Resolving Knudsen Layer by High Order Moment Expansion

Yuwei Fan\textsuperscript{*}, Jun Li\textsuperscript{†}, Ruo Li\textsuperscript{‡}, Zhonghua Qiao\textsuperscript{§}

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Abstract

We model the Knudsen layer in Kramers’ problem by linearized high order hyperbolic moment system. Due to the hyperbolicity, the boundary conditions of the moment system is properly reduced from the kinetic boundary condition. For Kramers’ problem, we give the analytical solutions of moment systems. With the order increasing of the moment model, the solutions are approaching to the solution of the linearized BGK kinetic equation. The velocity profile in the Knudsen layer is captured with improved accuracy for a wide range of accommodation coefficients.

1 Introduction

In the area of kinetic theory, Kramers’ problem \cite{Kramers} is generally considered as the most basic way to understand the fundamental flow physics of the wall, which defining the Knudsen layer \cite{Knudsen}, without some of the additional complications in other more realistic problems, such as flow in a plane channel \cite{PlanarChannel} or cylindrical tube \cite{CylindricalTube}. It is well known \cite{NSF1, NSF2} that the classical Navier-Stokes-Fourier(NSF) equations with appropriate boundary conditions can be used to describe the flow with satisfactory accuracy when the gas is close to a statistical equilibrium state. However, more accurate model is needed to depict the nonequilibrium effects near the wall, where the continuum assumption is essentially broken down and NSF equations themselves become inappropriate \cite{Knudsen, NSF3}. This is exactly the case in Knudsen layers.

During the past decades, various methods have been developed to investigate the Kramers’ problem based on the Boltzmann equation. Highly accurate results on the dependence of slip coefficient for the unmodeled Boltzmann equation and general boundary condition have been reported \cite{Boltzmann1, Boltzmann2, Boltzmann3}. Variable collision frequency models of the Boltzmann equation \cite{VariableCollision1, VariableCollision2, VariableCollision3, VariableCollision4} are extensively discussed. We note that the direct simulation Monte Carlo (DSMC) method \cite{DSMC} is widely used to solve the Boltzmann equation numerically. Unfortunately, DSMC calculations impose prohibitive computational demands for many applications of current interests. The intensive computational demands of DSMC method have motivated recent interests in the application of higher-order hydrodynamic models to simulate rarefied flows \cite{HigherOrder1, HigherOrder2, HigherOrder3, HigherOrder4}. There are many competing sets

\textsuperscript{*}Department of Mathematics, Stanford University, Stanford, CA 94305, email: ywfan@stanford.edu.
\textsuperscript{†}School of Mathematical Sciences, Peking University, Beijing, China, email: lijun609@pku.edu.cn.
\textsuperscript{‡}CAPT, LMAM & School of Mathematical Sciences, Peking University, Beijing, China, email: rli@math.pku.edu.cn.
\textsuperscript{§}Department of Applied Mathematics, the Hong Kong Polytechnic University, Hung Hom, Hong Kong, email:zhonghua.qiao@polyu.edu.hk.
of higher-order constitutive relations, which are derived from the fundamental Boltzmann equation using differing approaches. The classical approaches are the Chapman-Enskog technique and Grad’s moment method. Among these alternative macroscopic modeling and simulation strategies [12, 21], the moment method is quite attractive due to its numerous advantages [31, 33, 36]. It is regarded as a useful tool to extend classical fluid dynamics, and achieves highly accurate approximations with great efficiency.

The moment method for gas kinetic theory [12] has been applied on wall-bounded geometries which supplemented by slip and jump boundary conditions [28], while its application is seriously limited due to the lack of hyperbolicity [31, 6]. Particularly for the 3D case, the moment system is not hyperbolic in any neighborhood of the Maxwellian. Only recently this fatal defect has been remedied [4, 5, 10] that globally hyperbolic models can be deduced. The global hyperbolicity of the new models provides us the information propagation directions, and thus a proper boundary condition of the moment model may be proposed. This motivates us to study the Kramers’ problem using the new moment models.

Starting from the globally hyperbolic moment system (HME), we first derive a linearized hyperbolic moment model to depict the Kramers’ problem. We found that the linearized model is even simpler than one’s expectation, since the equations for velocity are decoupled from other equations in the system involving high order moments. The number of equations in the decoupled part related with velocity is the same as the moment expansion order only. Then we establish the boundary conditions for the linearized moment model according to physical and mathematical requirements for the system. Following Grad’s approach in [12] for the kinetic accommodation model by Maxwell [29], we propose the general boundary conditions for shear flows. After that, by linearizing the velocity jump and high order terms in the expression of the general boundary conditions, it is then adapted to the boundary condition for the linearized model. This makes us able to give the expression of velocity by solving the decoupled system related with velocity together with the corresponding boundary condition. It is extensively believed that the linearized system is accurate enough for low-speed flows, which encourages us to apply the solution of the velocity obtained to study Kramers’ problem.

To obtain the full velocity profile and the velocity slip coefficient in Kramers’ problem, one may adopt a certain direct numerical method to solve the linearized Boltzmann equation. However, the linearized moment system can depict the velocity profile in the Knudsen layer with analytical expressions. This can be used to provide a convenient correction near the wall [23] for the lower order macroscopic system, such as NSF equations. In the moment method, the Knudsen layer appears as superpositions of exponential layers [35]. For the result we give based on HME, the number of exponential layers is increasing. Comparing with the results given by direct numerical simulation, our solutions illustrate a significant improvement in accuracy than the results in references when more and more high order moments are considered. Particularly, our results can capture the velocity profile in the Knusen layer accurately for a wide range of accommodation coefficients. We note that our linearized model is of the same computational cost as the lower order moment system.

This paper is organized as follows. In Section 2 we reviewed HME for Boltzmann equations and derived the linearized HME. The boundary conditions for HME and linearized HME are established in Section 3. The solutions of linearized equations are solved in detail for Kramers’ problem in Section 4. With the solutions of the velocity profile in Knudsen layer, some important coefficients, such as defect velocity, are compared with the
other model of kinetic solution in the same section. We then draw some conclusions to end this paper.

2 Linearized HME for Boltzmann Equation

2.1 Boltzmann equation

In gas kinetic theory, the motion of particles of gas can be depicted by the Boltzmann equation [3]

\[ \frac{\partial f}{\partial t} + \xi \cdot \nabla_x f = Q(f, f), \quad (2.1) \]

where \( f(t, x, \xi) \) is the number density distribution function which depends on the time \( t \in \mathbb{R}^+ \), the spatial position \( x \in \mathbb{R}^3 \) and the microscopic particle velocity \( \xi \in \mathbb{R}^3 \), and \( Q(f, f) \) is the collision term. In this paper, we limit the discussion on the BGK collision model [1], which reads:

\[ Q(f, f) = \frac{\rho \theta}{\mu} (M - f), \quad (2.2) \]

where \( \mu \) is the viscosity and \( M \) is the local thermodynamic equilibrium, usually called the local Maxwellian, defined by

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

Here the density \( \rho \), the macroscopic velocity \( u \) and the temperature \( \theta \) are related to the distribution function as

\[ \rho = \int_{\mathbb{R}^3} f \, d\xi, \quad \rho u = \int_{\mathbb{R}^3} \xi f \, d\xi, \quad \rho |u|^2 + 3\rho \theta = \int_{\mathbb{R}^3} |\xi|^2 f \, d\xi. \quad (2.3) \]

Multiplying the Boltzmann equation by \((1, \xi, |\xi|^2)\) and integrating both sides over \( \mathbb{R}^3 \) with respect to \( \xi \), we obtain the conservation laws of mass, momentum and energy as

\[ \frac{D\rho}{Dt} + \rho \sum_{d=1}^{3} \frac{\partial u_d}{\partial x_d} = 0, \]

\[ \rho \frac{Du_i}{Dt} + \sum_{d=1}^{3} \frac{\partial p_{id}}{\partial x_d} = 0, \quad (2.4) \]

\[ 3 \frac{\rho}{2} \frac{D\theta}{Dt} + \sum_{k,d=1}^{3} p_{kd} \frac{\partial u_k}{\partial x_d} + \sum_{d=1}^{3} \frac{\partial q_d}{\partial x_d} = 0, \]

where \( \frac{D}{Dt} := \frac{\partial}{\partial t} + \sum_{d=1}^{3} u_d \frac{\partial}{\partial x_d} \) is the material derivative, and the pressure tensor \( p_{ij} \) and the heat flux \( q_i \) are defined by

\[ p_{ij} = \int_{\mathbb{R}^3} (\xi_i - u_i)(\xi_j - u_j) f \, d\xi, \quad q_i = \frac{1}{2} \int_{\mathbb{R}^3} |\xi - u|^2 (\xi_i - u_i) f \, d\xi, \quad i, j = 1, 2, 3. \quad (2.5) \]

For convenience, we define the pressure \( p \) and the stress tensor \( \sigma_{ij} \) by

\[ p = \sum_{d=1}^{3} \frac{p_{dd}}{3} = \rho \theta, \quad \sigma_{ij} = p_{ij} - p \delta_{ij}, \quad i, j = 1, 2, 3. \]
2.2 HME and its linearization

The moment method in kinetic theory is first proposed by Grad in 1949 [12]. The primary idea is to expand the distribution function around the Maxwellian into Hermite series

\[
f(t, x, \xi) = \frac{M}{\rho} \sum_{\alpha \in \mathbb{N}^3} f_\alpha(t, x) H_{\alpha}^{[u, \theta]}(\xi) = \sum_{\alpha \in \mathbb{N}^3} f_\alpha(t, x) H_{\alpha}^{[u, \theta]}(\xi),
\]

(2.6)

where \( \alpha = (\alpha_1, \alpha_2, \alpha_3) \in \mathbb{N}^3 \) is a 3D multi-index, and \( H_{\alpha}^{[u, \theta]}(\xi) \) are generalized Hermite polynomials defined by

\[
H_{\alpha}^{[u, \theta]}(\xi) = \frac{(-1)^{|\alpha|}}{M} \frac{\partial^{|\alpha|} M}{\partial \xi_1^{\alpha_1} \partial \xi_2^{\alpha_2} \partial \xi_3^{\alpha_3}},
\]

\(|\alpha| = \sum_{d=1}^{3} \alpha_d,
\]

and \( \mathcal{H}_{\alpha}^{[u, \theta]}(\xi) \) is the basis function defined by

\[
\mathcal{H}_{\alpha}^{[u, \theta]}(\xi) = \frac{M}{\rho} H_{\alpha}^{[u, \theta]}(\xi).
\]

Directly calculations yield, for \( i, j = 1, 2, 3, \)

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

\[
p_{ij} = p\delta_{ij} + (1 + \delta_{ij}) f_{e_i + e_j}, \quad q_i = 2 f_{3e_i} + \sum_{d=1}^{3} f_{e_i + 2e_d}.
\]

(2.9)

Substituting Grad’s expansion (2.6) into the Boltzmann equation, and matching the coefficient of the basis function \( \mathcal{H}_{\alpha}^{[u, \theta]}(\xi) \), one can obtain the governing equations of \( u, \theta \) and \( f_\alpha, \alpha \in \mathbb{N}^3 \). However, the resulting system contains infinite number of equations.

