AN APPROXIMATE ANALYTICAL SOLUTION TO KNUDSEN LAYERS

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Abstract. We apply moment methods to obtaining an approximate analytical solution to Knudsen layers. Based on the hyperbolic regularized moment system for the Boltzmann equation with the Shakhov collision model, we derive a linearized hyperbolic moment system to model the scenario with the Knudsen layer vicinity to a solid wall with Maxwell boundary condition. We find that the reduced system is in an even-odd parity form that the reduced system proves to be well-posed under all accommodation coefficients. We show that the system may capture the temperature jump coefficient and the thermal Knudsen layer well with only a few moments. With the increasing number of moments used, qualitative convergence of the approximate solution is observed.

Keywords. Moment method; Maxwell boundary condition; Shakhov collision model; Thermal Knudsen layer; Temperature jump

AMS subject classifications. 34B05; 35Q20; 76P05; 82C40

1. Introduction

The Knudsen layer is an important feature of the rarefied gas flow [24], where the continuum assumption does not hold so the Navier-Stokes-Fourier (NSF) equations fail to describe the gas behavior [32] but the model from a statistical viewpoint such as the Boltzmann equation [5] works. As introduced in the book [34], the moment equations, which are extend macroscopic transport equations reduced from the Boltzmann equation, provide a new description of rarefied gases. The model reduction methods are necessary partly because the direct simulation of the Boltzmann equation, such as the direct simulation Monte Carlo (DSMC) [4] and the discrete velocity method (DVM) [6], may be too expensive for applications in concern [30, 28].

This paper is aimed to obtain an approximate analytical solution to the Knudsen layer in some classical flow problems, based on the hyperbolic regularized moment equations (HME) developed in recent years [7, 8, 16, 10, 14]. Moment methods for the Boltzmann equation are first proposed by Grad [17] and success to simulate the nonequilibrium gas flow with high accuracy and high efficiency [29, 33, 36]. Nevertheless, the original Grad’s moment equations suffer the lack of hyperbolicity [9] and the hyperbolic model reduction remains an important issue in this area, whose long and rich history can be found in the review paper [11]. Following the regularization framework [10], the HME is globally hyperbolic regularized from the Grad’s moment system of arbitrary moment orders and has been studied in both theoretical and numerical aspects [12].

There have been exhaustive studies applying the linearized Boltzmann equation [38] with various collision models to Knudsen layers in classical flow problems, i.e. the temperature jump problem [37] and Kramers’ problem [21]. Many highly accurate numerical results have been reported [25, 26, 2] by the discrete-ordinates method. However, moment methods may bring different insights into the understanding of Knudsen layers, especially by their available analytical solutions. To our best knowledge, [35] first analyses a 1D linear kinetic equation for heat transfer by means of Grad’s moment methods. [19] presents analytical solutions of the temperature jump problem for linearized R13 and R26 moment methods. In the recent work [15], formal analytical solutions of the Kramers’ problem are obtained for the linearized HME with the BGK collision model [3].

In this paper, we rewrite the linearized HME as an even-odd parity form and present approximate analytical solutions of the temperature jump problem with the Shakhov collision model [31]. Compared to the early work [15] on Kramers’ problem, the even-odd parity form of the linearized HME is explicitly utilized in this paper and the moment equations’ boundary conditions are also imposed as an even-odd formulation. In this way, we improve the results in [15] that the well-posedness is attained under all accommodation coefficients. Furthermore, the numerical study confirms the effectiveness of our model. The idea of the even-odd formulation is inspired by analysis of the kinetic equations such as [13, 23].
Briefly, we first derive the HME from the Boltzmann equation then make linearization to get the linearized HME (LHME). Thanks to the assumptions of the temperature jump problem, we can decouple the equations including the temperature from the whole LHME, to get a system of linear ordinary differential equations (ODEs) with constant coefficients. We impose the boundary conditions of the moment system by multiplying Maxwell’s accommodation boundary condition [27] with some appropriate polynomials then integrating both sides. Finally, we separate the decaying and non-decaying unknowns, seeking the analytical solutions of the ODEs satisfying the boundary conditions and the boundedness of the decaying unknowns. For arbitrary moment order $M$, the explicit solutions can be determined via a simple algorithm and we then study the temperature jump coefficient, temperature defect, and effective thermal conductivity, etc.

This paper is organized as follows. In Section 2 we derive the LHME in the half-space with wall boundary conditions, and discuss its reduced version in some classical flow problems. In Section 3 we detailedly discuss the temperature jump problem, obtaining the analytical solutions, and proving the well-posedness of the reduced moment system. In Section 4 we briefly discuss the Kramers’ problem. In Section 5 we carefully compare our temperature profile with other kinetic models both theoretically and numerically. The paper ends with a conclusion.

2. The Linearized Moment System

2.1. The Basic Equations. We consider the following Boltzmann equation [5] with the Shakhov [31] collision model

$$
\frac{\partial f}{\partial t} + \xi \cdot \nabla_x f = Q^S(f),
$$

(2.1)

where $f = f(t, x, \xi)$ is the number density distribution function of particles at time $t \in \mathbb{R}^+$, location $x = (x_1, x_2, x_3) \in \mathbb{R}^3$, with velocity $\xi = (\xi_1, \xi_2, \xi_3) \in \mathbb{R}^3$. The Shakhov collision term $Q^S(f)$ is

$$
Q^S(f) = \frac{1}{\tau} (f^S - f), \quad f^S = \rho \omega^{[u, \theta]}(\xi) \left( 1 + \frac{(1 - \text{Pr})(\xi - u) \cdot q}{5 \rho \theta^2} \left( \frac{|\xi - u|^2}{\theta} - 5 \right) \right),
$$

(2.2)

where $\tau^{-1}$ measures frequency of the collision, $\text{Pr}$ is the Prandtl number. And the macroscopic variables such as density $\rho = \rho(t, x)$, macro velocity vector $u = u(t, x)$, temperature $\theta = \theta(t, x)$ and heat flux vector $q = q(t, x)$ are defined by the distribution $f$:

$$
\rho = \int_{\mathbb{R}^3} f d\xi, \quad \rho u = \int_{\mathbb{R}^3} \xi f d\xi, \quad \rho |u|^2 = 3 \rho \theta = \int_{\mathbb{R}^3} f |\xi|^2 d\xi, \quad q = \frac{1}{2} \int_{\mathbb{R}^3} f (|\xi - u|^2 - |\xi|^2) d\xi. \quad (2.3)
$$

$\omega^{[u, \theta]}(\xi)$ is the local Maxwellian, defined as

$$
\omega^{[u, \theta]}(\xi) = \frac{1}{(2\pi \theta^{3/2})^{3/2}} \exp \left( -\frac{|\xi - u|^2}{2\theta} \right).
$$

Remark 2.1. The Shakhov model, which in fact turns to the BGK model [3] when $\text{Pr} = 1$, may provide the correct Prandtl number of the flow. The Boltzmann operator with a more general collision kernel will be discussed in the future work but not in this paper.

Then we briefly introduce the deduction of the HME, whose more details can be found in [10]. First we make the Hermite expansion ansatz of the distribution function

$$
f(t, x, \xi) = \omega^{[u, \theta]}(\xi) \sum_{\alpha \in \mathbb{N}^3} f_\alpha(t, x) \text{He}_\alpha^{[u, \theta]}(\xi),
$$

(2.4)

where $\alpha := (\alpha_1, \alpha_2, \alpha_3) \in \mathbb{N}^3$. $\text{He}_\alpha^{[u, \theta]}(\xi)$ is the generalized 3D Hermite polynomial defined as

$$
\text{He}_\alpha^{[u, \theta]}(\xi) = \frac{(-1)^{|\alpha|}}{\omega^{[u, \theta]}(\xi)} \frac{\partial^{3|\alpha|}}{\partial \xi^\alpha}, \quad |\alpha| := \alpha_1 + \alpha_2 + \alpha_3.
$$
By Appendix A, \( \{ \text{He}_{\alpha}^{[u, \theta]}(\xi) \} \) are orthogonal polynomials with the weight function \( \omega^{[u, \theta]}(\xi) \), and

\[
f_\alpha = \frac{\theta^{\lvert \alpha \rvert}}{\alpha!} \int_{\mathbb{R}^3} f \text{He}_{\alpha}^{[u, \theta]}(\xi) \, d\xi, \quad \alpha! := \alpha_1! \alpha_2! \alpha_3!.
\]

If \( e_i \in \mathbb{R}^3 \) is the unit vector with the \( i \)-th component equaling one, from (2.3) we have

\[
f_0 = \rho, \quad f_{e_i} = 0, \quad 3 \sum_{d=1}^{3} f_{2e_d} = 0, \quad 2f_{3e_i} + \sum_{d=1}^{3} f_{e_i + 2e_d} = q_i.
\]

For any integer \( M \geq 2 \), we define a projection \( \mathcal{P}_M^{[u, \theta]} \) onto the space spanned by the first \( M \)-th order basis functions \( S_M^{[u, \theta]} := \text{span} \{ \omega^{[u, \theta]}(\xi)\text{He}_{\alpha}^{[u, \theta]}(\xi), \lvert \alpha \rvert \leq M \} \), as

\[
\mathcal{P}_M^{[u, \theta]} f := \omega^{[u, \theta]}(\xi) \sum_{\lvert \alpha \rvert \leq M} f(\xi, x) \text{He}_{\alpha}^{[u, \theta]}(\xi).
\]

Then substituting it into the Boltzmann equation, making the HME’s closure and matching the coefficients before the first \( M \)-th order basis functions, we have a closed system with finite terms which is called the \( M \)-th order HME:

\[
\mathcal{P}_M^{[u, \theta]} \left( \frac{\partial \mathcal{P}_M^{[u, \theta]} f}{\partial t} + \sum_{i=1}^{3} \xi_i \mathcal{P}_M^{[u, \theta]} \left( \frac{\partial \mathcal{P}_M^{[u, \theta]} f}{\partial x_i} \right) \right) = \mathcal{P}_M^{[u, \theta]} Q^S(\mathcal{P}_M^{[u, \theta]} f).
\]

