. Hu and G. Hu. An efficient steady-state solver for microflows with high-order moment model. J. Comput. Phys., 392:462–482, 2019.
[21] H. Kramers. On the behaviour of a gas near a wall. Il Nuovo Cimento (1943-1954), 6(2):297–304, 1949.
[22] P. Lax and R. Phillips. Local boundary conditions for dissipative symmetric linear differential operators. Comm. Pure Appl. Math., 13(3):427–455, 1960.
[23] Q. Li, J. Lu, and W. Sun. A convergent method for linear half-space kinetic equations. ESAIM: Math. Model. Numer. Anal., 51(5):1583–1615, 2017.
[24] Q. Li, J. Lu, and W. Sun. Half-space kinetic equations with general boundary conditions. Math. Comput., 86(305):1269–1301, 2017.
[25] C. Lilley and J. Sader. Velocity gradient singularity and structure of the velocity profile in the Knudsen layer according to the Boltzmann equation. Phys. Rev. E, 76:026315, 2007.
[26] S. Loyalka. Temperature jump and thermal creep slip: Rigid sphere gas. Phys. Fluids A, 1(2):403–408, 1989.
[27] S. Loyalka and K. Hickey. The Kramers problem: Velocity slip and defect for a hard sphere gas with arbitrary accommodation. Z. Angew. Math. Phys., 41:245–253, 1990.
[28] A. Rana, M. Torrilhon, and H. Struchtrup. A robust numerical method for the R13 equations of rarefied gas dynamics: Application to lid driven cavity. J. Comput. Phys., 236(1):169–186, 2013.
[29] J. Rauch. Symmetric positive systems with boundary characteristic of constant multiplicity. Trans. Amer. Math. Soc., 291(1):167–187, 1985.
[30] N. Sarna and M. Torrilhon. On stable wall boundary conditions for the Hermite discretization of the linearised Boltzmann equation. J. Stat. Phys., 170:101–126, 2018.
[31] E. Shakhov. Generalization of the Krook kinetic relaxation equation. Fluid Dyn., 3(5):95–96, 1968.
[32] C. Siewert. Kramers' problem for a variable collision frequency model. Eur. J. Appl. Math., 12(2):179–191, 2001.

[33] C. Siewert and F. Sharipov. Model equations in rarefied gas dynamics: Viscous-slip and thermal-slip coefficients. Phys. Fluids, 14(12):4123–4129, 2002.
[34] H. Struchtrup. Linear kinetic heat transfer: Moment equations, boundary conditions, and Knudsen layers. Physica A, 387(8-9):1750–1766, 2008.
[35] M. Torrilhon. Special issues on moment methods in kinetic gas theory. Contin. Mech. Thermodyn., 21(5):341–343, 2009.
[36] Y. Wang and Z. Cai. Approximation of the Boltzmann collision operator based on Hermite spectral method. J. Comput. Phys., 397:108815, 2019.
[37] P. Welander. On the temperature jump in a rarefied gas. Ark. Fys., 7(7):507, 1954.
[38] M. Williams. A review of the rarefied gas dynamics theory associated with some classical problems in flow and heat transfer. Z. Angew. Math. Phys., 52(3):500–516, 2001.
[39] W. Yang, X. Gu, D. Emerson, Y. Zhang, and S. Tang. Modelling thermally induced non-equilibrium gas flows by coupling kinetic and extended thermodynamic methods. Entropy, 21(8):816, 2019.
[40] W. Yong. Boundary stabilization of hyperbolic balance laws with characteristic boundaries. Automatica, 101:252–257, 2019.

Appendix A. Proofs of Lemmas

Proof of Lemma 1.

Proof. Since $\boldsymbol{Q}\boldsymbol{G} = \boldsymbol{0}$ and $\text{Null}(\boldsymbol{A}) \cap \text{Null}(\boldsymbol{Q}) = \{\boldsymbol{0}\}$, we have $\text{rank}(\boldsymbol{A}\boldsymbol{G}) = \text{rank}(\boldsymbol{G}) = p$. Thus $\boldsymbol{V}_2$ can be constructed by a Gram-Schmidt orthogonalization of $\boldsymbol{A}\boldsymbol{G}$. By definition,

$$(\boldsymbol{A}\boldsymbol{G})^T\boldsymbol{V}_1 = (\boldsymbol{A}\boldsymbol{G})^T\boldsymbol{G}\boldsymbol{X} = \boldsymbol{0} \quad \Rightarrow \quad \boldsymbol{V}_2^T\boldsymbol{V}_1 = \boldsymbol{0}.$$

Hence $[\boldsymbol{V}_1, \boldsymbol{V}_2] \in \mathbb{R}^{(m+n)\times(p+r)}$ is column orthogonal and there must be $m + n \geq p + r$. Then $\boldsymbol{V}_3 \in \mathbb{R}^{(m+n)\times(m+n-p-r)}$ can be chosen as an orthogonal complement of $[\boldsymbol{V}_1, \boldsymbol{V}_2]$.