Choosing a positive integer \( 3 \leq M \in \mathbb{N} \), and discarding all the equations including \( \frac{\partial f_\alpha}{\partial t} \), \( |\alpha| > M \), and setting \( f_\alpha = 0, |\alpha| > M \) to close the residual system, we obtain the \( M \)-th order Grad’s moment system. Since

\[
Q(f, f) = -\frac{p}{\mu} \sum_{|\alpha| \geq 2} f_{\alpha} \mathcal{H}_{\alpha}^{[u, \theta]}(\xi) = -\frac{p}{\mu} H(|\alpha| - 2) f_\alpha,
\]

where \( H(n) \) is the Heaviside step function

\[
H(n) = \begin{cases} 
0, & n < 0, \\
1, & n \geq 0,
\end{cases}
\]

the \( M \)-th order Grad’s moment system can be written as

\[
\frac{D f_\alpha}{Dt} + \sum_{d=1}^{3} \left( \theta \frac{\partial f_{\alpha-e_d}}{\partial x_d} + (1 - \delta_{|\alpha|,M})(\alpha_d + 1)\frac{\partial f_{\alpha-e_d}}{\partial x_d} \right)
\]

\[
+ \sum_{k=1}^{3} f_{\alpha-e_k} \frac{D u_k}{Dt} + \sum_{k,d=1}^{3} \frac{\partial u_k}{\partial x_d} (\theta f_{\alpha-e_k-e_d} + (\alpha_d + 1)f_{\alpha-e_k+e_d})
\]

\[
+ \frac{1}{2} \sum_{k=1}^{3} f_{\alpha-2e_k} \frac{D \theta}{Dt} + \sum_{k,d=1}^{3} \frac{1}{2} \frac{\partial \theta}{\partial x_d} (\theta f_{\alpha-2e_k-e_d} + (\alpha_d + 1)f_{\alpha-2e_k+e_d})
\]

\[
= -\frac{p}{\mu} f_\alpha H(|\alpha| - 2), \quad |\alpha| \leq M,
\]

(2.10)
where $\delta_{i,j}$ is Kronecker delta. Here and hereafter we agree that $(\cdot)_{\alpha}$ is taken as zero if any component of $\alpha$ is negative.

However, as is pointed in [31, 6], Grad’s moment system lacks global hyperbolicity and is not hyperbolic even in any neighborhood of local Maxwellian. The globally hyperbolic regularization proposed in [4, 5] figures the drawback out essentially, and results in globally Hyperbolic Moment Equations (HME) as

\[
\frac{D f_{\alpha}}{Dt} + \sum_{d=1}^{3} \left( \theta \frac{\partial f_{\alpha-e_d}}{\partial x_d} + (1 - \delta_{|\alpha|,M})(\alpha_d + 1) \frac{\partial f_{\alpha-e_d}}{\partial x_d} \right) \\
+ \sum_{k=1}^{3} f_{\alpha-e_k} \frac{Du_k}{Dt} + \sum_{k,d=1}^{3} \frac{\partial u_k}{\partial x_d} \left( \theta f_{\alpha-e_k-e_d} + (1 - \delta_{|\alpha|,M})(\alpha_d + 1) f_{\alpha-e_k+e_d} \right) \\
+ \frac{1}{2} \sum_{k=1}^{3} \sum_{d=1}^{3} \frac{1}{2} \frac{\partial \theta}{\partial x_d} \left( \theta f_{\alpha-e_k-e_d} + (1 - \delta_{|\alpha|,M})(\alpha_d + 1) f_{\alpha-e_k+e_d} \right)
\]

\[
= -\frac{\mu}{\mu} f_{\alpha} H(|\alpha| - 2), \quad |\alpha| \leq M.
\]

Next, we try to derive the linearized system of (2.11). This requires us to examine the case that the distribution function is in a small neighborhood of an equilibrium state

\[
f_0(\xi) = \frac{\rho_0}{(2\pi\theta_0)^{3/2}} \exp \left( -\frac{|\xi|^2}{2\theta_0} \right),
\]

given by $\rho_0, \theta_0, u = 0$. We introduce the dimensionless variables $\bar{p}, \bar{\theta}, \bar{u}, \bar{p}_{ij}$ and $\bar{f}_\alpha$ as

\[
\rho = \rho_0 (1 + \bar{p}), \quad u = \sqrt{\theta_0} \bar{u}, \quad \theta = \theta_0 (1 + \bar{\theta}), \quad p = p_0 (1 + \bar{p}), \\
\bar{p}_{ij} = p_0 (\delta_{ij} + \bar{p}_{ij}), \quad f_\alpha = \rho_0 \theta_0 |\alpha| \bar{f}_\alpha, \quad x = L \cdot \bar{x}, \quad t = \frac{L}{\sqrt{\theta_0}} \bar{t},
\]

where $L$ is a characteristic length, $\bar{x}$ and $\bar{t}$ are the dimensionless coordinates and time, respectively. Assume all the dimensionless variables $\bar{p}, \bar{\theta}, \bar{u}, \bar{p}_{ij}$ and $\bar{f}_\alpha$ are small quantities. Substituting (2.12) into the globally hyperbolic moment system (2.11), and discarding all the high-order small quantities, and noticing that $u_d \frac{\partial}{\partial x_d}$ is high-order small quantity, 

\[
\frac{D f_{\alpha}}{Dt} \approx \frac{\partial f_{\alpha}}{\partial t},
\]

we obtain the linearized HME as

\[
\frac{\partial \bar{p}}{\partial t} + \frac{3}{d=1} \frac{\partial \bar{u}_d}{\partial x_d} = 0, \\
\frac{\partial \bar{u}_k}{\partial t} + \frac{\partial \bar{p}}{\partial x_k} + \frac{3}{d=1} \frac{\partial \bar{\sigma}_{kd}}{\partial x_d} = 0, \\
\frac{\partial \bar{p}_{ij}}{\partial t} + \frac{3}{d=1} \delta_{ij} \frac{\partial \bar{u}_d}{\partial x_d} + \frac{\partial \bar{u}_i}{\partial x_j} + \frac{3}{d=1} (e_i + e_j + e_d) \frac{\partial \bar{f}_{e_i+e_j+e_d}}{\partial x_d} = -\frac{\bar{\sigma}_{ij}}{Kn}, \\
\frac{\partial \bar{f}_\alpha}{\partial t} + \frac{3}{d=1} \frac{\partial \bar{f}_{\alpha-e_d}}{\partial x_d} + \frac{3}{d=1} (\alpha_d + 1)(1 - \delta_{M})(\alpha_d + 1) \frac{\partial \bar{f}_{\alpha+e_d}}{\partial x_d} \\
+ \frac{3}{d=1} 2 \delta_{\alpha,e_d+2e_k} \frac{\partial \theta}{\partial x_d} = -\frac{\bar{f}_\alpha}{Kn}, \quad 3 \leq |\alpha| \leq M,
\]
where \( \hat{\sigma}_{ij} = \hat{p}_{ij} - \hat{p} \delta_{ij}, i, j = 1, 2, 3, \) and \( \delta_{\alpha, e_d + 2e_k} = 1 \) iff \( \alpha = e_d + 2e_k, \) otherwise is 0. The Knudsen number \( \text{Kn} \) is defined by

\[
\text{Kn} = \frac{\lambda}{L},
\]

where \( \lambda = \frac{m}{\rho_0^2} \sqrt{k_0} \) is the mean free path.

### 3 Boundary Condition

In this paper, we adopt Maxwell’s accommodation boundary condition \([29]\), which is the most commonly used boundary condition in gas kinetic theory. It is formulated as a linear combination of the specular reflection and the diffuse reflection. Wall boundary only requires the incoming half of the distribution function when \( \xi \cdot n > 0, \) where \( n \) is the unit normal vector pointing into the gas. With the given velocity \( u_W(t, x) \) and temperature \( \theta_W(t, x) \) of the wall, the boundary condition at the wall is

\[
f_W(t, x, \xi) = \begin{cases} \chi f_M^W(t, x, \xi) + (1 - \chi) f(t, x, \xi^*), & C_W^* \cdot n > 0, \\ f(t, x, \xi), & C_W^* \cdot n \leq 0, \end{cases}
\]

where

\[
\xi^* = \xi - 2(C_W^* \cdot n)n, \quad C_W^* = \xi - u_W(t, x),
\]

\[
f_M^W(t, x, \xi) = \frac{\rho_W(t, x)}{(2\pi \theta_W(t, x))^{3/2}} \exp \left(-\frac{|\xi - u_W(t, x)|^2}{2\theta_W(t, x)} \right),
\]

and \( \chi \in [0, 1] \) is the accommodation coefficient.

A boundary condition for general hyperbolic moment system was proposed in \([7]\), which is derived from the Maxwell boundary condition by calculating the expression of the moments at the wall. Here we are purposely considering only steady shear flow, thus we adopt an alternative approach to derive our boundary conditions. Let the unit normal vector of the wall \( n = (0, 1, 0)^T. \) The velocity of the wall \( u_W = (u_W, 0, 0), \) and velocity for steady shear flow is \( u = (u_1, 0, 0). \) For \( \xi^* = (\xi_1, -\xi_2, \xi_3), \) (3.1) is precisely as

\[
f_W(x, \xi) = \begin{cases} \chi f_M^W(x, \xi) + (1 - \chi) f(x, \xi^*), & \xi_2 > 0, \\ f(x, \xi), & \xi_2 \leq 0, \end{cases}
\]

Denote \( \Omega = \{ \xi \in \mathbb{R}^3 \}, \) \( \Omega^+ = \{ \xi_1 \in \mathbb{R}, \xi_2 \in \mathbb{R}^+, \xi_3 \in \mathbb{R} \} \) and \( \Omega^- = \{ \xi_1 \in \mathbb{R}, \xi_2 \in \mathbb{R}^-, \xi_3 \in \mathbb{R} \}. \) The integral of the wall distribution function (3.3) with any function \( \psi(C) \) gives us an equation

\[
\int_{\Omega} \psi(C) f_W(x, \xi) d\xi = \int_{\Omega^-} \psi(C) f(x, \xi) d\xi \\
+ \int_{\Omega^+} \psi(C) (\chi f_M^W(x, \xi - u_W) + (1 - \chi) f(x, \xi^*)) d\xi,
\]

where \( C = (\xi_1 - u_1, \xi_2, \xi_3). \)

Definitely, for HME one has to restrict the form of function \( \psi(C), \) otherwise (3.4) will produce too many boundary conditions. It is clear that we should restrict ourselves to those \( \psi \)'s that the moments in the equation can be retrieved. Thus those \( \psi \)'s are polynomials as \( C^\beta, |\beta| \leq M, \) where \( \beta = (\beta_1, \beta_2, \beta_3) \in \mathbb{N}^3 \) is a 3D multi-index. Moreover, the distribution function of shear flow is an even function in the \( \xi_3 \) direction, which leads to \( f_\beta = 0, \) for \( \beta_3 \) is odd. Following Grad’s theory \([12]\) to limit the number of boundary
condition in order to ensure the continuity of boundary conditions when $\chi \to 0$, only a subset of all the moments corresponding to

$$\{ C^\beta | \beta \in \mathbb{I} \}, \quad \mathbb{I} = \{ |\beta| \leq M \mid \beta_2 \text{ is odd and } \beta_3 \text{ is even} \}$$

(3.5)
can be used to construct the wall boundary conditions. Then we reformulate the equation (3.4) as

$$\int_{\Omega^+} C^\beta f^W_M (x, \xi - u^W) \, d\xi = \frac{1}{\chi} \left( \int_{\Omega^+} C^\beta \left( f(x, \xi) - (1 - \chi) f(x, \xi^*) \right) \, d\xi \right), \quad \beta \in \mathbb{I}. \quad (3.6)$$

Notice that the basis function defined in (2.8) is decoupled in components of $\xi$. We then substitute (2.6) into (3.6) to calculate the integral on both left and right hand side in (3.6), respectively. To give the results, we first make some simplification and define the following notations. Let

$$J_0(u, \theta) = 1, \quad J_1(u, \theta) = u, \quad J_{k+1}(u, \theta) = u J_k(u, \theta) + k \theta J_{k-1}, k \geq 1,$$

(3.7)

then

$$\frac{1}{\sqrt{2\pi \theta W}} \int_{-\infty}^{\infty} (\xi_1 - u_1)^k \exp \left( -\frac{|\xi_1 - u_1|^2}{2\theta W} \right) \, d\xi_1 = J_k(u_1^W - u_1, \theta W).$$

Let

$$K(k, m) := \int_{-\infty}^{\infty} \frac{1}{\sqrt{2\pi}} \exp \left( -\frac{|\xi|^2}{2} \right) \xi^k H_e_m(\xi) \, d\xi,$$

where $H_e_m(\xi)$ is $m$-th Hermite polynomial, then using the orthogonal relation of the Hermite polynomials, one can find $K(0, m) = \delta_{0, m}$. Denote the half space integral by

$$S^*(k, m) := \int_{0}^{\infty} \xi^k H_e_m(\xi) \exp \left( -\frac{\xi^2}{2} \right) \, d\xi,$$

(3.8)

and we have the following properties for $S^*(k, m)$.