The component form reads as

\[
\text{D}f_\alpha \text{D}t + \sum_{d=1}^{3} f_{\alpha - e_d} \text{D}t + \sum_{d=1}^{3} \sum_{k=1}^{3} \left( \theta f_{\alpha - e_d} + (1 - \delta_{\lvert \alpha \rvert, M}) (\alpha_d + 1) f_{\alpha + e_d} \right) + \sum_{k=1}^{3} f_{\alpha - 2e_k} \text{D}t + \frac{1}{2} \sum_{d=1}^{3} \sum_{k=1}^{3} \left( \theta f_{\alpha - e_k} + (1 - \delta_{\lvert \alpha \rvert, M}) (\alpha_d + 1) f_{\alpha + e_d} \right) = -Q_\alpha.
\]

where \( \text{D}t = \frac{\partial}{\partial t} + \sum_{d=1}^{3} u_d \frac{\partial}{\partial x_d} \) is the material derivative and \( (\cdot)_{\alpha} \) is taken as zero if any component of \( \alpha \) is negative or \( \lvert \alpha \rvert > M \). \( Q_\alpha \) is calculated directly as in [12],

\[
Q_\alpha = -\frac{\theta^{\lvert \alpha \rvert}}{\alpha!} \int_{\mathbb{R}^3} Q^S(f) \text{He}_{\alpha}^{[u, \theta]}(\xi) \, d\xi = \frac{1}{\tau} \left( \delta_{\lvert \alpha \rvert, 2} f_{\alpha} - \frac{1}{5} \sum_{i, j=1}^{3} \delta_{\alpha, e_i + 2e_j} q_i \right),
\]

where the Kronecker function \( \delta_{\alpha, e_i + 2e_j} \) equals 1 when \( \alpha = e_i + 2e_j \) and equals 0 otherwise; \( \delta_{\lvert \alpha \rvert, 2} \) equals 1 when \( \lvert \alpha \rvert \geq 2 \) and equals 0 otherwise.

**Remark 2.2.** The hyperbolicity of the moment system (2.3) is proved in [10]. And [10] clarifies that the keypoint of the regularization lies in the extra projection after the space derivatives in (2.3), which is also the only difference between Grad’s moment equations and the HME.

After the non-dimensionalization and linearization, we will get the linearized HME (LHME). The linearization is assumed to be around the Maxwellian \( \rho_{0\omega}^{[u, \theta]}(\xi) \) where \( \rho_0, u_0 = 0, \theta_0 \) are constants. Denote by \( L \) a characteristic length, then we introduce the dimensionless coordinates \( \tilde{x} \) and time \( t \) as \( \tilde{x} = L \tilde{x} \) and \( \tilde{t} = \frac{\gamma_{\theta_0}}{\sqrt{\theta_0}} t \). The corresponding dimensionless Knudsen number is defined as

\[
Kn = \frac{70}{L/\sqrt{\theta_0}}, \quad \text{where } \tau = \gamma_{\theta_0}(1 + \tilde{\tau}), \quad \tilde{\tau} = o(1).
\]
Analogously, we introduce the variables with a bar as dimensionless variables:

\[ \rho = \rho_0(1 + \bar{\rho}), \quad u = \sqrt{\bar{\rho}_0}\bar{u}, \quad \bar{\theta} = \theta_0(1 + \bar{\theta}), \quad f_\alpha = \rho_0\bar{\rho}_0^{\alpha_1}f_\alpha, \quad |\alpha| \geq 2, \]  

(2.9)

where \( Kn \) is assumed to be a small quantity, \( \bar{\rho}, \bar{u}, \bar{\theta} \) and \( f_\alpha \) assumed to be \( O(Kn) \). Substituting (2.9) into the HME (2.8) and discarding the higher order terms, we have \( M \)-th order LHME:

\[ \frac{\partial \bar{h}_\alpha}{\partial t} + \sum_{d=1}^{3} \left( \frac{\partial \bar{h}_\alpha}{\partial \bar{x}_d} + (1 - \delta_{|\alpha|, M})(\alpha_d + 1) \frac{\partial \bar{h}_\alpha}{\partial \bar{x}_d} \right) = -\frac{1}{Kn} \bar{Q}_\alpha, \quad |\alpha| \leq M, \]  

(2.10)

where \( \bar{h}_\alpha \) and \( \bar{Q}_\alpha \) are defined as

\[ \bar{h}_\alpha = \bar{f}_\alpha + \sum_{k=1}^{3} \delta_{\alpha, e_k} \bar{u}_k + \frac{1}{2} \sum_{k=1}^{3} \delta_{\alpha, 2e_k} \bar{\theta}, \quad \bar{Q}_\alpha = \delta_{|\alpha| \geq 2} \bar{f}_\alpha - \frac{1}{5} Pr \sum_{i,j=1}^{3} \delta_{\alpha, e_i + 2e_j} \bar{q}_i. \]  

(2.11)

**Remark 2.3.** We can see from the deduction that the extra projection in the HME only affects the higher order terms. So the difference between Grad’s moment equations and the HME vanishes in case of this linearization.

**Remark 2.4.** From another point of view, the linearized moment equations may be deduced directly from the linearized Boltzmann equation by the traditional Galerkin spectral expansion, i.e. under the basis functions independent on temporal and spatial variables \( t, x \).

### 2.2. Wall Boundary Conditions.

In this paper we will consider the half-space problem, where the gas flow is on the upper half plane of an infinite plate wall. Without loss of generality, we assume the coordinate of the wall \( x = (x_1, 0, x_3), x_1, x_3 \in \mathbb{R} \), the outer normal vector \( n = (0, -1, 0)^T \), the wall velocity \( u^W = (0, 0, 0)^T \) and the wall temperature \( \theta^W \) here and hereafter.

We use Maxwell’s accommodation boundary condition [27] to describe the diffuse-specular process between the wall and the gas flow, which in this case reads as

\[ f(t, x, \xi) = \chi M^W(x, \xi) + (1 - \chi) f(t, x, \xi^*), \quad \xi_2 > 0, \quad x_2 = 0, \]  

(2.12)

where \( \chi \in [0, 1] \) is the accommodation coefficient. \( \xi^* = \xi - 2n(\xi \cdot n) = (\xi_1, -\xi_2, \xi_3)^T \) comes from the specular reflection at the wall, and \( M^W(x, \xi) \) is the Maxwellian characterizing the wall:

\[ M^W(x, \xi) = \frac{\rho^W(x)}{(2\pi\theta^W(x))^{3/2}} \exp \left( -\frac{|\xi - u^W|^2}{2\theta^W(x)} \right), \]

where \( \rho^W \) is a normalizing factor to ensure \( (u - u^W) \cdot n = 0 \) at the wall.

To construct the boundary conditions of the moment equations, a traditional way is multiplying (2.12) by some polynomials \( p_\alpha(\xi) \) and taking integral in \( \mathbb{R}^3 \) about \( \xi \) both sides. To ensure the continuity when \( \chi \to 0 \), Grad [17, 18] suggests choosing the polynomials satisfying

\[ p_\alpha(\xi) = -p_\alpha(\xi^*), \quad \deg(p_\alpha) \leq M, \]  

(2.13)

i.e. the odd polynomials about \( \xi_2 \). Hence substituting \( \xi^* \) by \( \xi \) in the last integral and noting that \( M^W(x, \xi^*) = M^W(x, \xi) \), we have

\[ \int_{\mathbb{R}^3} p_\alpha(\xi) f \, d\xi = \int_{\mathbb{R}^3} \int_{-\infty}^{0} p_\alpha(\xi) f \, d\xi + \int_{\mathbb{R}^3} \int_{0}^{+\infty} p_\alpha(\xi) (\chi M^W + (1 - \chi) f(x, \xi^*)) \, d\xi = \chi \int_{\mathbb{R}^3} \int_{-\infty}^{0} p_\alpha(\xi) (f - M^W) \, d\xi. \]  

(2.14)

Since the equivalence of finite dimensional polynomial spaces, the specific choice of \( p_\alpha(\xi) \) can somehow be arbitrary in numeric, such as the Hermite polynomial [12], the Legendre polynomial [35], or even the monomial \( \xi^\alpha \) [15]. However, to analyse the well-posedness, it may be more convenient to rewrite the odd polynomial \( p_\alpha \) as \( \xi_2 \tilde{p}_\alpha \) where \( \tilde{p}_\alpha \) is an even polynomial. This is analogous
to the Marshak conditions which impose the continuity of fluxes in the domain decomposition methods [1] and its benefits will show naturally in the following sections.

According to this belief and note that when \( \alpha_2 \) is even, \( \bar{u}^{[u,\theta]}(\xi) = \bar{u}^{[u,\theta]}(\xi^*) \), we choose

\[
p_\alpha(\xi) = \xi_2 \theta^{\frac{|\alpha|}{2}} \bar{M}^{[u,\theta]}(\xi), \quad \alpha \in I = \{ |\alpha| \leq M - 1 \mid \alpha_2 \text{ is even} \}.
\]

Then assume \( f \) and \( M^W \) each has the expansion coefficients \( f_\alpha \) and \( m_\alpha \) defined as [25] under the basis functions \( \{\omega^{[u,\theta]}(\xi) \bar{u}^{[u,\theta]}(\xi)\} \). The even-odd symmetry shows that

\[
\int_{\mathbb{R}^2} \int_{-\infty}^0 p_\alpha \bar{H}^{[u,\theta]} \omega^{[u,\theta]} d\xi = \int_{\mathbb{R}^2} \int_0^{+\infty} p_\alpha \bar{H}^{[u,\theta]} \omega^{[u,\theta]} d\xi
\]

\[
= \frac{1}{2} \int_{\mathbb{R}^3} p_\alpha \bar{H}^{[u,\theta]} \omega^{[u,\theta]} d\xi, \quad \beta_2 \text{ is odd.}
\]

\[
- \int_{\mathbb{R}^2} \int_{-\infty}^0 p_\alpha \bar{H}^{[u,\theta]} \omega^{[u,\theta]} d\xi = \int_{\mathbb{R}^2} \int_0^{+\infty} p_\alpha \bar{H}^{[u,\theta]} \omega^{[u,\theta]} d\xi
\]

\[
= \frac{1}{2} \int_{\mathbb{R}^3} \xi_2 \theta^{\frac{|\alpha|}{2}} \bar{M}^{[u,\theta]} \bar{H}^{[u,\theta]} \omega^{[u,\theta]} d\xi, \quad \beta_2 \text{ is even.}
\]