Now we show that $\boldsymbol{U} = [\boldsymbol{U}_1, \boldsymbol{U}_2, \boldsymbol{V}_3]$ is invertible, where $\boldsymbol{U}_1 = \boldsymbol{G}$, $\boldsymbol{U}_2 = \boldsymbol{A}\boldsymbol{G}\boldsymbol{X}$. Since $\boldsymbol{V}_3^T\boldsymbol{V}_2 = \boldsymbol{0}$, we have $\boldsymbol{V}_3^T\boldsymbol{U}_2 = \boldsymbol{0}$. To make $\boldsymbol{U}$ invertible, it's enough to show that

$$\text{span}\{\boldsymbol{V}_3\} \cap \text{span}\{\boldsymbol{G}\} = \{\boldsymbol{0}\}. \tag{39}$$

In fact, if $\boldsymbol{G}\boldsymbol{c}_1 = \boldsymbol{V}_3\boldsymbol{c}_2$ for some $\boldsymbol{c}_1 \in \mathbb{R}^p$ and $\boldsymbol{c}_2 \in \mathbb{R}^{(m+n-p-r)}$, then $(\boldsymbol{G}\boldsymbol{c}_1)^T\boldsymbol{A}\boldsymbol{G} = \boldsymbol{0}$ since $\boldsymbol{V}_3^T\boldsymbol{V}_2 = \boldsymbol{0}$. So $\boldsymbol{c}_1 \in \text{span}\{\boldsymbol{X}\}$ and $\boldsymbol{V}_3\boldsymbol{c}_2 \in \text{span}\{\boldsymbol{G}\boldsymbol{X}\} = \text{span}\{\boldsymbol{V}_1\}$. Thus, from $\boldsymbol{V}_3^T\boldsymbol{V}_1 = \boldsymbol{0}$ we have $\boldsymbol{c}_2 = \boldsymbol{0}$, which implies (39).

Finally, we have $\text{rank}(\boldsymbol{U}_2^T\boldsymbol{A}\boldsymbol{V}_1) = \text{rank}(\boldsymbol{U}_2^T\boldsymbol{U}_2) = r$. Meanwhile, $\boldsymbol{V}_3^T\boldsymbol{A}\boldsymbol{V}_1 = \boldsymbol{V}_3^T\boldsymbol{U}_2 = \boldsymbol{0}$. Since $\text{span}\{\boldsymbol{V}_3\}\cap\text{span}\{\boldsymbol{G}\} = \{\boldsymbol{0}\}$ from (39), we have $\boldsymbol{V}_3^T\boldsymbol{Q}\boldsymbol{V}_3 > 0$. ☐

Proof of Lemma 3.

Proof. Suppose $\boldsymbol{Y}_3^T\boldsymbol{M}\boldsymbol{Z}_3\boldsymbol{x} = \boldsymbol{0}$ for some $\boldsymbol{x} \in \mathbb{R}^{n-r_2-p_1}$. Since $[\boldsymbol{Y}_1, \boldsymbol{Y}_2, \boldsymbol{Y}_3]$ is orthogonal, there exists $\boldsymbol{x}_1$ and $\boldsymbol{x}_2$ such that

$$\boldsymbol{M}\boldsymbol{Z}_3\boldsymbol{x} = \boldsymbol{Y}_1\boldsymbol{x}_1 + \boldsymbol{Y}_2\boldsymbol{x}_2, \quad \boldsymbol{x}_1 \in \mathbb{R}^{r_1},\ \boldsymbol{x}_2 \in \mathbb{R}^{p_2}. \tag{40}$$