- Recursion relation:
  $$S^*(k, m) = (k - 1)S^*(k - 2, m) + mS^*(k - 1, m - 1). \quad (3.9)$$

- The value of $S^*(k, m)$ is:
  1. If $m \leq k$:
     (a) If $k - m$ is even, $S^*(k, m) = \sqrt{2\pi} \cdot A$;
     (b) If $k - m$ is odd, $S^*(k, m) = B$;
     here $A$ and $B$ are two algebraic numbers.
  2. If $m > k$ and $k - m$ is even, $S^*(k, m) = 0$.

Let

$$S(k, m) := \frac{\chi^m}{\sqrt{2\pi}} S^*(k, m)$$

$$= \frac{\theta^{(m-k)/2}}{\chi} \int_{0}^{\infty} \xi^k \left( H_e_m(\xi) - (1 - \chi) H_e_m(-\xi) \right) \exp \left( -\frac{\xi^2}{2} \right) \, d\xi,$$

(3.10)
where
\[ \tilde{\chi} = \begin{cases} 1, & m \text{ is even}, \\ \frac{2}{\chi}, & m \text{ is odd}, \end{cases} \]
then for each \( \beta \in \mathbb{I} \) in (3.5), the left and right hand side of (3.6) can be represented by
\[ \text{lhs of (3.6)} = \frac{\rho^W (\theta^W)^{(\beta_2+\beta_3)/2}}{\sqrt{2\pi}} f_{\beta_1} \left( u_1^W - u_1, \theta^W \right) (\beta_2 - 1)!!(\beta_3 - 1)!!, \]
\[ \text{rhs of (3.6)} = \sum_{\alpha \in \mathbb{N}^3} \left( K(\beta_1, \alpha_1) S(\beta_2, \alpha_2) K(\beta_3, \alpha_3) \theta^{(\beta_2-\alpha_2)/2} \right) f_{\alpha}. \]

Noticing \( K(0, m) = \delta_{0,m} \), by setting \( \beta = e_2 \) in (3.11), we have
\[ \rho^W \sqrt{\theta^W} = \sum_{m=0}^{\infty} S(1, m) \frac{f_{me_2}}{\theta^{(m-1)/2}}. \]

Let \( p_w = \rho^W \sqrt{\theta^W} \), then we have
\[ p_w = \sqrt{2\pi} \sum_{m=0}^{\infty} S(1, m) \frac{f_{me_2}}{\theta^{(m-1)/2}} = p + f_{2e_2} - \frac{f_{4e_2}}{2} + \frac{3}{4} f_{6e_2} - \frac{15}{32} f_{8e_2} + \cdots. \]

The boundary condition for the case \( \beta = e_1 + e_2 \) is
\[ \frac{\rho^W}{\sqrt{2\pi}} (\theta^W)^{\beta_1/2} (u_1^W - u_1)(\beta_2 - 1)!! S(\beta_2, \alpha_2) f_{\epsilon_1+\alpha_2 e_2} \theta^{(\beta_2-\alpha_2)/2}. \]

Particularly, for the case \( \beta = e_1 + e_2 \), one has
\[ p_w \sqrt{\theta^W} (u_1^W - u_1) = S(1, 1) \sigma_{12} + \sum_{\alpha_2 > 1} S(1, \alpha_2) f_{\epsilon_1+\alpha_2 e_2} \theta^{(1-\alpha_2)/2}. \]

Here we only consider the boundary condition for the specific case that \( \beta = e_1 + e_2 \) in (3.14), which is
\[ p_w \left( \frac{\theta^W}{\sqrt{2\pi}} (\beta_2 - 1)!! (u_1^W - u_1) = \sum_{\alpha_2} \theta^{1+\beta_2-\alpha_2/2} S(\beta_2, \alpha_2) f_{\epsilon_1+\alpha_2 e_2}. \right. \]

We linearize this condition at \( \theta_0 \) as that in (2.12) for our purpose, and assume \( \theta^W - \theta_0 \) is a small quantity. By substituting (2.12) into (3.15), and applying the closure of HME, i.e \( f_\alpha = 0, |\alpha| > M \), the linearized boundary condition is arrived at as
\[ \frac{(\beta_2 - 1)!!}{\sqrt{2\pi}} (\bar{u}_1^W - \bar{u}_1) = \sum_{\alpha_2 \leq M} S(\beta_2, \alpha_2) \tilde{f}_{\epsilon_1+\alpha_2 e_2}, \]
where \( \bar{u}_1^W \) is defined as dimensionless variable \( u_1^W = \sqrt{\theta_0} \bar{u}_1^W \), and \( \beta_2 \) is odd and \( |\beta_2| \leq M \).

### 4 Kramers’ Problem

Our setup for Kramers’ problem is standard. The gas flow in a half-space over a flat wall is considered, and the coordinates are chosen such that \( x \) direction is parallel to the wall, and \( y \) direction is perpendicular to the wall. The solid wall is fixed on \( \bar{y} = 0 \) (\( \bar{u}_1^W = 0 \)). The temperature and density of the gas far from the wall are constant. Gas velocity is \( \bar{u} = (\bar{u}_1, 0, 0) \) and all derivatives in equations (2.13) in \( x \) and \( z \) direction are zero.
4.1 Formal solution of linearized HME

We give the formal solution of the linearized HME at first. The setup of Kramers’ problem makes the equations of linearized moment system (2.13) related to velocity decoupled from the whole linearized moment system, which enables us to investigate the velocity by studying a small system as

\[
\frac{d\bar{\sigma}_{12}}{d\bar{y}} = 0, \\
\frac{d\bar{u}_1}{d\bar{y}} + 2\frac{d\bar{f}_{e_1+2e_2}}{d\bar{y}} = -\frac{1}{Kn}\bar{\sigma}_{12}, \\
\frac{d\bar{\sigma}_{12}}{d\bar{y}} + 3\frac{d\bar{f}_{e_1+3e_2}}{d\bar{y}} = -\frac{1}{Kn}\bar{f}_{e_1+2e_2}, \\
\cdots \\
\frac{d\bar{f}_{e_1+(M-2)e_2}}{d\bar{y}} = -\frac{1}{Kn}\bar{f}_{e_1+(M-1)e_2},
\]

\[(4.1)\]

We collect the variables involved in (4.1) into a vector

\[
V = (\bar{u}_1, \bar{\sigma}_{12}, \bar{f}_{e_1+2e_2}, \bar{f}_{e_1+3e_2}, \cdots, \bar{f}_{e_1+(M-1)e_2})^T,
\]

and then (4.1) is formulated as

\[
M \frac{dV}{d\bar{y}} = -\frac{1}{Kn}QV,
\]

\[(4.2)\]

where

\[
M = \begin{pmatrix}
0 & 1 & 1 & 0 & 2 & 1 & 0 & 3 & \cdots & \cdots & \cdots \\
1 & 0 & 3 & 1 & 0 & M - 1 & 1 & 0 & \cdots & \cdots & \cdots \\
\end{pmatrix}, \quad Q = \begin{pmatrix}
0 & 1 & \cdots & \cdots & \cdots \\
1 & \cdots & \cdots & \cdots & \cdots \\
\end{pmatrix}.
\]

\[(4.3)\]

Easy to check that the matrix \(M\) is real diagonalizable. Actually, we have the eigen-decomposition of \(M\) as \(M = R\Lambda R^{-1}\), where \(R\) is the Hermite transformation matrix

\[
R = (r_{ij})_{M \times M}, \quad r_{ij} = \frac{He_{i-1}(\lambda_j)}{(i - 1)!}, \quad i, j = 1, \cdots, M,
\]

\[(4.4)\]

and \(\Lambda = \text{diag}\{\lambda_i; i = 1, \cdots, M\}\), where the eigenvalues \(\lambda_i, i = 1, \cdots, M\) are zeros of the \(M\)-th order Hermite polynomial \(He_M(x)\). We sort the eigenvalues \(\lambda_i\) in decending order, saying \(\lambda_i > \lambda_{i+1}\). The diagonal matrix \(\Lambda\) can then be written as

\[
\Lambda = \begin{pmatrix}
\Lambda_+ & \\
\Lambda_{\leq 0} & \\
\end{pmatrix},
\]

\[(4.5)\]

\[
\Lambda_+ = \text{diag}\left\{\lambda_i; i = 1, \cdots, \left\lfloor \frac{M}{2} \right\rfloor\right\},
\]

\[(4.6)\]

\[
\Lambda_{\leq 0} = \text{diag}\left\{\lambda_i; i = \left\lceil \frac{M}{2} \right\rceil + 1, \cdots, M\right\}.
\]
The first equation of (4.2) indicates $\tilde{\sigma}_{12}$ is a constant and the second equation of (4.2) gives that
\[
\tilde{u}_1(\tilde{y}) = -\frac{\tilde{y}}{Kn}\tilde{\sigma}_{12} - 2\tilde{f}_{e_1+2e_2}(\tilde{y}) + c_0,
\]
where $c_0$ is a constant to be determined. We denote
\[
\hat{V} = (\tilde{f}_{e_1+2e_2}, \tilde{f}_{e_1+3e_2}, \cdots, \tilde{f}_{e_1+(M-1)e_2})^T,
\]
which is the remaining part of $V$ excluded the first two variables $\tilde{u}_1$ and $\tilde{\sigma}_{12}$. Then the system with higher order moments is separated from (4.2), which reads as
\[
\hat{M} \frac{d\hat{V}}{d\tilde{y}} = -\frac{1}{Kn}\hat{V},
\]
where
\[
\hat{M} = \begin{pmatrix}
0 & 3 & \\
1 & 0 & 4 \\
& \ddots & \ddots \\
& & 1 & 0 & M-1 \\
& & & 1 & 0
\end{pmatrix}.
\]