Note that all the integral can calculate separately about \( \xi_1, \xi_2 \) and \( \xi_3 \). After some tedious computation using the properties of Hermite polynomials (Appendix A), and plugging the linearization [24] as well as \( \bar{m}_\alpha \) defined analogously (explicitly calculated in Appendix B), making the linearized HME’s closure \( f_\alpha = o(K \bar{u}) \), \( |\alpha| > M \), then discarding all the higher order small quantities, we have the linearized boundary conditions from (2.14):

\[
\alpha_2! \left( f_{\alpha-e_2} + (\alpha_2 + 1) f_{\alpha+e_2} \right) = b(\chi) \left( \sum_{\beta_2 = 0, \text{ even}}^{M-\alpha_2-\alpha_3} S(\alpha_2, \beta_2) \left( \bar{f}_{\beta_2} - \bar{m}_{\beta_2} \right) \right),
\]

where \( \alpha \in I = \{ |\alpha| \leq M - 1 \mid \alpha_2 \text{ is even} \} \) as in \(2.15\), \( k^{(\alpha)}_{\beta_2} := (\beta_2 - \alpha_2)e_2, b(\chi) := \frac{2\chi}{2-\chi} (2\pi)^{-\frac{3}{2}}. \)

\( S(\alpha_2, \beta_2) \) is a 1D half-space integral with two parameters \( \alpha_2, \beta_2 \in \mathbb{N} \), defined as

\[
S(\alpha_2, \beta_2) := \sqrt{\frac{2\pi}{\theta}} \int_{-\infty}^{\infty} \xi_2 \theta^{\frac{\alpha_2+\beta_2}{2}} \bar{M}^{[u,\theta]}(\xi_2) \bar{H}^{[0,\theta]}(\xi_2) \omega^{[0,\theta]}(\xi_2) d\xi_2.
\]

We put all the calculation in Appendix for brevity and just list some properties for completeness:

**Proposition 2.1.** \( S(\alpha_2, \beta_2) \) is independent of \( \theta \) and can be written explicitly. Especially, when \( \alpha_2 \) is even, \( \beta_2 \) is odd and \( |\beta_2 - \alpha_2| \neq 1 \), we have \( S(\alpha_2, \beta_2) = 0 \). (proof in Appendix [A])

**Proposition 2.2.** When \( \alpha \neq 0, e_i, 2e_i (1 \leq i \leq 3) \), \( \bar{m}_\alpha = 0 \). Especially, \( \bar{m}_{e_i} = \bar{u}^W - \bar{u} \), and \( \bar{m}_{2e_i} = \frac{1}{2}(\bar{u}^W - \bar{u}) \). (proof in Appendix [B])

**Remark 2.5.** The boundary conditions (2.16) are in an even-odd parity form, i.e, the left-hand side of (2.10) only involves \( f_\alpha \) where \( \alpha_2 \) is odd and the right-hand side \( \alpha_2 \) is even.

### 2.3. Reduced Moment System

Under the assumptions of the temperature jump problem proposed by Welander [37], we claim that the equations including \( \theta \) can decouple from the whole LHME. Thus, we only need to solve a smaller moment system, which is called the reduced moment system, to get solutions of the temperature jump problem.

In the temperature jump problem, we assume that the gas velocity is \( \bar{u} = (u_1, 0, 0)^T \) and all derivatives in \( x_1, x_3, t \) vanish. Further, we assume that there is a given constant gradient of the temperature normal to the wall at infinity. Thus, we just set \( \bar{\alpha} = 2e_k + i e_2, \ k = 1, 2, 3, 0 \leq i \leq M - 2 \) in the \( M \)-th order LHME (2.10), and set \( \alpha = 2e_k + i e_2, \ k = 1, 2, 3, 0 \leq i \leq M - 3, \ i \) even, in the linearized wall boundary conditions (2.16). Since \( h_{e_2} = \bar{u}_2 = 0 \), (2.16) and (2.11), we will have \( 3(M - 1) \) equations with the same number unknowns \( h_\alpha \), where \( \sum_{i=1}^{3} h_{2e_i} = \frac{3}{4} \). If we impose the remaining required boundary conditions by the boundedness of solutions, we will get a system of ODEs with the correct number of boundary conditions.
The details will be shown in the next section, and here we just mention two important tricks. First, the main focus in the temperature jump problem, i.e. $\Theta$, is only dependent on $x_2$, so we can add the corresponding terms on $x_1$ and $x_3$ to get a reduced system of $2(M-1)$ equations. This is similar as integrating in the $x_1$ and $x_3$ dimension when applying the linearized Boltzmann equation to the temperature jump problem [35]. Second, since the Boltzmann collision operator always has the nontrivial null space which means the conservation laws, we can only expect part of $f_\alpha$ to be bounded at infinity. So we dividedly consider what we call the decaying variables and non-decaying variables.

**Remark 2.6.** The Kramers’ problem [21], which can be seen as the velocity analogue of the temperature jump problem, would also be solved by a reduced moment system. For LHME with the BGK collision model, this is claimed in [13]. Here for the Shakhov collision model, $\bar{q}_1 = 3\bar{f}_{3e_1} + \bar{f}_{e_1+2e_2} + \bar{f}_{e_1+2e_3}$ will appear. So similarly we can set $\alpha = e_1 + ie_2$, $0 \leq i \leq M - 1$ and assume $\bar{f}_{3e_1} = 0$, $\bar{f}_{e_1+2e_3} = 0$ to get $M$ equations with the same number unknowns.

3. The Temperature Jump Problem

For simplicity, we write $x_2$ as $y$ and define $\tilde{w}(\xi) = \omega^{[0,1]}(\xi)$,

$$\tilde{g}_i = \tilde{f}_{2e_1+ie_2} + \tilde{f}_{2e_3+ie_2}, \quad \tilde{r}_i = \tilde{f}_{(i+2)e_2}, \quad \tilde{\Pi}_\alpha(\xi) = \Pi^{[0,1]}(\xi), \quad \langle \rangle_\omega = \int_{\mathbb{R}^3} \tilde{w} d\xi. \quad (3.1)$$

**Theorem 3.1.** Then if $\tilde{\theta}$ satisfies (2.10), it must satisfy the following $2(M-1)$ equations:

$$\frac{d\tilde{q}_2}{dy} = 0, \quad \frac{d\tilde{\theta}}{dy} = -\frac{2}{5} \frac{1}{Kn} \frac{4}{5} \frac{d(\tilde{r}_0 + (1 - \delta_{M,3})(6\tilde{q}_2 + \tilde{g}_2))}{dy}, \quad (3.2)$$

$$M \frac{d\tilde{w}}{dy} := \begin{bmatrix} 0 & M_0 \\ M_0^T & 0 \end{bmatrix} \frac{d}{dy} \begin{bmatrix} \tilde{w}_{\text{even}} \\ \tilde{w}_{\text{odd}} \end{bmatrix} = -\frac{1}{Kn} \frac{\tilde{w}}{\tilde{w}}, \quad (3.3)$$

where $M \geq 3$, $\tilde{q}_2 = 3\tilde{r}_1 + \tilde{g}_1$, $\tilde{w} = L\tilde{f} := (\tilde{w}_{\text{even}}, \tilde{w}_{\text{odd}})^T$ with $L = \text{diag}(L_1, L_2)$, $\tilde{f} = (\tilde{f}_{\text{even}}, \tilde{f}_{\text{odd}})^T$. Here $\tilde{f}_{\text{even}} = (\tilde{f}_{0}, \tilde{f}_{1}, \tilde{f}_{2}, \cdots, \tilde{f}_{m_{-1}, g_{m_{-1}}})^T \in \mathbb{R}^{m_0}$ collects unknowns with even subscripts, $\tilde{f}_{\text{odd}} = (\tilde{f}_1, \tilde{f}_2, \tilde{f}_3, \cdots, \tilde{f}_{m_{-1}, g_{m_{-1}}})^T \in \mathbb{R}^{m_0}$ collects the odd. The index $m_0 = 2[\frac{M-3}{2}] - 1$, $m_e = 2[\frac{M}{2}] - 1$, thus $m_0 + m_e = 2(M - 2)$. The matrix $M_0 = (m_{ij}^0) \in \mathbb{R}^{m_0 \times m_0}$, $L_1 = \text{diag}(a_i) \in \mathbb{R}^{m_0 \times m_0}$, $L_2 = \text{diag}(b_i) \in \mathbb{R}^{m_0 \times m_0}$ can write explicitly:

$$m_{ij}^0 = \frac{1}{a_i b_j} \langle \phi_i, \phi_j \rangle_\omega, \quad a_i := \sqrt{\langle \phi_i, \phi_i \rangle_\omega}, \quad b_i := \sqrt{\langle \varphi_i, \varphi_i \rangle_\omega}, \quad (3.4)$$

where $\phi = (\phi_i) \in \mathbb{R}^{m_0}$ and $\varphi = (\varphi_i) \in \mathbb{R}^{m_0}$ come from rearranging the Hermite polynomials:

$$\phi_1 = \Pi^{[2e_2]} - \frac{1}{2} (\Pi^{[2e_1]} + \Pi^{[2e_3]}), \quad \phi_{2k} = \Pi^{[2k+2]} + \Pi^{[2k+1]}, \quad \phi_{2k+1} = \frac{1}{2} (\Pi^{[2k+2]} + \Pi^{[2k+1]} + \Pi^{[2k+3]}) ; \quad \varphi_1 = \Pi^{[2e_2]} - \frac{3}{2} (\Pi^{[2e_1+2]} + \Pi^{[2e_3+2]}), \quad \varphi_{2k} = \Pi^{[2k+2]} + \Pi^{[2k+1]}, \quad \varphi_{2k+1} = \frac{1}{2} (\Pi^{[2k+2]} + \Pi^{[2k+1]} + \Pi^{[2k+3]}) .$$