Since $\boldsymbol{Z}_3^T\boldsymbol{M}^T\boldsymbol{Y}_1 = \boldsymbol{0}$ and $\boldsymbol{Y}_2^T\boldsymbol{Y}_1 = \boldsymbol{0}$, we have $\boldsymbol{x}_1 = \boldsymbol{0}$. Note that the result (39) implies $\text{span}\{\boldsymbol{Z}_3\} \cap \text{span}\{\boldsymbol{G}_o\} = \{\boldsymbol{0}\}$ and $\text{span}\{\boldsymbol{Y}_2\} = \text{span}\{\boldsymbol{M}\boldsymbol{G}_o\}$. Then since $\boldsymbol{M}$ and $\boldsymbol{Z}_3$ are of full column rank, there must be $\boldsymbol{x} = \boldsymbol{0}$. So $\boldsymbol{Y}_3^T\boldsymbol{M}\boldsymbol{Z}_3$ is of full column rank. ☐

Proof of Lemma 4.

Proof. According to the description before Lemma 4, we only need to show that $\mathrm{rank}(\boldsymbol{M}) = n$. If not, there must be not all zero coefficients $r_{\boldsymbol{\beta}}$, $\boldsymbol{\beta} \in \mathbb{I}_o$, s.t.

$$\left\langle \xi_2 \omega \sum_{\boldsymbol{\beta}\in\mathbb{I}_o} r_{\boldsymbol{\beta}} \phi_{\boldsymbol{\beta}},\ \phi_{\boldsymbol{\alpha}} \right\rangle = 0, \quad \forall \boldsymbol{\alpha} \in \mathbb{I}_e.$$

However, for any $\boldsymbol{\gamma} \in \mathbb{I}_e$ with $\gamma_2 = 0$, $\boldsymbol{M}[\boldsymbol{\gamma}, \boldsymbol{\beta}] \neq 0$ if and only if $\boldsymbol{\beta} = \boldsymbol{\gamma} + \boldsymbol{e}_2$. So $r_{\boldsymbol{\gamma}+\boldsymbol{e}_2} = 0$ from the above relations. By induction we have $r_{\boldsymbol{\gamma}+\beta_2\boldsymbol{e}_2} = 0$, $1 \le \beta_2 \le M - |\boldsymbol{\gamma}|$, β_2 odd. Because of (**C1**), any $\boldsymbol{\beta} \in \mathbb{I}_o$ can be represented in the above form $\boldsymbol{\gamma} + \beta_2\boldsymbol{e}_2$ and consequently, $r_{\boldsymbol{\beta}} = 0$, $\forall \boldsymbol{\beta} \in \mathbb{I}_o$. This contradiction shows that $\boldsymbol{M}$ must have a full column rank of n.

It's classical for the linearized Boltzmann operator (cf. [12, Chapter III]) that $\boldsymbol{Q} \ge 0$. It's also shown that $\langle \mathcal{L}[\omega\phi_{\boldsymbol{\beta}}]\phi_{\boldsymbol{\alpha}} \rangle = 0$, $\boldsymbol{\alpha} \in \mathbb{I}_e, \boldsymbol{\beta} \in \mathbb{I}_o$. So $\boldsymbol{Q}$ has a block diagonal structure.

Note that $\mathrm{Null}(\boldsymbol{Q})$ always has a constant dimension because of properties of the linearized Boltzmann operator. So direct calculations show $\mathrm{Null}(\boldsymbol{A}) \cap \mathrm{Null}(\boldsymbol{Q}) = \{\boldsymbol{0}\}$. When $\boldsymbol{J}$ is replaced by $\boldsymbol{J}_{Sh}$ in (15), direct calculation also shows the lemma right. □

Proof of Lemma 5.

Proof. By definition, $\boldsymbol{S}$ is symmetric. For any $\boldsymbol{z} \in \mathbb{R}^m$, denote by

$$f(\boldsymbol{\xi}) = \sum_{\boldsymbol{\alpha}\in\mathbb{I}_e} \boldsymbol{z}[\boldsymbol{\alpha}]\phi_{\boldsymbol{\alpha}}(\boldsymbol{\xi}),$$

then we have $\boldsymbol{z}^T\boldsymbol{S}\boldsymbol{z} = \dfrac{\sqrt{2\pi}}{2}\left\langle |\xi_2|\omega f^2 \right\rangle \ge 0$. If $\boldsymbol{z}^T\boldsymbol{S}\boldsymbol{z} = 0$, there must be $f = 0$. Due to the orthogonality, $f = 0$ means $\boldsymbol{z} = \boldsymbol{0}$. Hence, $\boldsymbol{S}$ is symmetric positive definite. □