Correspondingly to the matrix $\hat{M}$, the matrix $\hat{M}$ is real diagonalizable, too. Precisely, let
\[
\hat{H}e_0(x) = 1, \quad \hat{H}e_1(x) = x, \quad \hat{H}e_k(x) = x\hat{H}e_k(x) - (k+2)\hat{H}e_{k-1}(x), \quad k \geq 1,
\]
then the characteristic polynomial of $\hat{M}$ is $\hat{H}e_{M-2}(\lambda)$. The recursion relation implies that $\hat{H}e_k(x)$ has $k$ real and simple zeros, and thus $\hat{M}$ is real diagonalizable and the eigenvalues $\hat{\lambda}_i$, $i = 1, \cdots, M-2$, are the zeros of $\hat{H}e_{M-2}(\lambda)$. Furthermore, if $\hat{\lambda}_i$ is an eigenvalue of $\hat{M}$, then $-\hat{\lambda}_i$ has to be an eigenvalue of $\hat{M}$, since $\hat{H}e_{M-2}(x)$ is an odd function if $M$ is odd and is an even function if $M$ is even. As for the matrix $\hat{M}$, we sort the eigenvalues $\hat{\lambda}_i$ in descending order, too, to make the diagonal matrix
\[
\hat{\Lambda} = \begin{pmatrix}
\hat{\Lambda}_+ & \\
\hat{\Lambda}_{\leq 0}
\end{pmatrix},
\]
\[
\hat{\Lambda}_+ = \text{diag} \left\{ \hat{\lambda}_i; \quad i = 1, \cdots, \left\lfloor \frac{M}{2} \right\rfloor - 1 \right\},
\]
\[
\hat{\Lambda}_{\leq 0} = \text{diag} \left\{ \hat{\lambda}_i; \quad i = \left\lfloor \frac{M}{2} \right\rfloor, \cdots, M-2 \right\}.
\]

Then eigen-decomposition of $\hat{M}$ is $\hat{M} = \hat{R} \hat{\Lambda} \hat{R}^{-1}$, where
\[
\hat{R} = (\hat{r}_{ij})_{(M-2) \times (M-2)}, \quad \hat{r}_{ij} = \frac{\hat{H}e_{i-1}(\hat{\lambda}_j)}{(i+1)!}, \quad i, j = 1, \cdots, M-2.
\]

Let us define the matrix $\hat{R}_+$ as the left $\left\lfloor \frac{M}{2} \right\rfloor - 1$ columns of $\hat{R}$, $\hat{R}_-$ as the right $\left\lfloor \frac{M}{2} \right\rfloor - 1$ columns of $\hat{R}$ for latter usage, and precisely, we have
\[
\hat{R}_+ = \begin{pmatrix}
\frac{\hat{H}e_0(\hat{\lambda}_1)}{2!} & \cdots & \frac{\hat{H}e_0(\hat{\lambda}_{M-1})}{2!} \\
\vdots & \ddots & \vdots \\
\frac{\hat{H}e_{M-3}(\hat{\lambda}_1)}{(M-1)!} & \cdots & \frac{\hat{H}e_{M-3}(\hat{\lambda}_{M-1})}{(M-1)!}
\end{pmatrix}, \quad \hat{R}_- = \begin{pmatrix}
\frac{\hat{H}e_0(\hat{\lambda}_{M/2+1})}{2!} & \cdots & \frac{\hat{H}e_0(\hat{\lambda}_{M-1})}{2!} \\
\vdots & \ddots & \vdots \\
\frac{\hat{H}e_{M-3}(\hat{\lambda}_{M/2+1})}{(M-1)!} & \cdots & \frac{\hat{H}e_{M-3}(\hat{\lambda}_{M-2})}{(M-1)!}
\end{pmatrix}.
Let $\hat{\mathbf{R}}_{+,\text{even}}$, which is made with the even rows of $\hat{\mathbf{R}}_+$ as

$$
\hat{\mathbf{R}}_{+,\text{even}} \triangleq (\hat{r}_{ij}), \text{ where } i \text{ is even, } j = 1, \ldots, \lfloor \frac{M}{2} \rfloor - 1,
$$

be a $\lfloor \frac{M}{2} \rfloor - 1 \times \lfloor \frac{M}{2} \rfloor - 1$ square matrix. And corresponding to $\hat{\mathbf{R}}_{+,\text{even}}$, define $\hat{\mathbf{R}}_{+,\text{odd}}, \hat{\mathbf{R}}_{-,\text{odd}}, \hat{\mathbf{R}}_{-,\text{even}}$ as

$$
\hat{\mathbf{R}}_{+,\text{odd}} \triangleq (\hat{r}_{ij}), \text{ where } i \text{ is odd, } j = 1, \ldots, \lfloor \frac{M}{2} \rfloor - 1,
$$

and

$$
\hat{\mathbf{R}}_{-,\text{even}} \triangleq (\hat{r}_{ij}), \text{ where } i \text{ is even, } j = \lfloor \frac{M}{2} \rfloor, \ldots, M - 2,
$$

and

$$
\hat{\mathbf{R}}_{-,\text{odd}} \triangleq (\hat{r}_{ij}), \text{ where } i \text{ is odd, } j = \lfloor \frac{M}{2} \rfloor, \ldots, M - 2.
$$

We declare that

**Lemma 1.** $\hat{\mathbf{R}}_{+,\text{even}}$ is invertible.

**Proof.** Let $P_{\sigma}$ to be the permutation matrix of the permutation

$$
\sigma : \{1, 2, \ldots, M - 2\} \rightarrow \{1, 2, \ldots, M - 2\}, \quad (4.9)
$$

that

$$
\sigma(i) = \text{ mod } (i, 2) \times (\lfloor \frac{M}{2} \rfloor - 1) + \lfloor i/2 \rfloor.
$$

The permutation maps the list of numbers $1, 2, \ldots, M - 2$ to

$$
2, 4, 6, \ldots, 1, 3, 5, \ldots
$$

that the even numbers are ahead of the odd numbers. Then matrix $\hat{\mathbf{R}}$ is re-organized by the permutation matrix as

$$
P_{\sigma}^{-1} \hat{\mathbf{R}} = \begin{pmatrix}
\hat{\mathbf{R}}_{+,\text{even}} & \hat{\mathbf{R}}_{-,\text{even}} \\
\hat{\mathbf{R}}_{+,\text{odd}} & \hat{\mathbf{R}}_{-,\text{odd}}
\end{pmatrix}.
$$

Notice that each eigenvalue $\hat{\lambda}_i \in \hat{\Lambda}_+, -\hat{\lambda}_i \in \hat{\Lambda}_{\leq 0}$. Then for any eigenvector

$$
\hat{\mathbf{r}}_i = (\hat{r}_{i,\text{even}} | \hat{r}_{i,\text{odd}})^T \in (\hat{\mathbf{R}}_{+,\text{even}} | \hat{\mathbf{R}}_{+,\text{odd}})^T,
$$

there exists a column vector

$$
\hat{\mathbf{r}}_j = (\hat{r}_{j,\text{even}} | \hat{r}_{j,\text{odd}})^T \in (\hat{\mathbf{R}}_{-,\text{even}} | \hat{\mathbf{R}}_{-,\text{odd}})^T.
$$

Then

$$
\hat{\mathbf{r}}_i - \hat{\mathbf{r}}_j = 2(\hat{r}_{i,\text{even}} | 0)^T.
$$

The set of vectors $\hat{\mathbf{r}}_i - \hat{\mathbf{r}}_j$ are linearly independent since $\hat{\mathbf{r}}_i, \hat{\mathbf{r}}_j$ are eigenvectors of $\hat{\mathbf{R}}$, then columns of $\hat{\mathbf{R}}_{+,\text{even}}$ are linearly independent. Thus $\hat{\mathbf{R}}_{+,\text{even}}$ is invertible. $\square$
4.1.1 Illustrative examples: \( M \leq 5 \)

We examine the cases for small \( M \) to find out the formal solution for generic \( M \). The simplest system is the case for \( M = 3 \). The variables are \( V = (\bar{u}_1, \bar{\sigma}_{12}, \bar{f}_{e_1+2e_2})^T \), and matrices \( M \) and \( Q \) in (4.2) are

\[
M = \begin{pmatrix}
0 & 1 & 0 \\
1 & 0 & 2 \\
0 & 1 & 0
\end{pmatrix}, \quad Q = \begin{pmatrix}
0 & 1 \\
1 & 1
\end{pmatrix}.
\]

Since \( \bar{\sigma}_{12} \) is constant and the velocity is

\[
\bar{u}_1 = -\bar{\sigma}_{12} \frac{\bar{y}}{Kn} + c_0,
\]

it is clear that the solution of \( \bar{u}_1 \) is not able to capture the boundary layer since here \( \bar{u}_1 \) is a linear function of \( \bar{y} \). To capture the boundary layer of velocity, we need more moments thus we turn to the case \( M = 4 \). For \( M = 4 \), the equations (4.1) are

\[
\begin{align*}
\frac{d\bar{\sigma}_{12}}{d\bar{y}} &= 0, \\
\frac{d\bar{u}_1}{d\bar{y}} + 2\frac{d\bar{f}_{e_1+2e_2}}{d\bar{y}} &= -\frac{1}{Kn} \bar{\sigma}_{12}, \\
\frac{d\bar{\sigma}_{12}}{d\bar{y}} + 3\frac{d\bar{f}_{e_1+3e_2}}{d\bar{y}} &= -\frac{1}{Kn} \bar{f}_{e_1+2e_2}, \\
\frac{d\bar{f}_{e_1+2e_2}}{d\bar{y}} &= \frac{1}{Kn} \bar{f}_{e_1+3e_2}.
\end{align*}
\]

The solution gives us the expression of velocity as

\[
\bar{u}_1 = -\bar{\sigma}_{12} \frac{\bar{y}}{Kn} - 2\bar{f}_{e_1+2e_2} + c_0
\]

from the second equation in (4.10). Here we need to solve the equations (4.7) for \( \hat{V} = (\hat{f}_{e_1+2e_2}, \hat{f}_{e_1+3e_2})^T \), where

\[
\hat{M} = \begin{pmatrix}
0 & 3 \\
1 & 0
\end{pmatrix}.
\]

The matrix \( \hat{M} \) can be decomposed as \( \hat{M} = \hat{R} \hat{\Lambda} \hat{R}^{-1} \),

\[
\hat{\Lambda} = \begin{pmatrix}
\sqrt{3} \\
-\sqrt{3}
\end{pmatrix}, \quad \hat{R} = \begin{pmatrix}
\frac{1}{\sqrt{3}} & -\frac{1}{\sqrt{3}} \\
\frac{1}{\sqrt{3}} & \frac{1}{\sqrt{3}}
\end{pmatrix}.
\]

Hence, the solution of system (4.7) is

\[
\hat{V} = \hat{R} \exp \left( -\frac{\bar{y}}{Kn} \hat{\Lambda}^{-1} \right) \hat{R}^{-1} \hat{V}^{(0)}.
\]

By setting \( \hat{c} = (\hat{c}_1, \hat{c}_2)^T = \hat{R}^{-1} \hat{V}^{(0)} \), the equations above result in

\[
\hat{V} = \begin{pmatrix}
\hat{f}_{e_1+2e_2} \\
\hat{f}_{e_1+3e_2}
\end{pmatrix} = \hat{R} \exp \left( -\frac{\bar{y}}{Kn} \hat{\Lambda}^{-1} \right) \hat{c} = \begin{pmatrix}
\hat{c}_1 \exp(-\frac{\bar{y}}{\sqrt{3}Kn}) + \hat{c}_2 \exp(\frac{\bar{y}}{\sqrt{3}Kn}) \\
\frac{\sqrt{3}}{3} \hat{c}_1 \exp(-\frac{\bar{y}}{\sqrt{3}Kn}) - \frac{\sqrt{3}}{3} \hat{c}_2 \exp(\frac{\bar{y}}{\sqrt{3}Kn})
\end{pmatrix}.
\]
The exponential terms provide us the boundary layer. Since all the variables have to remain finite as \( \bar{y} \to \infty \), the term \( \exp\left(-\frac{1}{\sqrt{3}Kn} \bar{y}\right) \) has to be dropped. Therefore,

\[
\left( \frac{\bar{f}_{e_1+2e_2}}{\bar{f}_{e_1+3e_2}} \right) = \hat{\mathbf{R}} \left( \begin{array}{c}
\exp\left(-\frac{\bar{y}}{Kn} \bar{\Lambda}_+^{-1}\right) \\
0
\end{array} \right) \hat{c}_1 \exp\left(-\frac{\bar{y}}{\sqrt{3}Kn} \right) \left( \begin{array}{c}
\frac{1}{\sqrt{3}}
\end{array} \right).
\]