**Proof.** As mentioned before, we set $\alpha = 2e_k + ie_2$, $k = 1, 2, 3$, $0 \leq i \leq M - 2$, $M \geq 3$ in (2.10). For each $i$, add the equations with $k = 1$ and $k = 3$, then we have

$$\frac{d}{dy}(\tilde{g}_{i-1} + \delta_{i,1}\tilde{\theta}) + (1 - \delta_{i, M-2})(i + 1) \frac{d}{dy} \tilde{g}_{i+1} = -\frac{1}{Kn} \left( \tilde{g}_{i} - \frac{2}{5} \frac{1}{Pr} \delta_{i,1} \tilde{q}_2 \right),$$

where $\tilde{g}_{i-1} = 0$. And for $k = 2$ we have

$$\frac{d}{dy} \left( \tilde{r}_{i-1} + \frac{1}{2} \delta_{i,1}\tilde{\theta} \right) + (1 - \delta_{i, M-2})(i + 3) \frac{d}{dy} \tilde{r}_{i+1} = -\frac{1}{Kn} \left( \tilde{r}_{i} - \frac{2}{5} \frac{1}{Pr} \delta_{i,1} \tilde{q}_2 \right),$$

where $\tilde{r}_{i-1} = 0$ because $\tilde{f}_{e_2} = \tilde{u}_2 = 0$ in this case. Note that $\tilde{g}_0 + \tilde{r}_0 = 0$ and $\tilde{q}_2 = 3\tilde{r}_1 + \tilde{g}_1$ from (2.6), so add the equations with $i = 0$, we have

$$\frac{d\tilde{q}_2}{dy} = 0 \quad \Rightarrow \quad \tilde{q}_2 \text{ is a constant.}$$
Add the equations with \( i = 1 \) by proportion 3:1 to make the right hand side a constant, we have

\[
\frac{d\hat{\theta}}{dy} = -\frac{2}{5} \frac{1}{Kn} Pr \hat{q}_2 - \frac{4}{5} \frac{d(\hat{t}_0 + (1 - \delta_{M,\beta})(6\hat{t}_2 + \hat{y}_2))}{dy}.
\]

Note Appendix [A] tells us \( \xi \bar{H}_\alpha = \alpha d \bar{H}_\alpha - e_d + \bar{H}_\alpha + e_d \), \( \langle \bar{H}_\alpha, \bar{H}_\beta \rangle = \alpha! \delta_{\alpha,\beta} \), so direct computation shows that from \( [3.4] \),

\[
a_1 = \sqrt{3}, \quad a_{2k} = \sqrt{(2k + 2)!}, \quad a_{2k+1} = \sqrt{(2k)!},
\]

\[
b_1 = \sqrt{15}, \quad b_{2k} = \sqrt{(2k + 3)!}, \quad b_{2k+1} = \sqrt{(2k + 1)!},
\]

\[
\langle \phi_1, \xi_2 \varphi_1 \rangle = 0, \quad \langle \phi_2, \xi_2 \varphi_1 \rangle = 24, \quad \langle \phi_3, \xi_2 \varphi_1 \rangle = -6,
\]

\[
\langle \phi_{2k}, \xi_2 \varphi_{2k} \rangle = (2k + 3)!; \quad \langle \phi_{2k}, \xi_2 \varphi_{2k-2} \rangle = (2k + 2)!,
\]

\[
\langle \phi_{2k+1}, \xi_2 \varphi_{2k+1} \rangle = (2k + 1)!, \quad \langle \phi_{2k+1}, \xi_2 \varphi_{2k-1} \rangle = (2k)!.
\]

And the other entries of \( M_0 \) are zero. So if we eliminate \( \hat{\theta} \) in the later equations, we can verify that \( \theta \) satisfies \( [3.2], [3.3] \).

Since the special structure of \( M \) from the even-odd parity form, immediately we have

**Lemma 3.1.** \( M \) has \( m_o \) positive, \( m_o \) negative and \( m_e - m_o \) zero eigenvalues.

**Proof.** Evidently, if

\[
\begin{bmatrix}
0 & M_0 \\
M_0^T & 0
\end{bmatrix}
\begin{bmatrix}
x_1 \\
x_2
\end{bmatrix} = \lambda \begin{bmatrix}
x_1 \\
x_2
\end{bmatrix}, \quad \text{then} \quad \begin{bmatrix}
0 & M_0 \\
M_0^T & 0
\end{bmatrix}
\begin{bmatrix}
x_1 \\
-x_2
\end{bmatrix} = -\lambda \begin{bmatrix}
x_1 \\
-x_2
\end{bmatrix}.
\]

So the positive and negative eigenvalues of \( M \) appear in pairs. \( M \) is real symmetric so it can be real diagonalized. What’s more, we claim that \( M_0 \) has a column full rank of \( m_o \). If suppose the contrary, there exists non-trivial coefficients \( r_j \in \mathbb{R}, 1 \leq j \leq m_o \) such that

\[
\langle \phi_1, \xi_2 \sum_{j=1}^{m_o} r_j \varphi_j \rangle = 0, \quad \forall 1 \leq i \leq m_e.
\]

But if we let \( i = 1 \), the trinomial recurrence and orthogonality tell us

\[
\langle \phi_1, \xi_2 \sum_{j=1}^{m_o} r_j \varphi_j \rangle = \langle \phi_1, \xi_2 r_1 \varphi_1 \rangle = 9 r_1,
\]

so \( r_1 = 0 \). By induction, we can see that \( r_j = 0, 1 \leq j \leq m_o \). Thus the lemma is proved.

From the process of the proof we immediately have

**Corollary 3.1.** There exist an orthogonal diagonalization \( MR = RA \) where \( R^T R = R R^T = I_{2(M-2)} \) is the \( 2(M-2) \)-th order identity matrix and

\[
R := \begin{bmatrix}
R_{\text{even}} & R_0 & R_{\text{even}} \\
R_{\text{odd}} & 0 & -R_{\text{odd}}
\end{bmatrix}, \quad A := \begin{bmatrix}
A_+ & 0_{m_e-m_o} \\
0_{m_o} & -A_+
\end{bmatrix},
\]

(3.5)

where \( R_{\text{even}} \in \mathbb{R}^{m_e \times m_o}, \quad R_{\text{odd}} \in \mathbb{R}^{m_o \times m_e}, \quad R_0 \in \mathbb{R}^{m_o \times (m_e - m_o)}, \quad A_+ := \text{diag}(\lambda_i) \in \mathbb{R}^{m_o \times m_o} \) and \( \lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_{m_o} > 0 \).

As mentioned in Section \( [2.3] \) we shall impose boundary conditions from two parts: one is to ensure the boundedness of the decaying variables \( \hat{w} \), the other is from the wall-gas interaction. Define \( \hat{v} = R^{-\frac{1}{2}} \hat{w} \), we have characteristic equations

\[
\Lambda \frac{d\hat{v}}{dy} = -\frac{1}{Kn} \hat{v},
\]

Assume \( \hat{v} = (\hat{v}_+, \hat{v}_0, \hat{v}_-)^T \) where \( \hat{v}_+, \hat{v}_- \in \mathbb{R}^{m_e}, \hat{v}_0 \in \mathbb{R}^{m_o - m_e} \). Then if we don’t allow the exponential blow up of \( \hat{v} \) at infinity, we would get \( m_e \) boundary conditions:

\[
\hat{v}_-(0) = \mathbf{0}, \quad \hat{v}_0(0) = \mathbf{0}.
\]

(3.7)

As a remark, from \( \hat{w} = R\hat{v} \) and \( [3.7] \) we have

\[
\hat{w}_{\text{even}} = R_{\text{even}} \hat{v}_+, \quad \hat{w}_{\text{odd}} = R_{\text{odd}} \hat{v}_+.
\]

(3.8)
THEOREM 3.2. From (2.16), \( \hat{v}(0) \) and \( \hat{\theta}(0) \) satisfy the following \( m_o + 1 \) boundary conditions:

\[
\hat{q}_c + E \begin{bmatrix} 0 \\ M_0 \end{bmatrix} \begin{bmatrix} \hat{\theta}(0) - \hat{\theta}^W \\ \hat{w}_{\text{odd}}(0) \end{bmatrix} = b(\chi) ET \begin{bmatrix} \hat{\theta}(0) - \hat{\theta}^W \\ \hat{w}_{\text{even}}(0) \end{bmatrix},
\]

where \( c_r = (1, 1/\sqrt{5}, 2/\sqrt{5}, 2/\sqrt{5}, 0, ..., 0)^T \in \mathbb{R}^{m_o + 1} \), \( E := [I_{m_o + 1}, 0] \in \mathbb{R}^{(m_o + 1) \times (m_o + 1)}. \) \( \hat{w}_{\text{even}}, \hat{w}_{\text{odd}} \) are related to \( \hat{v}_+ \) by (3.8). And

\[
T = \begin{bmatrix} 1 \\ L_1^{-1} \end{bmatrix} \begin{bmatrix} P_1 & I_{m_x - 1} \end{bmatrix} \begin{bmatrix} P_1 \\ I_{m_x - 1} \end{bmatrix} \begin{bmatrix} 1 \\ L_1^{-1} \end{bmatrix}, \quad P_1 = \begin{bmatrix} 0.5 & 1 \\ 1 & -1 \end{bmatrix}.
\]

Here \( T^b := (t_i^b) \in \mathbb{R}^{(m_o + 1) \times (m_o + 1)} \) is a square matrix with nonzero entries

\[
t_i^{2k, 2l} = S(2k - 2, 2l - 2), \quad t_i^{2k - 1, 2l - 1} = S(2k, 2l) - S(2k, 0) \frac{S(0, 2l)}{S(0, 0)} S(0, 2l), \quad k, l \geq 1, \quad (3.10)
\]

where \( S(\alpha, \beta) \) is the half-space integral (2.17).