Appendix B. Derivation of the Knudsen layer equations (12)

The system (12) can be derived in several ways. We put one method to derive it in the Appendix for completeness. With notations in Definition 3.2, we consider the linearized Boltzmann equation

$$\frac{\partial f}{\partial t} + \sum_{d=1}^{D} \xi_d \frac{\partial f}{\partial x_d} = \mathcal{L}[f].$$

Choose an integer $M \ge 3$ and test the above equation with the orthonormal Hermite polynomials $\phi_{\boldsymbol{\alpha}}$, $|\boldsymbol{\alpha}| \le M$, then we have an unclosed moment system

$$\frac{\partial \langle f\phi_{\boldsymbol{\alpha}} \rangle}{\partial t} + \sum_{d=1}^{D} \frac{\partial \langle \xi_d f \phi_{\boldsymbol{\alpha}} \rangle}{\partial x_d} = \langle \mathcal{L}[f]\phi_{\boldsymbol{\alpha}} \rangle.$$

Assume $\boldsymbol{f} \in \mathbb{R}^N$ with $N = \#\{\boldsymbol{\alpha} \in \mathbb{N}^D, |\boldsymbol{\alpha}| \le M\}$ and $\boldsymbol{f}[\boldsymbol{\alpha}] = \langle f\phi_{\boldsymbol{\alpha}} \rangle$. Grad's ansatz assumes $f = \omega \sum_{|\boldsymbol{\alpha}|\le M} \boldsymbol{f}[\boldsymbol{\alpha}]\phi_{\boldsymbol{\alpha}}$, which would close the above moment system, as

$$\frac{\partial \boldsymbol{f}}{\partial t} + \sum_{d=1}^{D} \boldsymbol{A}_d \frac{\partial \boldsymbol{f}}{\partial x_d} = -\boldsymbol{J}\boldsymbol{f},$$

where $\boldsymbol{A}_d$ is analogous to $\boldsymbol{A}_2$ in (13) and $\boldsymbol{J}$ is defined in (14). After some careful definition, macroscopic variables can be related to $\boldsymbol{f}$ by similar formulas like (16).

Putting aside the detailed boundary condition, we make some Knudsen layer assumptions. Due to the rotation invariance, we consider the plane-boundary lying at $\{\boldsymbol{x} \in \mathbb{R}^D : x_2 = 0\}$, introducing $\boldsymbol{x}^w = (x_1, x_3, ..., x_D)$ and rewriting variables in the local coordinates, i.e. $\boldsymbol{f}(t, \boldsymbol{x}) = \boldsymbol{f}(t, \boldsymbol{x}^w; x_2)$. Assume ε is a small parameter representing the Knudsen number, then a typical Knudsen layer ansatz could be

$$\begin{aligned} \boldsymbol{f}(t, \boldsymbol{x}) = \boldsymbol{f}_B(t, \boldsymbol{x}^w; x_2) + \varepsilon \boldsymbol{f}_K(t, \boldsymbol{x}^w; y); \\ \boldsymbol{f}_K(t, \boldsymbol{x}^w; +\infty) = 0; \quad y = x_2/\varepsilon, \end{aligned} \tag{41}$$

where $\boldsymbol{f}_B$ and $\boldsymbol{f}_K$ represent the bulk and Knudsen layer solutions respectively with $\boldsymbol{f}_K = O(\boldsymbol{f}_B)$. Formally expand all variables into series on ε, with $h^{(j)}$ representing the j-th order term of h, e.g.

$$\boldsymbol{f}_B = \boldsymbol{f}_B^{(0)} + \varepsilon \boldsymbol{f}_B^{(1)} + o(\varepsilon \boldsymbol{f}_B), \quad \boldsymbol{f}_K = \boldsymbol{f}_K^{(0)} + o(\boldsymbol{f}_K). \tag{42}$$

Assume that there are no initial layers and variations of $\boldsymbol{f}_B$ are of the same order of $\boldsymbol{f}_B$, while variations of $\boldsymbol{f}_K$ are relatively large in the direction normal to the boundary, i.e.