Here \( \bar{\Lambda}_+ \) is a 1 \( \times \) 1 matrix with its entry as \( \sqrt{3} \). Applying the linearized boundary condition \([3.16]\), i.e.

\[
-\frac{1}{\sqrt{2\pi}} \bar{u}_1 = S(1, 1)\bar{\sigma}_{12} + S(1, 2)\bar{f}_{e_1+2e_2} + S(1, 3)\bar{f}_{e_1+3e_2},
\]

\[
-\frac{2}{\sqrt{2\pi}} \bar{u}_1 = S(3, 1)\bar{\sigma}_{12} + S(3, 2)\bar{f}_{e_1+2e_2} + S(3, 3)\bar{f}_{e_1+3e_2},
\]

we can obtain

\[
\hat{c}_1 = -\frac{\sqrt{\pi}(\chi - 2)}{2(3\sqrt{7}\pi(\chi - 2) - 10\sqrt{2}\chi)} \bar{\sigma}_{12}, \quad c_0 = \sqrt{\frac{\pi}{2}} \frac{\chi - 2}{\chi} \left( 1 + \frac{\sqrt{2}\chi}{4\sqrt{2}\chi + 2\sqrt{3}\pi(2 - \chi)} \right) \bar{\sigma}_{12}.
\]

Then the solution of velocity is

\[
\bar{u}_1 = -\bar{\sigma}_{12} \frac{\bar{y}}{Kn} - 2\hat{c}_1 \exp\left(-\frac{\bar{y}}{\sqrt{3}Kn}\right) + c_0.
\]

Similar procedure can be carried out for greater \( M \). For example, if we set \( M = 5 \), then \( V = (\bar{u}_1, \bar{\sigma}_{12}, \bar{f}_{e_1+2e_2}, \bar{f}_{e_1+3e_2}, \bar{f}_{e_1+4e_2})^T \) and \( \hat{V} = (\bar{f}_{e_1+2e_2}, \bar{f}_{e_1+3e_2}, \bar{f}_{e_1+4e_2})^T \). The matrix \( \hat{\mathbf{M}} = \mathbf{R} \hat{\mathbf{M}} \mathbf{R}^{-1} \) in \([4.17]\) is

\[
\hat{\mathbf{M}} = \left( \begin{array}{ccc}
0 & 3 & 0 \\
1 & 0 & 1 \\
0 & 0 & 1
\end{array} \right) \quad \text{with} \quad \hat{\mathbf{A}} = \left( \begin{array}{cc}
\sqrt{7} & 0 \\
0 & -\sqrt{7}
\end{array} \right), \quad \hat{\mathbf{R}} = \left( \begin{array}{ccc}
1 & 1 & 1 \\
\sqrt{7}/3 & 0 & -\sqrt{7}/3 \\
1/3 & -1/4 & 1/3
\end{array} \right).
\]

Notice that \( M = 5 \) is odd, so zero is a simple eigenvalue of \( \hat{\mathbf{M}} \). This vanished eigenvalue provides a constant factor in the exponential terms in the boundary layer, while the eigenvalue \( \sqrt{7} \) of matrix \( \hat{\mathbf{M}} \) provides the only term still which survives in the solution. The solution of \([4.17]\) is

\[
\hat{V} = \left( \begin{array}{c}
\bar{f}_{e_1+2e_2} \\
\bar{f}_{e_1+3e_2} \\
\bar{f}_{e_1+4e_2}
\end{array} \right) = \hat{\mathbf{R}} \left( \begin{array}{c}
\exp\left(-\frac{\bar{y}}{Kn} \bar{\Lambda}_+^{-1}\right) \\
0
\end{array} \right) \hat{c}_1 \exp\left(-\frac{\bar{y}}{\sqrt{7}Kn} \right) \left( \begin{array}{c}
\frac{1}{\sqrt{7}}
\frac{1}{3}
\frac{1}{3}
\end{array} \right),
\]

where \( \hat{c} = (\hat{c}_1, \hat{c}_2, \hat{c}_3)^T = \mathbf{R}^{-1} \hat{V}^{(0)} \) and the entry of the 1 \( \times \) 1 matrix \( \hat{\Lambda}_+ \) is \( \sqrt{7} \). Similar as in the case \( M = 4 \), there are 2 coefficients \( c_0 \) and \( \hat{c}_1 \) to be determined. To fix the coefficients, we utilize two boundary conditions by setting \( \beta_2 = 1, 3 \) in \([3.16]\)

\[
-\frac{1}{\sqrt{2\pi}} \bar{u}_1 = S(1, 1)\bar{\sigma}_{12} + S(1, 2)\bar{f}_{e_1+2e_2} + S(1, 3)\bar{f}_{e_1+3e_2} + S(1, 4)\bar{f}_{e_1+4e_2},
\]

\[
-\frac{2}{\sqrt{2\pi}} \bar{u}_1 = S(3, 1)\bar{\sigma}_{12} + S(3, 2)\bar{f}_{e_1+2e_2} + S(3, 3)\bar{f}_{e_1+3e_2} + S(3, 4)\bar{f}_{e_1+4e_2}.
\]

Direct calculations yield

\[
\hat{c}_1 = -\frac{3\sqrt{\pi}(\chi - 2)}{2(3\sqrt{7}\pi(\chi - 2) - 10\sqrt{2}\chi)} \bar{\sigma}_{12}, \quad c_0 = \sqrt{\frac{\pi}{2}} \frac{\chi - 2}{\chi} \left( 1 - \frac{2\sqrt{2}\chi}{3\sqrt{7}\pi(\chi - 2) - 10\sqrt{2}\chi} \right) \bar{\sigma}_{12}.
\]
Then the solution of velocity is given by

$$\bar{u}_1 = -\bar{\sigma}_{12} \frac{\bar{y}}{Kn} - 2\hat{c}_1 \exp \left( -\frac{\bar{y}}{\sqrt{7Kn}} \right) + c_0.$$  

4.1.2 General case: arbitrary $M$

Now we are ready to present the formal solution for arbitrary $M$. Following the examples above, we have to drop those unbounded factors to attain a stable solution that only the terms contributed from the positive eigenvalues of $\hat{M}$ are kept. Thus the stable solution of (4.7) is

$$\hat{V}(\bar{y}) = \hat{R} \left( \exp \left( -\frac{\bar{y}}{Kn} \hat{\Lambda}^{-1} \right) 0 \right) \hat{c},$$  

(4.14)

where $\hat{c} = (\hat{c}_1, \cdots, \hat{c}_{M-2})^T = \hat{R}^{-1} \hat{V}(0)$. Clearly, there are only the beginning $\left\lfloor \frac{M}{2} \right\rfloor - 1$ entries in $\hat{c}$ appears in $\hat{V}(\bar{y})$. With the expression of $\hat{f}_{e_1+2e_2}(\bar{y})$ provided as the first entry of $\hat{V}(\bar{y})$, the velocity is again given by the second equation in (4.1) as

$$\bar{u}_1(\bar{y}) = -\bar{\sigma}_{12} \frac{\bar{y}}{Kn} - 2 e_1^T \hat{V}(\bar{y}) + c_0,$$  

(4.15)

where $e_1 = (1, 0, \cdots, 0)^T$. Since $c_0$ in the expression of $\bar{u}_1(\bar{y})$ is also to be determined, there are in total $\left\lfloor \frac{M}{2} \right\rfloor$ indeterminate coefficients in $V(\bar{y})$.

Combining (4.14) and (4.15) with linearized boundary condition (3.16), we can obtain the boundary condition for (4.7) as

$$- \frac{(\beta_2 - 1)!!}{\sqrt{2\pi}} \bar{u}_1 = S(\beta_2, 1) \bar{\sigma}_{12} + \sum_{\alpha_2=2}^{M-1} S(\beta_2, \alpha_2) \hat{f}_{e_1+2e_2}, \quad \beta_2 = 1, 3, \cdots, 2 \left\lfloor \frac{M}{2} \right\rfloor - 1. \quad (4.16)$$

The total number of boundary condition is $\left\lfloor \frac{M}{2} \right\rfloor$, which may fix all coefficients in the solution of $V(\bar{y})$. Once these coefficients are fixed by the boundary conditions, we eventually attain $\bar{u}_1$ formulated as

$$\bar{u}_1(\bar{y}) = -\bar{\sigma}_{12} \frac{\bar{y}}{Kn} - 2 e_1^T \hat{V}(\bar{y}) + c_0$$

$$= -\bar{\sigma}_{12} \frac{\bar{y}}{Kn} - 2 e_1^T \hat{R} \left( \exp \left( -\frac{\bar{y}}{Kn} \hat{\Lambda}^{-1} \right) 0 \right) \hat{c} + c_0$$

$$= -\bar{\sigma}_{12} \frac{\bar{y}}{Kn} - 2 \sum_{i=1}^{\left\lfloor \frac{M}{2} \right\rfloor} \hat{c}_i \exp \left( -\frac{\bar{y}}{Kn\lambda_i} \right) + c_0. \quad (4.17)$$

We let $\bar{y} = 0$ in (4.17) to have $\bar{u}_1 = -2 \sum_{i=1}^{\left\lfloor \frac{M}{2} \right\rfloor} \hat{c}_i + c_0$ and substitute it into (4.16) to
obtain the following linear system

\[
-2 \sum_{i=1}^{[\frac{M}{2}]-1} \hat{c}_i + c_0 \begin{pmatrix}
\frac{1}{(3-1)!!} \\
\vdots \\
\frac{1}{(2[\frac{M}{2}]-2)!!}
\end{pmatrix} = \sigma_{12} \begin{pmatrix}
S(1,1) \\
S(3,1) \\
\vdots \\
S(2[\frac{M}{2}]-1,1)
\end{pmatrix}
\]

\[
= \begin{pmatrix}
S(1, 2) & S(1, 3) & \cdots & S(1, M - 1) \\
S(3, 2) & S(3, 3) & \cdots & S(3, M - 1) \\
\vdots & \vdots & \ddots & \vdots \\
S(2[\frac{M}{2}]-1, 2) & S(2[\frac{M}{2}]-1, 3) & \cdots & S(2[\frac{M}{2}]-1, M - 1)
\end{pmatrix} \hat{\mathbf{R}} \begin{pmatrix}
\hat{c}_1 \\
\vdots \\
\hat{c}_{[\frac{M}{2}]-1} \\
0
\end{pmatrix}
\]

Clearly, this is a linear system of for \(c = (c_0, \hat{c}_1, \ldots, \hat{c}_{[\frac{M}{2}]-1})^T\). Precisely, we let

\[
h = \frac{1}{\sqrt{2\pi}} \begin{pmatrix}
1 \\
(3-1)!! \\
\vdots \\
(2[\frac{M}{2}]-2)!!
\end{pmatrix}, \quad b = \begin{pmatrix}
S(1,1) \\
S(3,1) \\
\vdots \\
S(2[\frac{M}{2}]-1,1)
\end{pmatrix}
\]

\[
S = \begin{pmatrix}
S(1, 2) & S(1, 3) & \cdots & S(1, M - 1) \\
S(3, 2) & S(3, 3) & \cdots & S(3, M - 1) \\
\vdots & \vdots & \ddots & \vdots \\
S(2[\frac{M}{2}]-1, 2) & S(2[\frac{M}{2}]-1, 3) & \cdots & S(2[\frac{M}{2}]-1, M - 1)
\end{pmatrix}
\]

then the system \((4.18)\) is formulated as

\[
A c = -\sigma_{12} b,
\]

where \(A = \left(h, (S - 2he_1^T)\hat{\mathbf{R}}_+\right)\).