Proof. We just set \( \alpha = 2e_k + ie_2 \), where \( i \) is even and \( 0 \leq i \leq M - 3 \), in the linearized boundary conditions (2.16). For each \( i \), add the conditions with \( k = 1 \) and \( k = 3 \), then we will have \( 2(\frac{M}{2} - 1) = m_o + 1 \) more boundary conditions. Since \( t_0 + g_0 = 0 \), we have

\[
P_1 \begin{bmatrix} \hat{\theta} \\ t_0 \end{bmatrix} = \begin{bmatrix} \hat{\theta} + \hat{\theta}^W/2 \\ g_0 + \hat{\theta}^W/2 \end{bmatrix}.
\]

From Appendix B we know that \( \bar{m}_{2e_k} = \frac{1}{2} (\hat{\theta}^W - \hat{\theta}) \), \( \bar{m}_\alpha = 0 \) when \( \alpha_2 \) is even and \( |\alpha| > 2 \), and

\[
S(0, 0)(\bar{m}_\alpha - \bar{\rho}) = \sum_{\beta_2 = 2, \text{even}}^{M} S(0, \beta_2)(\bar{f}_{\beta_2 e_2} - \bar{m}_{\beta_2 e_2}).
\]

So direct computation will show (3.9) right. \( \square \)

REMARK 3.1. Here when \( M \) is odd, \( m_o = m_n = M - 2 \). So \( M \) has no zero eigenvalues and \( E = I_{m_x + 1} \) is an identity matrix which can be ignored. When \( M \) is even, \( m_o = M - 1, m_n = M - 3 \). So \( M \) has two zero eigenvalues and \( E \) ensures the correct number of boundary conditions.

LEMMA 3.2. \( T^b \) is negative symmetric definite, so is \( T \).

Proof. By definition \( S(\alpha, \beta, \alpha) = S(\beta, \alpha) \), so \( T^b \) is symmetric. For any \( x = (x_i) \in \mathbb{R}^{m_x + 1} \), define

\[
f_o(\xi_2) := \sum_{i=1}^{(m_o + 1)/2} x_{2i-1} \overline{H}_{e_2}(\xi_2), \quad f_o(\xi_2) := \sum_{i=1}^{(m_o + 1)/2} x_{2i} \overline{H}_{e_2}(\xi_2),
\]

where \( \overline{H}_{e_2}(\xi_2) := H_{e_2}^{(0, 1)}(\xi_2) \). By definition (2.17) and Cauchy-Schwartz inequality, we have

\[
x^T T^b x = \frac{2\pi}{\theta} \int_{-\infty}^{0} \xi_2 (f_o^2 + f_o^2) \omega^{0, \theta} d\xi_2 = \frac{1}{S(0, 0)} \frac{2\pi}{\theta} \left( \int_{-\infty}^{0} \xi_2 f_2^{0, \theta} d\xi_2 \right)^2 \leq \frac{1}{S(0, 0)} \frac{2\pi}{\theta} \left( \int_{-\infty}^{0} \xi_2 f_2^{0, \theta} d\xi_2 \right)^2 \leq 0.
\]

Note that here \( S(0, 0) = \sqrt{\frac{2\pi}{\theta} \int_{-\infty}^{0} \xi_2^{0, \theta} d\xi_2} = -1 \). If \( x^T T^b x = 0 \), there must have \( f_o = 0 \) and \( f_o \) a constant function, which means \( x = 0 \in \mathbb{R}^{m_x + 1} \) because \( f_o \) is at least a polynomial of degree 2 if it’s not zero. Thus \( T^b \) is negative definite. So is \( T \) by definition. \( \square \)

DEFINITION 3.1. We call the ODEs (3.2) (3.3) with the boundary conditions (3.8) (3.9) and a given constant \( \hat{q}_2 \) the \( M \)-th order reduced moment system for the temperature jump problem.
Note that if $M$ has zero eigenvalues, i.e., $M$ is even, the matrix $E$ in (3.9) would make the analysis more complicated. And for our purpose, we just need to choose odd $M$ to obtain a series of temperature solutions for the temperature jump problem. Thus, we have:

**Theorem 3.3.** For any given constant $q_2$, accommodation coefficient $\chi \in (0, 1]$ and odd moment order $M \geq 3$, $M \in \mathbb{N}$, (3.9) has a unique solution of $\theta(0)$ and $\tilde{v}_+(0)$.

**Proof.** By the orthogonal diagonalization (3.5), $M_0 R_{odd} = R_{even} A_+ + R_{even}^T R_{even} = \frac{1}{2} I_{m_o}$.

Note the diagonal matrix $L_1 = \text{diag}(a_i)$ is invertible, we can write (3.9) as

$$
EK(\chi) \begin{bmatrix} 1 \\ R_{even} \end{bmatrix} \begin{bmatrix} \theta(0) - \theta^W \\ \tilde{v}_+(0) \end{bmatrix} = \tilde{q}_2 c_r, \quad K(\chi) := b(\chi) T - 2 \begin{bmatrix} 0 \\ R_{even} A_+ + R_{even}^T \end{bmatrix}, \quad (3.11)
$$

where $b(\chi) = \frac{2\chi}{(3-\chi)\sqrt{2\pi}} > 0$ when $\chi \in (0, 1]$, we immediately know that $K(\chi)$ is negative symmetric definite by Lemma 3.2. When $M$ is odd, we further have $m_o = m_e = M - 2$, $E = I_{m_o+1}$ is just the identity matrix and $R_{even}$ is a square matrix. So $R_{even}$ is invertible and (3.11) immediately implies that the coefficient matrix is non-singular.

**Remark 3.2.** The well-posedness of the linear kinetic equations is widely studied. We note that for the non-stationary problem, when $M$ is odd, the reduced system with the given boundary conditions is symmetric hyperbolic with dissipative boundary conditions. Many classical results such as [22] have studied the well-posedness of this type of linear problems.

**Remark 3.3.** When $M$ is even, the zero eigenvalues of $M$ will make the case more complicated. For two reasons, we think it unnecessary to consider this case. One is mentioned previously: the odd $M$ can already give a series of solutions. The other is inspired from [15], which shows that when $M$ is even, alternative spaces should be used to ensure the stability, i.e., multiplying even polynomials $p_m$ when imposing the boundary conditions.

**Remark 3.4.** Nevertheless, numerically we verify that (3.9) has a unique solution when $M$ is even, varying from 4 to 4000. In fact the coefficient matrix can write as a form $b(\chi) S_1 - S_2$ where $S_1, S_2$ is the constant matrix. We can calculate a generalized eigenvalue problem to get $b(\chi)$ such that $|b(\chi) S_1 - S_2| = 0$ in numeric.

Now for arbitrary odd moment order $M \geq 3$, we have the formal analytical solutions of the temperature profile:

$$
\tilde{\theta}(\bar{y}) = \frac{2 Pr}{K_n q_2 \bar{y}} + c_0 - \frac{4}{5} \begin{bmatrix} \sqrt{3} \sqrt{2} \sqrt{2} \end{bmatrix} R_{even}[1 : 3 ;] \exp \left( -\frac{1}{K_n} \chi \frac{1}{\sqrt{2}} \right) \tilde{v}_+(0) \\
:= -\frac{2 Pr}{5 K_n} \bar{q}_2 \bar{y} + c_0 + \sum_{i=1}^{m_o} \tilde{r}_i \exp \left( -\frac{1}{K_n} \chi \frac{1}{\sqrt{2}} \right), \quad (3.12)
$$

where $\bar{q}_2$ is the given constant. $R_{even}[1 : 3 ;]$ is the first three rows of $R_{even}$, $c_0, \tilde{r}_i$ are some constants calculated from the previous process.

Qualitatively, we can see that the temperature profile are superpositions of Knudsen layers of various widths, which is shown similarly in [35, 15]. When $\bar{y}$ goes to infinity, $\bar{\theta}$ oscillates periodically and finally approach a linear function, which is exactly the classical Fourier’s Law. While as $\bar{y}$ goes to zero, the phenomenon of temperature jump will occur.

**Corollary 3.2.** From (3.9) we can see that $\tilde{v}_+(0)$ and $\tilde{\theta}(0) - \theta^W$ depend linearly on $\bar{q}_2$, where the coefficients depend on $\chi$, the moment order $M$ but not on $\bar{q}_2$. Further we can see from (3.12) that $\tilde{\theta}(\bar{y}) - \theta^W$ is depend linearly on $\bar{q}_2$.

**Case $M=3$.** As an illustrative example, we show the case $M = 3$ in some detail. When $M = 3, m_o = m_e = 1, \bar{f} = (t_0, l_1 - 0.2\bar{q}_2)^T$, and the eigenvalue decomposition gives

$$
M = \begin{bmatrix} 0 & 0 \\ \frac{3}{5} & 0 \end{bmatrix}, \quad \Lambda = \begin{bmatrix} \frac{3}{5} & 0 \\ 0 & -\frac{3}{5} \end{bmatrix}, \quad R = \begin{bmatrix} -\sqrt{2} & -\sqrt{2} \\ \frac{3}{2} & \frac{3}{2} \end{bmatrix}.
$$

The boundary condition (3.7) is $\bar{t}_0(0) = \sqrt{5}(\bar{t}_1(0) - 0.2\bar{q}_2)$ and (3.9) becomes

$$
\begin{bmatrix} 1 \\ 0.8 \end{bmatrix} \bar{q}_2 + \begin{bmatrix} 0 \\ 9 \end{bmatrix} \begin{bmatrix} \tilde{\theta}(0) - \theta^W \\ \bar{t}_1(0) - 0.2\bar{q}_2 \end{bmatrix} = b(\chi) \begin{bmatrix} -2 & 1 \\ -1 & -5 \end{bmatrix} \begin{bmatrix} \tilde{\theta}(0) - \theta^W \\ \bar{t}_0(0) \end{bmatrix}.
$$
where $\tilde{\ell}_0(0) = -\frac{\bar{\eta}_2}{\sqrt{5(6 + 3\sqrt{5b(\chi)})}}$, $c_0 = -\frac{\bar{\eta}_2}{2b(\chi)} + \bar{\eta}_W + 0.3\tilde{\ell}_0(0)$.