$$\frac{\partial \boldsymbol{f}_K}{\partial s} = O(\boldsymbol{f}_K),\ s = t, x_d,\ d \neq 2; \quad \frac{\partial \boldsymbol{f}_K}{\partial y} = \frac{\partial \boldsymbol{f}_K}{\partial x_2}\varepsilon = O(\boldsymbol{f}_K); \quad \text{when } y = O(1).$$

Substitute the ansatz into the moment system and match the order of ε, then we would get equations about $\boldsymbol{f}_K^{(0)}$. If we omit the arguments t and $\boldsymbol{x}^w$, rewriting $\boldsymbol{f}_K^{(0)}(t, \boldsymbol{x}^w; y)$ as $\boldsymbol{h}(y)$, then we obtain the Knudsen layer equations (12).

Appendix C. Derivation of the boundary condition (21)

First we make an ansatz that $f = \sum_{|\boldsymbol{\alpha}| \le M} \omega f_{\boldsymbol{\alpha}} \phi_{\boldsymbol{\alpha}}$ and $\mathcal{M}^w = \sum_{|\boldsymbol{\alpha}| \le M} \omega m_{\boldsymbol{\alpha}} \phi_{\boldsymbol{\alpha}}$, where the coefficients

$$f_{\boldsymbol{\alpha}} = \langle f \phi_{\boldsymbol{\alpha}} \rangle, \quad m_{\boldsymbol{\alpha}} = \langle \mathcal{M}^w \phi_{\boldsymbol{\alpha}} \rangle.$$

Note that we assume the outward normal vector $\boldsymbol{n} = (0, -1, 0, .., 0)$ and $\boldsymbol{u}^w \cdot \boldsymbol{n} = 0$. So $\boldsymbol{\xi}^* = (\xi_1, -\xi_2, \xi_3, .., \xi_D)$ and we test the kinetic boundary condition (19) with $\xi_2 \phi_{\boldsymbol{\alpha}}(\boldsymbol{\xi})$ to have

$$\langle \xi_2 \phi_{\boldsymbol{\alpha}} f \rangle = \langle I_{\xi_2 > 0} \xi_2 \phi_{\boldsymbol{\alpha}} f \rangle + \chi \langle I_{\xi_2 < 0} \xi_2 \phi_{\boldsymbol{\alpha}} \mathcal{M}^w \rangle + (1 - \chi) \langle I_{\xi_2 < 0} \xi_2 \phi_{\boldsymbol{\alpha}} f(\boldsymbol{\xi}^*) \rangle,$$

where $I_{\xi_2 < 0} = I_{\xi_2 < 0}(\boldsymbol{\xi})$ equals one when $\xi_2 < 0$ and otherwise zero. Substituting the ansatz into the above formula and noting that $\mathcal{M}^w(\boldsymbol{\xi}) = \mathcal{M}^w(\boldsymbol{\xi}^*)$, $\phi_{\boldsymbol{\alpha}}(\boldsymbol{\xi}) = (-1)^{\alpha_2} \phi_{\boldsymbol{\alpha}}(\boldsymbol{\xi}^*)$, we collect the formula into an even-odd parity form:

$$\left(1 - \frac{\chi}{2}\right) \sum_{\boldsymbol{\beta} \in \mathbb{I}_o} \langle \xi_2 \omega \phi_{\boldsymbol{\alpha}} \phi_{\boldsymbol{\beta}} \rangle f_{\boldsymbol{\beta}} = -\frac{\chi}{2} \sum_{\boldsymbol{\beta} \in \mathbb{I}_e} \langle |\xi_2| \omega \phi_{\boldsymbol{\alpha}} \phi_{\boldsymbol{\beta}} \rangle (f_{\boldsymbol{\beta}} - m_{\boldsymbol{\beta}}), \quad \boldsymbol{\alpha} \in \mathbb{I}_e,$$

where we use the fact that $\langle \xi_2 \omega \phi_{\boldsymbol{\alpha}} \phi_{\boldsymbol{\beta}} \rangle = 0$ when $\boldsymbol{\alpha}, \boldsymbol{\beta} \in \mathbb{I}_e$. According to the Knudsen layer ansatz, we attach the subscripts B and K to discriminate the bulk solution and the Knudsen layer solution. Then we write

$$f_{\boldsymbol{\alpha}} = f_{\boldsymbol{\alpha},B} + \varepsilon f_{\boldsymbol{\alpha},K},$$

where ε is a small quantity representing the Knudsen number. Expand all the variables formally into series on ε, and we assume