To fix the parameters in \(c\), the unique solvability of \((4.19)\) is required. Currently, we can only claim the system \((4.19)\) is uniquely solvable when \(\chi\) is an algebraic number. Precisely, we have the following theorem:

**Theorem 1.** \(|A| \neq 0\) if \(\chi\) is an algebraic number.

**Proof.** We times \(A\) by \(\begin{pmatrix} 1 & 2e_1^T \hat{\mathbf{R}}_+ \end{pmatrix}\) to obtain \((h, SR_+)\). Thus \(|A| = |(h, SR_+)|\).

We retrieve the coefficient \(h_m(\chi)\) in \(S(k, m)\) to have

\[
S = S_0^* H
\]

where \(H = \frac{1}{\sqrt{2\pi}} \text{diag}\{h_2(\chi), h_3(\chi), \ldots, h_{M-1}(\chi)\}\) and

\[
S_0^* = \begin{pmatrix}
S^*(1, 2) & S^*(1, 3) & \cdots & S^*(1, M - 1) \\
S^*(3, 2) & S^*(3, 3) & \cdots & S^*(3, M - 1) \\
\vdots & \vdots & \ddots & \vdots \\
S^*(2[\frac{M}{2}]-1, 2) & S^*(2[\frac{M}{2}]-1, 3) & \cdots & S^*(2[\frac{M}{2}]-1, M - 1)
\end{pmatrix}
\]

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By the recursion relation (3.9) of $S^*(k, m)$, we have that
\[
LS_0^* = \begin{pmatrix} S^*(1, 2), & S^*(1, 3), & \cdots, & S^*(1, M - 1) \end{pmatrix},
\]
where
\[
L = \begin{pmatrix} 1 & -2 & 1 & \cdots & 1 \\ 0 & 1 & -4 & \cdots & 1 \\ & & \ddots & \ddots & \ddots \\ & & & 0 & -(2 \frac{M}{2} - 2) & 1 \\
\end{pmatrix},
\]
and
\[
S_1^* = \begin{pmatrix} 2S^*(2, 1) & 3S^*(2, 2) & \cdots & (M - 1)S^*(2, M - 2) \\ 2S^*(4, 1) & 3S^*(4, 2) & \cdots & (M - 1)S^*(4, M - 2) \\ \vdots & \vdots & \ddots & \vdots \\ 2S^*(2 \frac{M}{2} - 2, 1) & 3S^*(2 \frac{M}{2} - 2, 2) & \cdots & (M - 1)S^*(2 \frac{M}{2} - 2, M - 2) \\
\end{pmatrix}.
\]
Noticing that $Lh = (1/\sqrt{2\pi}, 0, \cdots, 0)^T$, we have that
\[
(h, S\hat{R}_+) = L^{-1} \begin{pmatrix} 1/\sqrt{2\pi} \\ (S^*(1, 2), \cdots, S^*(1, M - 1)) \\ S_1^* \\
\end{pmatrix} \begin{pmatrix} 1 \\ H\hat{R}_+ \\
\end{pmatrix}.
\]
Thus we need only to verify the determinant of $S_1^*H\hat{R}_+$ is not vanished. Consider the permutation matrix in [13], we then see that
\[
S_1^*P_\sigma = (S_{\text{even}}^*, S_{\text{odd}}^*),
\]
where $S_{\text{even}}^*$ is made with the even columns of $S_1^*$ as
\[
S_{\text{even}}^* = \begin{pmatrix} 3S^*(2, 2) & 5S^*(2, 4) & 7S^*(2, 6) & \cdots \\ 3S^*(4, 2) & 5S^*(4, 4) & 7S^*(4, 6) & \cdots \\ \vdots & \vdots & \vdots & \vdots \\ 3S^*(2 \frac{M}{2} - 2, 2) & 5S^*(2 \frac{M}{2} - 2, 4) & 7S^*(2 \frac{M}{2} - 2, 6) & \cdots \\
\end{pmatrix},
\]
and $S_{\text{odd}}^*$ is made with the odd columns of $S_1^*$ as
\[
S_{\text{odd}}^* = \begin{pmatrix} 2S^*(2, 1) & 4S^*(2, 3) & 6S^*(2, 5) & \cdots \\ 2S^*(4, 1) & 4S^*(4, 3) & 6S^*(4, 5) & \cdots \\ \vdots & \vdots & \vdots & \vdots \\ 2S^*(2 \frac{M}{2} - 2, 1) & 4S^*(2 \frac{M}{2} - 2, 3) & 6S^*(2 \frac{M}{2} - 2, 5) & \cdots \\
\end{pmatrix}.
\]
With the integral properties of $S^*(k, m)$ in [3], $S_{\text{even}}^*$ is a lower triangular matrix and each entry in its lower triangular part is an algebraic number $\times \sqrt{2\pi}$.

The diagonal matrix $H$ is turned into
\[
P_\sigma^{-1}HP_\sigma = \frac{1}{\sqrt{2\pi}} \begin{pmatrix} I \\ -\chi I \\
\end{pmatrix}.
\]
We then have that
\[
S_1^*HP_\sigma P^{-1}_\sigma R_+^\dagger = S_1^* P_\sigma P^{-1}_\sigma R_+^\dagger,
\]
\[
= \frac{1}{\sqrt{2\pi}} \left( S_{\text{even}}^* S_{\text{odd}}^* \left( \begin{array}{c} I \\ 2 - \chi I \end{array} \right) \right) \left( \begin{array}{c} R_{+\text{,even}}^\dagger \\ R_{+\text{,odd}}^\dagger \end{array} \right)
\]
\[
= \frac{1}{\sqrt{2\pi}} \left( S_{\text{even}}^* \hat{R}_{+\text{,even}}^\dagger + \frac{2 - \chi}{\chi} S_{\text{odd}}^* \hat{R}_{+\text{,odd}}^\dagger \right).
\]

Since \( \hat{R}_{+\text{,even}}^\dagger \) is invertible by Lemma 1,
\[
S_1^*HP_\sigma P^{-1}_\sigma R_+^\dagger = \frac{1}{\sqrt{2\pi}} \left( S_{\text{even}}^* + \frac{2 - \chi}{\chi} S_{\text{odd}}^* \hat{R}_{+\text{,odd}}^{-1} \hat{R}_{+\text{,even}} \right) \hat{R}_{+\text{,even}}, \tag{4.20}
\]
and we only need to verify the matrix \( S_{\text{even}}^* + \frac{2 - \chi}{\chi} S_{\text{odd}}^* \hat{R}_{+\text{,odd}}^{-1} \hat{R}_{+\text{,even}} \) in (4.20) is not singular. Considering the polynomial of \( \lambda \) defined by
\[
p(\lambda) \triangleq \left| \frac{\lambda}{\sqrt{2\pi}} S_{\text{even}}^* + \frac{2 - \chi}{\chi} S_{\text{odd}}^* \hat{R}_{+\text{,odd}}^{-1} \hat{R}_{+\text{,even}} \right|,
\]
we point out that \( p(\lambda) \) is a polynomial with all coefficients to be algebraic numbers, since \( \chi \) is assumed to be algebraic, and entries of matrices \( \frac{1}{\sqrt{2\pi}} S_{\text{even}}^* \), \( \hat{R}_{+\text{,even}}^{-1} \), \( S_{\text{odd}}^* \), \( \hat{R}_{+\text{,odd}} \) are all algebraic numbers. Particularly, the coefficient of the leading term of \( p(\lambda) \) is the product of all diagonal entries in matrix \( \frac{1}{\sqrt{2\pi}} S_{\text{even}}^* \) and thus is not vanished. Therefore, \( p(\lambda) = 0 \) can only valid for \( \lambda \) to be an algebraic number, too. Thus \( p(\sqrt{2\pi}) \neq 0 \) and consequently \( |A| \neq 0 \). We conclude that the linear system (4.19) is uniquely solvable. \( \square \)

**Remark 1.** Definitely, we speculate that \( |A| \neq 0 \) for all \( \chi \), while currently we can not prove it unfortunately. If we take \( |A| \) as a function of \( \chi \), it is clearly a continuous function. The theorem above declares that the value of the function is not zero on all algebraic numbers, and by the continuity of the function, the roots for \( |A| = 0 \) can not be dense on \( \mathbb{R} \) at least.

### 4.2 Convergence in moment order

Let us reveal below the connection of the linearized HME and the linearized Boltzmann equation in [37]. For Kramers’ problem, the boundary condition we proposed is related with that in [37], either. Roughly speaking, our system is illustrated to be a particular discretization of the equation in [37]. This allows to examine the convergence of the solution of our systems to the numerical results of the equation in [37]. It is demonstrated that the solution converges to that of the linearized Boltzmann equation in [37] with the increasing of moment order. Let us start from a brief review of the main result on the Kramers’ problem in [37].

For the time independent Boltzmann equation
\[
\xi \cdot \nabla_x f = Q(f,f), \tag{4.21}
\]
considering here only Kramers’ problem is studied, we linearize the distribution function \( f \) as
\[
f(x,\xi) = M(x,\xi)[1 + h(x,\xi)], \tag{4.22}
\]
where $h(x, \xi)$ is a disturbance term caused by the small perturbation near the local equilibrium Maxwellian $\mathcal{M}(x, \xi)$, which has the form

$$
\mathcal{M}(x, \xi) = \frac{\rho_0(x, y)}{(2\pi \theta_0(x, y))^{3/2}} \exp \left( -\frac{(\xi_x - u(y))^2 + \xi_y^2 + \xi_z^2}{2\theta_0(x, y)} \right).
$$

Here $\rho_0$ and $\theta_0$ are same as that in (2.12), and

$$
u = Ky.
$$

Inserting (4.22) into the time independent Boltzmann equation (4.21), and discarding the high-order small quantities, we can obtain

$$
\xi \cdot \nabla_x \mathcal{M} + \mathcal{M} \xi \cdot \nabla_x h = J(\mathcal{M}, h),
$$

where $J(\mathcal{M}, h)$ is the linearized BGK collision

$$
J(\mathcal{M}, h) = -\mathcal{M} \left\{ \nu h - \frac{\nu}{\sqrt{2\pi \theta_0}} \int h(y, \xi') \left[ 1 + \frac{1}{\theta_0} \xi \cdot \xi' + \frac{2}{3} \left( \frac{\xi'^2}{2\theta_0} - \frac{3}{2} \right) \right] \exp \left( -\frac{\|\xi\|^2}{2\theta_0} \right) d\xi' \right\},
$$

where $\nu$ is the collision frequency of BGK model. For convenience, we introduce the dimensionless variables

$$
\xi_i = \sqrt{\theta_0} \xi_i, \quad K = \sqrt{\theta_0} K_0, \quad x = Lx, \quad Kn = \frac{\sqrt{\theta_0}}{L\nu}.
$$

Then direct calculations and some simplification yield

$$
\bar{\xi} \xi_y K_0 + \bar{\xi} \frac{\partial h(\bar{y}, \bar{\xi})}{\partial y}