For general $M$, we need to determine the coefficients in the solutions numerically. Since $M_0$ is lower-triangular with bandwidth three, the eigenvalue decomposition will somehow be standard. And when $M$ is odd, the linear system (3.11) can be symmetric definite, which benefits the linear solver too.

4. The Kramers’ Problem

Before the quantitative study of the temperature profile, we will briefly represent the results of the Kramers’ problem for further reference convenience. All the proof is analogous to the quantitative study of the temperature profile, with the BGK collision model.

In this section, we will use the script $k$ to represent Kramers’ problem. As mentioned in Section 2.3, we set $\mathbf{e}_i = e_{i*}, 0 \leq i \leq M - 1$ in the $M$-th order ($M > 3$) LHEME (2.10) to decouple the following $M$ equations involving $\bar{a}_1$:

$$\frac{d\bar{a}_{12}}{dy} = 0, \quad \frac{d\bar{u}_1}{dy} = -\frac{1}{K_n} \bar{q}_{12} - 2\frac{d\bar{f}_{e_1+2e_2}}{dy},$$

$$M_k \frac{d\bar{w}_k}{dy} := \begin{bmatrix} 0 & M_k^0 \end{bmatrix} \begin{bmatrix} 0 \\ \bar{\eta}_k \end{bmatrix} = -\frac{1}{K_n} \bar{w}_k, \tag{4.2}$$

where $\bar{w}_k = L_k \bar{f}_k := (\bar{u}_{k,\text{even}}, \bar{u}_{k,\text{odd}})^T$, $L_k = \text{diag}(L_1^k, L_2^k)$, $\bar{f}_k = (\bar{f}_{\text{even}}, \bar{f}_{\text{odd}})^T$. The index $m_k^0 = \lfloor \frac{M}{2} \rfloor$, $m_k^\pm = \lfloor \frac{M-1}{2} \rfloor$. Similarly $\bar{f}_{\text{even}} := (f_{e_1+2e_2}, f_{e_1+4e_2}, ..., f_{e_1+(2m_k^+ + 1)e_2})^T \in \mathbb{R}^{m_k^e}$ collects the even subscripts, and $\bar{f}_{\text{odd}} := (f_{e_1+3e_2}, f_{e_1+5e_2}, ..., f_{e_1+(2m_k^+ + 1)e_2})^T \in \mathbb{R}^{m_k^o}$ collects the odd. Here $M_k^0 = (m_{ij}^0) \in \mathbb{R}^{m_k^e \times m_k^o}$, $L_1^k = \text{diag}(a_{1i}^k)_{i=1}^{m_k^0}$, $L_2^k = \text{diag}(b_i^k)_{i=1}^{m_k^0}$ have the entries:

$$m_{ij}^{0} = \frac{1}{a_{ij}^k} \langle \phi_i^k, \xi_{2e_2} \rangle, \quad a_i^k = \sqrt{(1 - \frac{1 - Pr}{5}) \delta_{i,1} + \langle \phi_i^k, \phi_i^k \rangle}, \quad b_i^k = \sqrt{\langle \phi_i^k, \phi_i^k \rangle},$$

where $\phi_i^k := \frac{\mathcal{H}e_{e_1+2i+e_2}}{\mathcal{H}e_{e_1+(2i+1)e_2}}$.

**Lemma 4.1.** $M_k$ has $m_k^0$ positive, $m_k^o$ negative and $m_k^+ - m_k^- = 0$ zero eigenvalues.

**Corollary 4.1.** There exists a real orthogonal diagonalization $M_k R_k = R_k \Lambda_k$ where

$$R_k := \begin{bmatrix} R_{k,\text{even}}^T & 0 \\ 0 & -R_{k,\text{odd}}^T \end{bmatrix}, \quad \Lambda_k := \begin{bmatrix} \Lambda_+^k & 0_{m_k^+ - m_k^-} \\ 0_{m_k^+} & -\Lambda_-^k \end{bmatrix}$$

Here $R_k$ is orthogonal, $R_{k,\text{even}} \in \mathbb{R}^{m_k^e \times m_k^+}$, $R_{k,\text{odd}} \in \mathbb{R}^{m_k^o \times m_k^+}$, $R_0^k \in \mathbb{R}^{m_k^+ \times (m_k^0 - m_k^-)}$, and $\Lambda_+^k := \text{diag}(\lambda_{k,i}) \in \mathbb{R}^{m_k^+ \times m_k^+}$ with $\lambda_{k,1} \geq \lambda_{k,2} \geq \cdots \geq \lambda_{k,m_k^+} > 0$.

Similarly define $\tilde{v}_k = R_k^{-1} \bar{w}_k = (\tilde{v}_{k,+}, \tilde{v}_{k,0}, \tilde{v}_{k,-})^T$, then (4.1) will turn to $\Lambda_k \frac{d\tilde{v}_k}{dy} = -\frac{1}{K_n} \tilde{v}_k$. The boundedness and consistency asks $m_k^+$ boundary conditions:

$$\tilde{v}_{k,0}(0) = 0, \quad \tilde{v}_{k,-}(0) = 0.$$
Setting $\alpha = e_1 + i e_2$, $0 \leq i \leq M - 2$, $i$ even, in (4.10) to get wall boundary conditions:

$$\bar{\sigma}_{12} r_k + E_k \begin{bmatrix} 0 \\ M_0^k \end{bmatrix} \begin{bmatrix} \bar{u}_1(0) - \bar{u}_1^W \\ \bar{w}_{d,dd}(0) \end{bmatrix} = b(\chi) E_k \hat{S}_k \begin{bmatrix} \bar{u}_1(0) - \bar{u}_1^W \\ \bar{w}_{\text{even}}(0) \end{bmatrix},$$

where $r_k = (1, 2/a_0^k, 0, ..., 0)^T$, $\hat{S}_k := \text{diag}(1, L_1^k)^{-1} S_k \text{diag}(1, L_1^k)^{-1}$, $E_k = [I_{m_o^k+1}, 0]$ is a $(m_o^k + 1) \times (m_o^k + 1)$ matrix. Here $S_k = (s_{ij}^k) \in \mathbb{R}^{(m_o^k+1) \times (m_o^k+1)}$ has the entries

$$s_{ij}^k = S(2i - 2, 2j - 2), \ i, j \geq 1.$$

Thus substituting $\hat{w}_k = R_k \hat{e}_k$ and (4.5) into (4.6), we can determine $\hat{v}_{k,+}(0)$ and $\bar{u}_1(0)$.

**Lemma 4.2.** $S_k$ is negative symmetric definite.

**Theorem 4.1.** For any given constant $\bar{\sigma}_{12}$, accommodation coefficient $\chi \in (0, 1]$ and even moment order $M \geq 4, M \in \mathbb{N}$, (4.4) has a unique solution of $\bar{u}_1(0)$ and $\bar{v}_{k,+}(0)$.

Finally the velocity solution has the form

$$\bar{u}_1(\bar{y}) = -\frac{1}{Kn} \bar{\sigma}_{12} \bar{y} + e_0^k - \frac{2}{a_1^k} R^k_{\text{even}}[1,] \exp \left(-\frac{1}{Kn} (\Lambda^k)^{-1} \bar{y} \right) \hat{v}_{k,+}(0),$$

where all constants can be determined by eigenvalue decomposition and linear solvers.

### 5. Numerical Validation

In this section, we will represent some numerical results in the temperature jump problem. As in the kinetic theory, we consider the normalized temperature combined by three parts

$$\hat{\theta}(\bar{y}) = \bar{y} + \xi - \theta_d(\bar{y}),$$

where $\bar{y}$ is the linear part, $\theta_d(\bar{y})$ is the temperature defect satisfying $\lim_{\bar{y} \to \infty} \theta_d(\bar{y}) = 0$ and $\xi$ is the temperature jump coefficient. In our model,

$$\xi = -\frac{5Kn}{2Pr \hat{q}_2} c_0, \quad \theta_d = \frac{2Kn}{Pr \hat{q}_2} (\ell_0 + (1 - \delta_{M,3})(6\ell_2 + \hat{s}_2)).$$

As shown in Corollary 3.2, $c_0 - \bar{\theta}_d^W$, $\ell_0$, $\ell_2$, $\hat{s}_2$ are linear dependent on $\hat{q}_2$, so we may as well set $\bar{\theta}_d^W = 0$ and $\hat{q}_2 = 1$. Since the reasons in Remark 3.3, we just consider the case when $M$ is odd.

### 5.1. Temperature Jump Coefficient $\xi$

We compare the temperature jump coefficient when $M = 2k + 1$, $1 \leq k \leq 6$ with the results solved by discrete-ordinates methods of linearized Boltzmann-BGK model [2] in Table 5.1. The parameters are chosen to be consistent with [2], i.e. $Kn = \frac{27}{4}, Pr = 1$.

| $\chi$ | Siewert’s $M = 3$ | $M = 5$ | $M = 7$ | $M = 9$ | $M = 11$ | $M = 13$ |
|--------|-------------------|---------|---------|---------|---------|---------|
| 0.1    | 21.45012          | 21.086  | 21.396  | 21.412  | 21.421  | 21.426  |
| 0.3    | 6.630514          | 6.3116  | 6.5542  | 6.5870  | 6.6003  | 6.6074  | 6.6118  |
| 0.5    | 3.629125          | 3.3538  | 3.5680  | 3.5951  | 3.6057  | 3.6114  | 3.6149  |
| 0.6    | 2.867615          | 2.6134  | 2.8135  | 2.8378  | 2.8473  | 2.8522  | 2.8553  |
| 0.7    | 2.317534          | 2.0840  | 2.2698  | 2.2916  | 2.3000  | 2.3043  | 2.3070  |
| 0.9    | 1.570264          | 1.3768  | 1.5342  | 1.5513  | 1.5576  | 1.5608  | 1.5628  |
| 1.0    | 1.302716          | 1.1287  | 1.2718  | 1.2867  | 1.2921  | 1.2949  | 1.2965  |

As can be seen, when $\chi$ becomes smaller the temperature jump coefficient will go larger. And for the given $\chi$, the LHME solutions seem to agree with the reference solutions with not too many moments. In fact when $M = 13$ the relative error between the LHME solution and the reference
solution is less than 1% in most cases. There is also a convergence trend when $M$ grows. In fact if $\zeta_k$ is the LHME solution when $M = 2^k + 1$, we can define the numerical convergence order as

$$\beta_k = -\log_2 \left( \frac{\zeta_{k+2} - \zeta_{k+1}}{\zeta_{k+1} - \zeta_k} \right).$$

Table 5.2 shows $\beta_k$ when $\chi$ is different and $k = 6, 7, 8$. The results imply about one order convergence when $M \to \infty$ and the accuracy of the linear solver may impact on $\beta_k$ when $M$ is large.