$$\begin{aligned} f_{\boldsymbol{\alpha},B} &= f_{\boldsymbol{\alpha},B}^{(0)} + \varepsilon f_{\boldsymbol{\alpha},B}^{(1)} + o(\varepsilon f_{\boldsymbol{\alpha}}), \\ f_{\boldsymbol{\alpha},K} &= f_{\boldsymbol{\alpha},K}^{(0)} + o(f_{\boldsymbol{\alpha}}), \\ m_{\boldsymbol{\alpha}} &= m_{\boldsymbol{\alpha}}^{(0)} + \varepsilon m_{\boldsymbol{\alpha}}^{(1)} + o(\varepsilon f_{\boldsymbol{\alpha}}), \end{aligned}$$

where $f_{\boldsymbol{\alpha},B}^{(j)},\ f_{\boldsymbol{\alpha},K}^{(j)}$ and $m_{\boldsymbol{\alpha}}^{(j)}$ have the same magnitude for $j \in \mathbb{N},\ j \geq 0$. When χ itself is not a small quantity, we can match the order of ε in the boundary condition and get

$$\left(1 - \frac{\chi}{2}\right) \sum_{\boldsymbol{\beta}\in\mathbb{I}_o} \langle \xi_2 \omega \phi_{\boldsymbol{\alpha}} \phi_{\boldsymbol{\beta}} \rangle \left(f_{\boldsymbol{\beta},B}^{(1)} + f_{\boldsymbol{\beta},K}^{(0)}\right) = -\frac{\chi}{2} \sum_{\boldsymbol{\beta}\in\mathbb{I}_e} \langle |\xi_2| \omega \phi_{\boldsymbol{\alpha}} \phi_{\boldsymbol{\beta}} \rangle \left(f_{\boldsymbol{\beta},B}^{(1)} - m_{\boldsymbol{\beta}}^{(1)} + f_{\boldsymbol{\beta},K}^{(0)}\right).$$

According to the derivation of Knudsen layer equations, $f_{\boldsymbol{\beta},K}^{(0)}$ would relate to $\boldsymbol{w}$ in (17), and $m_{\boldsymbol{\beta}}$ is calculated in Appendix E. Hence, we get boundary conditions in the form of (21).

Appendix D. Explicit expressions of (22)

We first introduce two differential relations of the one-dimensional Hermite polynomials (cf. [9]):

$$\frac{\partial}{\partial \xi} \phi_{\alpha+1}(\xi) = \sqrt{\alpha+1}\phi_\alpha(\xi), \qquad \frac{\partial}{\partial \xi}(\omega\phi_\alpha) = -\sqrt{\alpha+1}\omega\phi_{\alpha+1},$$

where $\alpha \in \mathbb{N}$ and $\xi \in \mathbb{R}$. Due to the orthogonality, we only need to calculate

$$\begin{aligned} S(\alpha,\beta) &:= -\sqrt{2\pi}\int_{-\infty}^{0} \xi \phi_\alpha \phi_\beta \omega \,\mathrm{d}\xi, \quad \alpha, \beta \text{ are even numbers.} \\ &= -\sqrt{2\pi}\int_{-\infty}^{0} \left(\sqrt{\alpha}\phi_{\alpha-1} + \sqrt{\alpha+1}\phi_{\alpha+1}\right)\phi_\beta \omega \,\mathrm{d}\xi. \end{aligned} \tag{43}$$

Denote by

$$I(\alpha,\beta) := \sqrt{2\pi}\int_{-\infty}^{0} \phi_\alpha \phi_\beta \omega \mathrm{d}\xi.$$

Integrate by parts using $\mathrm{d}\left(\omega\phi_\beta\right) = -\sqrt{\beta+1}\omega\phi_{\beta+1}\mathrm{d}\xi$ or $\mathrm{d}\left(\omega\phi_\alpha\right) = -\sqrt{\alpha+1}\omega\phi_{\alpha+1}\mathrm{d}\xi$, and we should have two equivalent results:

$$\begin{aligned} I(\alpha+1,\beta+1) &= \left(-\sqrt{2\pi}\phi_{\alpha+1}(0)\phi_\beta(0)\omega(0) + \sqrt{\alpha+1}I(\alpha,\beta)\right)/\sqrt{\beta+1} \\ &= \left(-\sqrt{2\pi}\phi_{\beta+1}(0)\phi_\alpha(0)\omega(0) + \sqrt{\beta+1}I(\alpha,\beta)\right)/\sqrt{\alpha+1}. \end{aligned}$$