= -\frac{1}{Kn} \left\{ h(\bar{y}, \bar{\xi}) - \frac{1}{\sqrt{2\pi}} \int h(\bar{y}, \bar{\xi}') \left[ 1 + \bar{\xi} \cdot \bar{\xi}' + \frac{2}{3} \left( \frac{\|\bar{\xi}'\|^2}{2\theta_0} - \frac{3}{2} \right) \right] \exp \left( -\frac{\|\bar{\xi}'\|^2}{2\theta_0} \right) d\bar{\xi}' \right\},
$$

and

$$
\bar{u}_1(\bar{y}) = K_0 \bar{y} + \frac{1}{\sqrt{2\pi}} \int_\infty Z(\bar{y}, \bar{\xi}) \exp \left( -\frac{\|\bar{\xi}\|^2}{2} \right) d\bar{\xi},
$$

where

$$
Z(\bar{y}, \bar{\xi}) = \frac{1}{2\pi} \int_\infty \int_\infty \bar{\xi} x h(\bar{y}, \bar{\xi}) \exp \left( -\frac{\bar{\xi}_x^2 + \bar{\xi}_z^2}{2} \right) d\bar{\xi}_x d\bar{\xi}_z.
$$

Then we have

$$
K_0 \bar{\xi} + \bar{\xi} \frac{\partial Z(\bar{y}, \bar{\xi})}{\partial y} = \frac{1}{Kn} \left( -Z(\bar{y}, \bar{\xi}) + \frac{1}{\sqrt{2\pi}} \int_\mathbb{R} Z(\bar{y}, \bar{\xi}') \exp \left( -\frac{\|\bar{\xi}'\|^2}{2} \right) d\bar{\xi}' \right).
$$

From (4.17) and (4.24) we notice that

$$
K_0 = \frac{\sigma_{12}}{Kn},
$$

and

$$
\int_{\xi_1 + i\epsilon_2} = \frac{1}{i!} \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}^3} H e_1(\bar{\xi}_x) H e_i(\bar{\xi}_y) h(\bar{y}, \bar{\xi}) \exp \left( -\frac{\|\bar{\xi}\|^2}{2} \right) d\bar{\xi}, \quad i = 1, \ldots, M - 1,
$$

$$
= \frac{1}{i!} \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} H e_i(\bar{\xi}) Z(\bar{y}, \bar{\xi}) \exp \left( -\frac{\|\bar{\xi}\|^2}{2} \right) d\bar{\xi}, \quad i = 1, \ldots, M - 1.
$$
Following [37], we use the model which is also based on the diffuse-specular process, and boundary condition can be written as

\[ f(0, \xi) = \chi N f_M^W(x, \xi) + (1 - \chi) f(0, \xi^*), \]

where \( f_M^W, \xi^* \) is defined in [3.2]. \( N \) is a normalizing factor to be determined [37]. Using the zero mass flux condition

\[ \int_{\xi_y < 0} \xi_y f(0, \xi) \, d\xi + \int_{\xi_y > 0} \xi_y f(0, \xi) \, d\xi = 0 \]

at \( y = 0 \) to calculate the \( N \). After the linearization and nondimensionalization, the boundary condition in Cartesian velocity coordinates as follows

\[ h(0, \xi_x, \xi_y, \xi_z) = \chi [\xi_x \bar{u}_1^W + \delta(\xi^2/2 - 2)] + (1 - \chi) h(0, \xi_x, -\xi_y, \xi_z) \]

\begin{align*}
- \frac{\chi}{2\pi} & \int_{-\infty}^{0} \xi_y' \, d\xi_y' \int_{R^2} h(0, \xi_x', \xi_y', \xi_z') \exp(-\frac{\xi_y'^2}{y}) \, d\xi_x' \xi_z'; \quad \xi_y > 0.
\end{align*}

Consider the Kramers’ problem with boundary condition \( \bar{u}_1^W = 0 \) and \( \delta = (\theta_W - \theta_0)/\theta_W = 0 \), then we have

\[ Z(0, \xi) = (1 - \chi) Z(0, -\xi); \quad \xi > 0. \quad (4.27) \]

The equation (4.25) is an integral equation on \( \xi \) and differential equation on \( y \). Here we discretize it on \( \xi \). Consider the Gauss-Hermite quadrature with \( M \in \mathbb{N} \) points, and denote the weights and integral points by \( \omega_i \) and \( \tilde{\xi}_i, \), \( i = 1, \cdots, M \). If we sort the \( \tilde{\xi} \) in descending order, then \( \tilde{\xi}_i = \lambda_i \) in (4.6). Let \( Z(\bar{y}) = Z(\bar{y}, \tilde{\xi}_k) \) and \( Z(\bar{y}) = (Z(\bar{y})_1, \cdots, Z(\bar{y})_M)^T \) and \( \omega = (\omega_1, \cdots, \omega_M)^T \), then we have

\[ K_0 \Lambda 1 + \Lambda \frac{dZ(\bar{y})}{d\bar{y}} = \frac{1}{Kn} (1\omega^T - \mathbf{I}) Z(\bar{y}), \quad (4.28) \]

where \( \Lambda \) is same as the (4.3) and \( \mathbf{I} \) is the \( M \times M \) identity matrix, and \( \mathbf{I} = (1, \cdots, 1)^T \in \mathbb{R}^M \). Let \( \mathbf{W} = \text{diag}\{\omega_i; \ i = 1, \cdots, M\} \), since \( \mathbf{W} \) is independent of \( \bar{y} \) and \( \mathbf{W} \) and \( \Lambda \) are both diagonal matrices, the upper formulation can be rewritten as

\[ K_0 \mathbf{W} \Lambda 1 + \Lambda \frac{dWZ(\bar{y})}{d\bar{y}} = \frac{1}{Kn} (\mathbf{W} \omega^T \mathbf{W}^{-1} - \mathbf{I}) \mathbf{W} Z(\bar{y}). \quad (4.29) \]

Noticing \( \tilde{\xi}_i, i = 1, \cdots, M \) are Gauss-Hermite integral points, we have \( H_{jM}(\tilde{\xi}_i) = 0 \), which indicates \( \Lambda = R^{-1} M R \), where \( M \) and \( R \) are defined in (4.3) and (4.4), respectively. The originality of the Hermite polynomial indicates \( \sum_{i=1}^{M} w_i H_{jM}(\tilde{y}_i) = \delta_{j,0} \), thus we have

\[ \mathbf{R} \mathbf{W} = e_1, \quad \omega^T = e_1^T \mathbf{R} \mathbf{W}. \]

Now (4.29) can be rewritten as

\[ K_0 e_2 + M \frac{d[RWZ(\bar{y})]}{d\bar{y}} = M \frac{dV}{d\bar{y}} \]

\begin{align*}
&= \frac{1}{Kn} R (\mathbf{W} \omega^T \mathbf{W}^{-1} - \mathbf{I}) \mathbf{W} Z(\bar{y}) \\
&= \frac{1}{Kn} (\mathbf{RW} \omega^T \mathbf{W}^{-1} - \mathbf{I}) \mathbf{W} Z(\bar{y}) \\
&= \frac{1}{Kn} (e_1 e_1^T - \mathbf{I}) \mathbf{W} Z(\bar{y}) \\
&= -\frac{1}{Kn} Q \mathbf{W} Z(\bar{y}) = -\frac{1}{Kn} Q V,
\end{align*}
where $Q$ is defined in (4.3) and it is readily shown that $V$ can be written as

$$V = \begin{cases} \bar{u}_1(\bar{y}) = K_0 \bar{y} + \sum_{j=1}^{M} \omega_j Z^j(\bar{y}), \\ \bar{f}_{i+1} = (\mathbf{R} \mathbf{W} Z(\bar{y}))_{i+1} = \frac{1}{i!} \sum_{j=1}^{M} \omega_j H_{\text{e}_i}(\xi_j^i) Z^j(\bar{y}), & i = 1, \ldots, M-1, \end{cases}$$

which is the discrete form of (4.24) and (4.26).

Similar discretization can be carried out for boundary condition (4.27). It can be written as

$$Z(0, \bar{\xi}_i) = (1 - \chi) Z(0, -\bar{\xi}_i), \quad (i = 1, \ldots, \lfloor \frac{M}{2} \rfloor).$$

Since the zeros of Hermite polynomials are symmetric, the equation

$$\omega_i Z(0, \bar{\xi}_i) = (1 - \chi) \omega_j Z(0, \bar{\xi}_j), \quad (i = 1, \ldots, \lfloor \frac{M}{2} \rfloor)$$

has to be satisfied for $j = M + 1 - i$. Thus we have

$$\mathbf{H}_\chi \mathbf{W} \mathbf{Z}(0) = 0,$$  \hspace{1cm} (4.31)

where $\mathbf{Z}(0) = (Z(0, \bar{\xi}_1), \ldots, Z(0, \bar{\xi}_M))^T$ and

$$\begin{align*}
\text{when } M \text{ is even: } & \quad \mathbf{H}_\chi = \begin{pmatrix} 1 & \cdots & \chi - 1 \\ \vdots & \ddots & \vdots \\ 1 & \chi - 1 & \chi - 1 \end{pmatrix}, & |\frac{M}{2}| \times M \\
\text{when } M \text{ is odd: } & \quad \mathbf{H}_\chi = \begin{pmatrix} 1 & \cdots & \chi - 1 \\ \vdots & \ddots & \vdots \\ 1 & \chi - 1 & \chi - 1 \end{pmatrix}, & |\frac{M}{2}| \times M
\end{align*}$$

Let

$$\mathbf{K}_v = \frac{1}{\chi} \begin{pmatrix} \bar{\xi}_1 & \bar{\xi}_2 & \cdots & \bar{\xi}_{\lfloor \frac{M}{2} \rfloor} \\ \bar{\xi}_1^2 & \bar{\xi}_2^2 & \cdots & \bar{\xi}_{\lfloor \frac{M}{2} \rfloor}^2 \\ \vdots & \vdots & \ddots & \vdots \\ \bar{\xi}_1^{2(\lfloor \frac{M}{2} \rfloor - 1)} & \bar{\xi}_2^{2(\lfloor \frac{M}{2} \rfloor - 1)} & \cdots & \bar{\xi}_{\lfloor \frac{M}{2} \rfloor}^{2(\lfloor \frac{M}{2} \rfloor - 1)} \end{pmatrix} \in |\frac{M}{2}| \times |\frac{M}{2}|$$

Since $\bar{\xi}_1, \ldots, \bar{\xi}_{\lfloor \frac{M}{2} \rfloor}$ are distinct, $\mathbf{K}_v$ is invertible due to the invertibility of Vandermonde matrix. Let $\mathbf{R} = (\bar{r}_{ij})_{M \times M}$ with $\bar{r}_{ij} = H_{\text{e}_{i-1}}(\lambda_j)$, $i, j = 1, \ldots, M$, then from (4.4) we have $\mathbf{R} = \text{diag}\{1, 1, \frac{1}{2!}, \ldots, \frac{1}{(M-1)!}\} \cdot \mathbf{R}$. Using the orthogonality of Hermite polynomials

$$\frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} H_{\text{e}_j}(x) H_{\text{e}_k}(x) \exp\left(-\frac{x^2}{2}\right) dx = j! \delta_{jk},$$

we have

$$\mathbf{W} \mathbf{R}^T \mathbf{R} = \mathbf{I}.$$
Then we multiply matrix (4.31) by \( K \), and the matrix form of boundary condition becomes
\[
K_v H \chi W Z(0) = [K_v H \chi W \tilde{R}^T] \cdot [RWZ(0)] = 0. \tag{4.32}
\]
The discretization of \( S(l, m) \) in (3.10) is
\[
S(l, m) = \frac{1}{\chi} \sum_j \{ \xi_j^l \omega_j [He_m(\tilde{\xi}_j) - (1 - \chi)He_m(-\tilde{\xi}_j)] \}
= \frac{1}{\chi} (\xi_1^l, \xi_2^l, \ldots, \xi_{\lceil M/2 \rceil}^l) \cdot H \chi W \cdot (He_m(\tilde{\xi}_1), He_m(\tilde{\xi}_2), \ldots, He_m(\tilde{\xi}_M))^T,
\]
then
\[
K_v H \chi W \tilde{R}^T = \begin{pmatrix}
S(1, 0) & S(1, 1) & \cdots & S(1, M - 1) \\
S(3, 0) & S(3, 1) & \cdots & S(3, M - 1) \\
\vdots & \vdots & \ddots & \vdots \\
S(2\lfloor M/2 \rfloor - 1, 0) & S(2\lfloor M/2 \rfloor - 1, 1) & \cdots & S(2\lfloor M/2 \rfloor - 1, M - 1)
\end{pmatrix}.
\]