Table 5.2: The numerical convergence order of the temperature jump coefficient

| $\chi$ | 0.1 | 0.3 | 0.5 | 0.6 | 0.7 | 0.9 | 1.0 |
|--------|-----|-----|-----|-----|-----|-----|-----|
| $k = 6$ | 0.984 | 0.995 | 1.006 | 1.012 | 1.018 | 1.029 | 1.036 |
| $k = 7$ | 0.976 | 0.985 | 0.993 | 0.998 | 1.003 | 1.012 | 1.017 |
| $k = 8$ | 0.974 | 0.981 | 0.988 | 0.991 | 0.995 | 1.002 | 1.006 |

**Remark 5.1.** For the linearized moment system, we think its capacity to describe the Knudsen layer mainly lies in the approximation of basis function spaces, i.e. similarly as in Galerkin spectral methods, but is rarely dependent on the hyperbolic regularization. For the HME, we can see from Remark 2.3 that the hyperbolic regularization does not affect the linearized moment system. Beyond, it may be also true for 13 or 26 moment methods.

Since $Pr$ only occurs in (3.2) and does not affect the other equations or boundary conditions, if we seem $\zeta$ as a function of $Pr$, immediately we have

$$\zeta(Pr) = Pr^{-1} \zeta(1).$$

(5.2)

So we can just consider the BGK model when studying the jump coefficient. We note this relation is also shown in [20] when studying the Shakhov model.

Fig. 5.1 shows the value $b(\chi)\zeta$ when $\chi$ is different and $M$ is fixed.

![Fig. 5.1: The value of $b(\chi)\zeta$ for the LHME solutions.](image)

In fact we can formally show the convergence results when $\chi \to 0$. When $\chi \to 0$, $b(\chi) = \frac{2^k}{\chi} (2\pi)^{-\frac{k}{2}}$ also goes to zero. Note that $\hat{w}_{\text{odd}} = R_{\text{odd}} \hat{v}_+^\dagger$ and $\hat{w}_{\text{even}} = R_{\text{even}} \hat{v}_+^\dagger$ should have the same order since $R$ remains the same when $\chi$ varies. So to make both sides of (3.2) the same
order, one must assume \( \hat{w}(0) = O(b\hat{\theta}(0)) \). Thus, the first row of the leading order equations will be

\[
-2b\hat{\theta}(0) = \hat{q}_2.
\]

After the normalization and note that \( c_0(0) = \bar{\theta}(0) + o(\bar{\theta}(0)) \), we have

\[
\lim_{\chi \to 0} b\zeta = \frac{5}{8}\sqrt{2} \quad \Rightarrow \quad \lim_{\chi \to 0} \frac{x}{2 - x}\zeta = \frac{5}{8}\sqrt{\pi}.
\]

The limit \( (5.3) \) exactly agrees with the result in linearized Boltzmann-BGK model as in [26].

In a word, the numerical results tell that we may only need a moment system with moderate moment order (such as \( M = 11, 13 \)) to describe the Knudsen layer in this problem. Since the 1D assumptions, the number of moments is linearly correlated with the moment order \( M \), so this scale may be affordable in practice.

### 5.2. Temperature Defect \( \theta_d(\bar{y}) \)

Fig.5.2 presents the profile of the temperature defect \( \theta_d(\bar{y}) \) for the LHME when \( M = 3, 7, 11, 15 \) and \( \chi = 0.1, 1.0 \). The reference solution is from the linearized Boltzmann-BGK model [2]. As we can see, the result of \( M = 3 \) is away from the reference solution but when \( M \) becomes larger our results quickly agree with the reference solution well. When \( M \geq 7 \), the gap seems to mainly occur only near the wall, i.e. \( \bar{y} \) close to zero.

In fact the analytical expressions of \( \theta_d(\bar{y}) \) are available in our model, by (3.12),

\[
\theta_d(\bar{y}) = -\frac{2Kn}{Pr\hat{q}_2} \left[ \frac{\sqrt{3}}{3}, \frac{\sqrt{5}}{2}, \frac{\sqrt{2}}{2} \right] R_{even}[1 : 3, \cdot] \exp \left( -\frac{1}{Kn} A_{-1} \bar{y} \right) \hat{v}_+ (0)
\]

\[
:= -\frac{2Kn}{Pr} \sum_{i=1}^{m_o} \tilde{c}_i \exp \left( -\frac{1}{Kn} \lambda_{-1} \bar{y} \right),
\]

where \( \tilde{c}_i \) is only dependent on the moment order \( M \) and accommodation coefficient \( \chi \). The profile of the temperature defect in Fig. 5.2 is obtained by solving the constants in (5.4) then plotting the analytical expressions.

Again we find that if we want to capture the behavior of the gas near the wall, it may be necessary to enlarge the moment order \( M \), but a modest \( M \) such as 11 may be enough considering the balance of accuracy and efficiency. In other problems, the moment order \( M \) should be of concrete analysis.
5.3. Effective Thermal Conductivity. The Fourier law fails in the Knudsen layer and we can formally write the Fourier law by the effective thermal conductivity $\kappa_{\text{eff}}$:

$$q_2 = -\kappa_{\text{eff}} \frac{d\theta}{dy}.$$  \hspace{1cm} (5.5)

So if we denote by $\kappa_0$ the original thermal conductivity, we have

$$\frac{\kappa_{\text{eff}}}{\kappa_0} = \left( \frac{d\theta}{dy} \right)^{-1} = \left( 1 - \frac{d\theta}{dy} \right)^{-1}.$$  \hspace{1cm} (5.6)

Fig. 5.3: Profile of the effective thermal conductivity in the Knudsen layer.

Here we choose $Pr = \frac{2}{3}$ for the Maxwell molecules and study the effective thermal conductivity of different $M$ and accommodation coefficients numerically in Fig. 5.3. We notice that [19] obtained a similar form of $\kappa_{\text{eff}}/\kappa_0$ with exponential terms by the R26 moment system and compare our results with it. We can find that the LHME captures all the qualitative trends of $\kappa_{\text{eff}}$ mentioned in [19] in the Knudsen layer, such as $\kappa_{\text{eff}}$ will reduce as $\bar{y} \to 0$ or $\chi \to 0$.

These analytical expressions may be used to correct the boundary conditions of the NSF equations. But since $\kappa_{\text{eff}}$ relies on the flow conditions [19], we must be very careful in the application. This may be the future study and we don’t plan to deal with it in this paper.

6. Conclusions

We have derived an approximate analytical solution for the Knudsen layer using arbitrary high order LHME. A class of well-posed boundary conditions for the LHME under all accommodation coefficients has been imposed. And the formal analytical solutions with some constants determined by numerical solvers have been presented. In the temperature jump problem, we have compared the temperature defect, temperature jump coefficient and effective thermal conductivity of our model with the existing models. It’s shown that the LHME with a few moments can capture the thermal Knudsen layer well. Although we restricted us mainly in the temperature jump problem (and Kramers’ problem), it is straightforward to extend the method to other boundary layer problems as well as other collision models.

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Appendix A. Hermite polynomials and the half-space integral.

Definition A.1. Given \( u \in \mathbb{R}^N, \theta \in \mathbb{R}, \theta > 0 \), we define the weight function \( \omega^{[u,\theta]}(\xi) \), the generalized N-D Hermite function \( H^{[u,\theta]}_\alpha(\xi) \) and the Hermite polynomial \( H^{[u,\theta]}_\alpha(\xi) \) as follows:

\[
\omega^{[u,\theta]}(\xi) = \frac{1}{(2\pi \theta)^{N/2}} \exp\left(-\frac{|\xi - u|^2}{2\theta}\right), \quad (A.1)
\]

\[
H^{[u,\theta]}_\alpha(\xi) = \frac{(-1)^{|\alpha|}}{\omega^{[u,\theta]}(\xi)} \frac{\partial^{|\alpha|}}{\partial \xi^{|\alpha|}} \omega^{[u,\theta]}(\xi), \quad (A.2)
\]

\[
H^{[u,\theta]}_\alpha(\xi) = H^{[u,\theta]}_\alpha(\xi) H^{[u,\theta]}(\xi), \quad (A.3)
\]

where \( \alpha = (\alpha_i)_{i=1}^N \in \mathbb{N}^N, |\alpha| := \sum_i \alpha_i, \xi \in \mathbb{R}^N \) and \( \xi^\alpha := \prod_i \xi_i^{\alpha_i} \). From the definition we have

\[
\omega^{[u,\theta]}(\xi) = \prod_{i=1}^N \omega^{[u,\theta]}(\xi_i), \quad H^{[u,\theta]}_\alpha(\xi) = \prod_{i=1}^N H^{[u,\theta]}_{\alpha_i}(\xi_i), \quad (A.4)
\]

so properties of N-D Hermite polynomials will reduce to the 1D case.

Proposition A.1. When \( N = 1 \), i.e. \( u, \xi \in \mathbb{R}, \alpha \in \mathbb{N} \), we have (proof in [38] or anywhere)

- Recursion relation: \( (\xi - u)H^{[u,\theta]}_{\alpha+1}(\xi) = (\alpha + 1)H^{[u,\theta]}_{\alpha}(\xi) + \theta H^{[u,\theta]}_{\alpha+2}(\xi) \).

- Differential relation I: \( \frac{\partial}{\partial \xi} H^{[u,\theta]}_{\alpha+1}(\xi) = \frac{\alpha + 1}{\theta} H^{[u,\theta]}_{\alpha}(\xi) \).