Noting that $\omega(0) = (2\pi)^{-1/2}$, we denote by $z_\alpha = \phi_\alpha(0)$ and have

$$I(\alpha,\beta) = \begin{cases} \dfrac{1}{\alpha-\beta}\left(\sqrt{\alpha+1}z_{\alpha+1}z_\beta - \sqrt{\beta+1}z_{\beta+1}z_\alpha\right), & \alpha \neq \beta, \\ \dfrac{\sqrt{2\pi}}{2}, \quad \alpha = \beta, \end{cases} \tag{44}$$

where $z_0 = 1,\ z_1 = 0$ and $z_{n+1} = -\sqrt{n} z_{n-1}/\sqrt{n+1}$. Since $z_n = 0$ when n is odd, we have

$$\begin{aligned} S(\alpha,\beta) &= -\sqrt{\alpha} I(\alpha-1,\beta) - \sqrt{\alpha+1} I(\alpha+1,\beta) \\ &= \frac{\alpha+\beta+1}{1-(\alpha-\beta)^2} z_\alpha z_\beta, \qquad \alpha,\beta \text{ even.} \end{aligned} \tag{45}$$

Appendix E. Moments of $\mathcal{M}^w$

We may calculate

$$m_{\boldsymbol{\alpha}} = \int_{\mathbb{R}^3} \frac{\rho^w}{\sqrt{2\pi\theta^w}^3} \exp\left(-\frac{|\boldsymbol{\xi} - \boldsymbol{u}^w|^2}{2\theta^w}\right) \phi_{\boldsymbol{\alpha}}(\boldsymbol{\xi}) \mathrm{d}\boldsymbol{\xi} := \rho^w \prod_{i=1}^{D} J_{\alpha_i}(u_i^w), \tag{46}$$

where $J_m(x)$ is a one-dimensional integral defined for $m \in \mathbb{N}$ and $x \in \mathbb{R}$ as

$$J_m(x) := \int_{\mathbb{R}} (2\pi\theta^w)^{-\frac{1}{2}} \exp\left(-\frac{|\xi - x|^2}{2\theta^w}\right) \phi_m(\xi) \mathrm{d}\xi. \tag{47}$$

Integrate by parts using $\mathrm{d}\left(\phi_{m+1}\right) = \sqrt{m+1}\phi_m \mathrm{d}\xi$, then we have

$$\begin{aligned} J_m(x) &= \frac{1}{\sqrt{m+1}} \int_{\mathbb{R}} (2\pi\theta^w)^{-\frac{1}{2}} \exp\left(-\frac{|\xi - x|^2}{2\theta^w}\right) \phi_{m+1}(\xi) \frac{\xi - x}{\theta^w} \mathrm{d}\xi \\ &= \frac{1}{\theta^w \sqrt{m+1}} \left(-x J_{m+1} + \sqrt{m+1} J_m(x) + \sqrt{m+2} J_{m+2}(x)\right), \quad m \geq 0. \end{aligned}$$

This gives the recurrence relation

$$J_m(x) = \frac{1}{\sqrt{m}} \left((\theta^w - 1)\sqrt{m-1} J_{m-2}(x) + x J_{m-1}(x)\right), \quad m \geq 2, \tag{48}$$

with $J_0(x) = 1$ and $J_1(x) = x$ since $\phi_0(\xi) = 1,\ \phi_1(\xi) = \xi$.

If $\mathcal{M}^w$ is linearized around the Maxwellian given by $\theta_0 = 1$ and $\boldsymbol{u}_0 = \boldsymbol{0}$, we would have $\theta^w - 1 = O(\varepsilon)$ and $u_i^w = O(\varepsilon)$ where ε is a small quantity. So

$$J_m(u_i^w) = o(\varepsilon),\ m > 2.$$

Thus, the linearization of $m_{\boldsymbol{\alpha}}$ would all be higher-order small quantities except the first two-order.

CAPT, LMAM & School of Mathematical Sciences, Peking University, Beijing 100871, China
E-mail: rli@math.pku.edu.cn

School of Mathematical Sciences, Peking University, Beijing 100871, China
E-mail: yichenyang@pku.edu.cn