- Differential relation II: \( \frac{\partial}{\partial \xi} H^{[u,\theta]}_{\alpha}(\xi) = -H^{[u,\theta]}_{\alpha+1}(\xi) \).

- Orthogonal relation: \( \int_{\mathbb{R}} H^{[u,\theta]}_{\alpha}(\xi) H^{[u,\theta]}_{\beta}(\xi) d\xi = \langle H^{[u,\theta]}_{\alpha}, H^{[u,\theta]}_{\beta} \rangle_{\omega^{[u,\theta]}} = \alpha!\theta^{-\alpha} \delta_{\alpha,\beta} \).

Proposition A.2. The half-space integral \( S(\alpha_2, \beta_2) \) defined as (2.17) is independent of \( \theta \). And

\[
S(\alpha_2, \alpha_2 + 1) = \frac{\sqrt{2\pi}}{2} (\alpha_2 + 1)!; \quad S(\alpha_2, \alpha_2 - 1) = \frac{\sqrt{2\pi}}{2} \alpha_2! \quad (\alpha_2 > 0).
\]

Otherwise when \( \beta_2 \neq \alpha_2 - 1, \alpha_2 + 1 \), we have

\[
S(\alpha_2, \beta_2) = \frac{\alpha_2 + \beta_2 + 1}{(\alpha_2 - \beta_2)^2 - 1} z_0 z_{\alpha_2} z_{\beta_2},
\]

where \( z_0 = 1, z_1 = 0, z_{n+1} = -nz_n, n \geq 1 \).

Corollary A.1. Since \( z_n = 0 \) when \( n \) is odd, from Property [A.2] we have \( S(\alpha_2, \beta_2) = 0 \) if \( \alpha_2 \) is even, \( \beta_2 \) is odd and \( |\beta_2 - \alpha_2| \neq 1 \).

Proof. (Proof of Proposition A.2) First for \( \alpha, \beta \in \mathbb{N} \), we denote by

\[
I(\alpha, \beta) = \sqrt{2\pi} \int_{-\infty}^{\infty} \theta^{\frac{|\alpha|}{2}} H^{[0,\theta]}_{\alpha}(\xi) H^{[0,\theta]}_{\beta}(\xi) \omega^{[0,\theta]}(\xi) d\xi.
\]

So \( I(\alpha, \beta) = I(\beta, \alpha) \). Integrate by parts using \( d\left(H^{[0,\theta]}_{\beta}(\xi)\right) = -H^{[0,\theta]}_{\beta+1}(\xi) d\xi \) or \( d\left(H^{[0,\theta]}_{\alpha}(\xi)\right) = -H^{[0,\theta]}_{\alpha+1}(\xi) d\xi \), then we should get the equivalent results by these two ways:

\[
I(\alpha + 1, \beta + 1) = -\sqrt{2\pi} \theta^{\frac{|\alpha+1|}{2}} H^{[0,\theta]}_{\alpha+1}(0) H^{[0,\theta]}_{\beta+1}(0) + (\alpha + 1)I(\alpha, \beta) \quad (A.5)
\]

\[
I(\alpha + 1, \beta - 1) = -\sqrt{2\pi} \theta^{\frac{|\alpha+2|}{2}} H^{[0,\theta]}_{\alpha+1}(0) H^{[0,\theta]}_{\beta-1}(0) + (\beta + 1)I(\alpha, \beta). \quad (A.6)
\]

Noting that \( H^{[0,\theta]}_{\alpha}(0) = (2\pi \theta)^{-\frac{1}{2}} H^{[0,\theta]}_{\alpha}(0) \). If we denote by \( z_\alpha = \theta^{\frac{1}{2}} H^{[0,\theta]}_{\alpha}(0) \), when \( \alpha \neq \beta \) we have

\[
I(\alpha, \beta) = \frac{1}{\alpha - \beta} (z_{\alpha+1} z_\beta - z_{\beta+1} z_\alpha), \quad (A.7)
\]
where \( z_0 = 1, z_1 = 0 \) and \( z_{n+1} = -nz_{n-1} \) by recursion relation in Proposition A.1. By definition,

\[
S(\alpha, \beta) = \beta I(\alpha, \beta - 1) + I(\alpha, \beta + 1),
\]

(A.8)

which turns to \( S(\alpha, 0) = I(\alpha, 1) \) when \( \beta = 0 \). So when \( \beta \neq \alpha + 1 \) and \( \beta \neq \alpha - 1 \), we have

\[
S(\alpha, \beta) = -\frac{\beta}{\alpha - \beta + 1}z_\alpha z_\beta - \frac{1}{\alpha - \beta - 1}z_\alpha z_{\beta+2} = \frac{\alpha + \beta + 1}{(\alpha - \beta)^2 - 1}z_\alpha z_\beta.
\]

(A.9)

For the special case \( \beta = \alpha + 1 \), we calculate by (A.3) to get

\[
S(\alpha, \alpha + 1) = (\alpha + 1)I(\alpha, \alpha) = (\alpha + 1)!I(0, 0) = \frac{\sqrt{2\pi}}{2}(\alpha + 1)!.
\]

Similarly when \( \alpha > 1 \) we have \( S(\alpha, \alpha - 1) = I(\alpha, \alpha) = \frac{\sqrt{2\pi}}{\alpha!} \).

**Appendix B. Calculation of \( \bar{m}_\alpha \).** Assume \( u^W = (u_1^W, u_2^W, u_3^W)^T \) and \( u_2^W = 0 \). Then from \( u \cdot n = 0 \) we have \( u_2 = 0 \). By definition

\[
m_\alpha = \frac{\partial^{\alpha+1}}{\alpha!} \int_{\mathbb{R}^3} \frac{\rho^W}{\sqrt{2\pi \theta^W}} \exp\left(-\frac{|\xi - u^W|^2}{2\theta^W}\right) H_{0}^{[\alpha, \theta]}(\xi)\,d\xi
\]

\[
= \rho^W J_\alpha(u_1^W - u_1)J_{\alpha+1}(0)J_{\alpha+2}(u_3^W - u_3),
\]

(B.1)

where the 1D integral \( J_m(x) \) is defined for \( m \in \mathbb{N} \) and \( x, u \in \mathbb{R} \) as

\[
J_m(x) := \frac{1}{m!} \theta^m \int_{\mathbb{R}} (2\pi \theta^W)^{-\frac{1}{2}} \exp\left(-\frac{|\xi - u - x|^2}{2\theta^W}\right)H_{m}^{[\alpha, \theta]}(\xi)\,d\xi.
\]

**Proposition B.1.** \( J_m(x) \) is independent of \( u \) and satisfy a recursion relation.

**Proof.** Use \( \frac{d}{d \theta} \left( H_{m+1}^{[\alpha, \theta]} \right) = \frac{m+1}{\theta}H_{m}^{[\alpha, \theta]} \) in the integration by parts formula, then we have

\[
J_m(x) = \frac{\theta^{m+1}}{(m+1)!} \int_{\mathbb{R}} (2\pi \theta^W)^{-\frac{1}{2}} \exp\left(-\frac{|\xi - u - x|^2}{2\theta^W}\right)H_{m+1}^{[\alpha, \theta]}(\xi)\,d\xi
\]

\[
= \frac{1}{\theta^W} (-xJ_{m+1} + \theta J_m(x) + (m+2)J_{m+2}(x)), \quad m \geq 0.
\]

(B.2)

Note that \( H_{0}^{[\alpha, \theta]}(\xi) = 1, \) \( H_{1}^{[\alpha, \theta]}(\xi) = (\xi - u)/\theta \), so if we substitute \( m \) by \( m - 2 \) in (B.2), we have

\[
J_m(x) = \frac{1}{m!} \left( (\theta^W - \theta)J_{m-2}(x) + xJ_{m-1}(x) \right), \quad m \geq 2,
\]

(B.3)

with \( J_0(x) = 1 \) and \( J_1(x) = x \).

If we introduce a formal small quantity \( \varepsilon \) and assume \( \rho = \rho_0(1+\bar{\rho}), m_0 = \rho^W = \rho_0(1+\bar{\rho}^W) \), \( u_1 = \sqrt{\theta_0}\bar{u}_1, u_i^W = \sqrt{\theta_0}\bar{u}_i^W, \theta = \theta_0(1+\bar{\theta}), \bar{\theta}^W = \theta_0(1+\bar{\theta}^W) \), \( m_\alpha = \rho_0\theta_0^{\alpha} \bar{m}_\alpha \), where the variables with a bar are \( O(\varepsilon) \), then discarding the higher order small quantities we have

**Proposition B.2.** \( \bar{m}_{e_i} = \bar{u}_i^W - \bar{u}_i, \bar{m}_{2e_i} = \frac{1}{2}(\bar{\theta}^W - \bar{\theta}). \) \( \bar{m}_\alpha = 0 \) when \( \alpha \neq 0, e_1, 2e_1 \). And

\[
S(0, 0)(\bar{\rho}^W - \bar{\theta}) = \sum_{\beta_2 = 2, \text{even}}^M S(0, \beta_2)(\bar{\beta}_2\bar{e}_2 - \bar{m}_{\beta_2\bar{e}_2}).
\]

(B.4)

**Proof.** Set \( \alpha = (0, 0, 0) \) in (2.10) and immediately we have (B.4). Since \( J_1(x) = x \) and \( J_2(x) = \frac{1}{2}(\theta_0(\bar{\theta}^W - \bar{\theta}) + x^2) \), from (B.1) we have \( \bar{m}_{e_i} = \bar{u}_i^W - \bar{u}_i, \bar{m}_{2e_i} = \frac{1}{2}(\bar{\theta}^W - \bar{\theta}) \). Further from (B.3) we can induce that \( J_m(x) = O(\varepsilon^{|m|}) \) if \( x = O(\varepsilon) \) and \( \bar{\theta}^W - \bar{\theta} = O(\varepsilon) \). So when \( \alpha \neq 0, e_1, 2e_1 \), from (2.11) we have \( \bar{m}_\alpha = o(\varepsilon) \).