And (4.32) is then turned into
\[
\begin{pmatrix}
S(1, 0) & S(1, 1) & \cdots & S(1, M - 1) \\
S(3, 0) & S(3, 1) & \cdots & S(3, M - 1) \\
\vdots & \vdots & \ddots & \vdots \\
S(2\lfloor M/2 \rfloor - 1, 0) & S(2\lfloor M/2 \rfloor - 1, 1) & \cdots & S(2\lfloor M/2 \rfloor - 1, M - 1)
\end{pmatrix} \cdot V^{(0)} = 0,
\]
which is same as the boundary condition in (3.16).

5 Quantity Validification

In this section, we numerically study the convergence of the solutions of the linearized HME to that of the linearized Boltzmann equation, and Knudsen layer effect of the velocity and effective viscosity, and compare them with the existing results. In all the tests, high precision computation in Maple\(^1\) is used to reduce the numerical error.

5.1 Convergence in moment order

In order to compare the results with linearized Boltzmann equation \([37]\), we normalized the velocity in (4.17) as
\[
\tilde{u}(\bar{y}) = -\frac{\text{Kn}}{\tilde{\sigma}_{12}} \bar{u} = \bar{y} + \text{Kn} \frac{\bar{y}}{\tilde{\sigma}_{12}} \left( \sum_{i=1}^{\lfloor M/2 \rfloor - 1} \hat{c}_i \exp \left( -\frac{\bar{y}}{\text{Kn}\lambda_i} \right) - c_0 \right). \tag{5.1}
\]
The normalized velocity can be split into three parts \([37, 33]\)
\[
\tilde{u}(\bar{y}) = \bar{y} + \zeta - \tilde{u}_d(\bar{y}), \tag{5.2}
\]
\(^1\)Maple is a trademark of Waterloo Maple Inc.
where \( \tilde{u}_d(\bar{y}) \) is the velocity defect, satisfying \( \lim_{\bar{y} \to +\infty} \tilde{u}_d(\bar{y}) = 0 \), and \( \zeta \) is the slip coefficient, which is
\[
\zeta = \lim_{\bar{y} \to +\infty} (\tilde{u}(\bar{y}) + \tilde{u}_d(\bar{y}) - \bar{y}) = -\text{Kn} \cdot \frac{c_0}{\bar{\sigma}_{12}}.
\] (5.3)

Then the velocity defect is
\[
\tilde{u}_d(\bar{y}) = 2\text{Kn} \sum_{i=1}^{\lfloor \frac{M-2}{2} \rfloor} \hat{c}_i \bar{\sigma}_{12} \exp\left( -\frac{\bar{y}}{\text{Kn} \lambda_i} \right).
\] (5.4)

Here we notice that there is always a factor \( \bar{\sigma}_{12} \) in the expression of \( \hat{c}_i \) and \( c_0 \) in (4.17). In this subsection, we fix \( \text{Kn} = \frac{1}{\sqrt{2}} \) as a constant for convenience. Next we study the convergence of the velocity defect and slip coefficient, respectively.

![Profiles of the defect velocity \( \tilde{u}_d(\bar{y}) \) of the linearized HME for different \( M \) with \( \chi = 0.1 \). The reference solution is Siewert’s result in [33] for linearized BGK model.](image)

Figure 5.1: Profile of the defect velocity \( \tilde{u}_d(\bar{y}) \) of the linearized HME for different \( M \) with \( \chi = 0.1 \). The reference solution is Siewert’s result in [33] for linearized BGK model.

For the velocity defect \( \tilde{u}_d(\bar{y}) \), the analytical results with \( M \) ranging from 5 to 80 are presented in Fig. 5.1 for \( \chi = 0.1 \) and Fig. 5.2 for \( \chi = 0.9 \), which are compared with the Siewert’s numerical results in [33] for the linearized BGK model. It is clear that the results of the linearized HME converge to Siewert’s result as \( M \) increasing, which is consistent with the theoretical analysis in Sec. 4.2. Meanwhile, one can find that the defect velocity of even order converges faster to the reference solution than that of odd order. This can
Figure 5.2: Profile of the defect velocity $\tilde{u}_d(\bar{y})$ of the linearized HME for different $M$ with $\chi = 0.9$. The reference solution is Siewert’s result in [33] for linearized BGK model.

be understood based on the smallest width of the boundary layer, which is represented by $w_M := \min\{\hat{\lambda}_i : i = 1, \ldots, \lfloor \frac{M}{2} - 1 \rfloor\}$. The smaller $w_M$, the closer of the defect velocity of the linearized HME to the reference solution. Fig. 5.3 gives all the $\hat{\lambda}_i$ for $M$ ranging from 3 to 40. One can observe that $w_M$ for even $M$ is quite smaller than that for the adjacent odd $M$.

Moreover, comparing with Fig. 5.1 and 5.2, one can find that for a given $M$, the relative error in Fig. 5.1 is a little larger than that of Fig. 5.2. Actually, for smaller $\chi$, the diffusion interaction between gas and the wall turns weak, then the distribution function is expected to be more far from the equilibrium, which indicates more moment is needed.

For the slip coefficient $\zeta$, the analytical results for different $M$ are plotted in Fig. 5.4. Similar convergence can be readily observed in Fig. 5.4. All the phenomena observed in Fig. 5.1 and 5.2 are also valid in Fig. 5.4.

5.2 Knudsen layer

In this subsection, we study the Knudsen layer of Kramers’ problem in three aspects. The first one is the profile of the normalized velocity $\tilde{u}(\bar{y})$ [5.1]. For convergence, here we also fix Kn as a constant $1/\sqrt{2}$. Fig. 5.5 gives the profile of $\tilde{u}(\bar{y})$ in [5.1] of linearized HME with $M = 8$ and $M = 9$. Compared with numerical results of linearized Boltzmann equation
Even order of Linearized HME
Odd order of Linearized HME
Siewert
ζ
M
(α)
χ = 0

Figure 5.3: The value \( \hat{\lambda}_i \) for different \( M \).

(a) \( \chi = 0.1 \)  
(b) \( \chi = 0.3 \)  
(c) \( \chi = 0.5 \)

(d) \( \chi = 0.7 \)  
(e) \( \chi = 0.9 \)  
(f) \( \chi = 1.0 \)

Figure 5.4: Values of the slip coefficient \( \zeta \) for different \( M \) and \( \chi \). The reference solution is Siewert’s result in [33] for linearized BGK model.

in [27], the good agreement of the solutions of the linearized HME in Fig. 5.5 indicates the moment system with a small \( M \) is good enough to describe the velocity profile in the Knudsen layer. Moreover, the value of \( \tilde{u}(\bar{y}) \) increases, as \( \chi \) decreasing. This is because the coefficients \( \hat{c}_i \) and \( c_0 \) are dependent on \( \frac{2 - \chi}{\chi} \). As discussed in the Section 5.1, the diffusion interaction between gas and the wall is weaker for smaller \( \chi \).

The second one is the profile of the velocity defect \( \tilde{u}_d(\bar{y}) \) in (5.2). Fig. 5.6 shows the profile of \( \tilde{u}_d(\bar{y}) \) with \( M = 20 \) for different Knudsen number. The thickness of the Knudsen layer largens as \( Kn \) increasing and the strength of of the Knudsen layer enhances. In practical application, more moments are needed for large \( Kn \).

The third one is the effective viscosity. The Navier-Stokes law indicates \( \sigma_{12} = -\mu \frac{\partial u}{\partial y} \). However, in the Knudsen layer, the Navier-Stokes does not hold anymore. To describe the non-Newtonian behavior inherent in the Knudsen layer, we formally write the Navier-
Stokes law on the shear stress \( \sigma_{12} \) as

\[
\sigma_{12} = -\mu_{\text{eff}} \frac{\partial u}{\partial y},
\]

where \( \mu_{\text{eff}} \) is called the “effective viscosity”. Since the shear stress \( \sigma_{12} \) is constant in the Kramers’ problem, we have

\[
\frac{\mu_{\text{eff}}}{\mu} = -\left( \frac{\sigma_{12}}{\partial u/\partial y} \right) / \left( \frac{\lambda \rho_0}{\sqrt{\theta_0}} \right) = -\frac{1}{\text{Kn}} \frac{\sigma_{12}}{\partial u/\partial y} = \frac{1}{\partial \tilde{u}/\partial \tilde{y}}. \tag{5.6}
\]

Noticing the definition of the normalized velocity \( \tilde{y} \), one can directly calculate

\[
\mu_{\text{eff}} = \frac{\mu}{1 + \sum_{i=1}^{M-2} c_i \exp \left( -\frac{\tilde{y}}{\lambda_\text{i} \text{Kn}} \right)}, \quad c_i = \frac{2\hat{c}_i}{\lambda_i \sigma_{12}}. \tag{5.7}
\]

In the past, the effective viscosity is well studied. For example, in \[14\], Gu investigated the R26 moment equations and predicted the effective viscosity as

\[
\mu_{\text{eff}} = \left[ 1 - \left( 1.3042C_1 \exp \left( -\frac{1.265\tilde{y}}{\text{Kn}} \right) + 1.6751C_2 \exp \left( -\frac{0.5102\tilde{y}}{\text{Kn}} \right) \right) \right]^{-1} \mu, \tag{5.8}
\]
where
\[ C_1 = \frac{\chi - 2}{\chi} \frac{0.81265 \times 10^{-1} \chi^2 + 1.2824}{0.48517 \times 10^{-2} \chi^2 + 0.64884 \chi + 8.0995}, \]
\[ C_2 = \frac{\chi - 2}{\chi} \frac{0.8565 \times 10^{-3} \chi^2 + 0.362 \chi}{0.48517 \times 10^{-2} \chi^2 + 0.64884 \chi + 8.0995}. \]

This model is similar as the linearized HME. Actually, since R26 moment system can be derived from HME, Gu’s result can be treated as a special case of the linearized HME. In [23], Lockerby et al. studied the effective viscosity based on the two low-Kn BGK results, and proposed an empirical expression as
\[ \mu_{eff} = (1 + 0.1859 \bar{y}^{-0.464} \exp(-0.7902 \bar{y}))^{-1} \mu. \quad (5.9) \]

For Lockerby’s model, we have \( \mu_{eff} \to 0 \) as \( y \to 0^+ \), which indicates the velocity gradient to approach infinity at the wall.

For convenience, here we let \( \chi = 1 \) and \( Kn = 1/\sqrt{2} \). Fig. 5.7 shows the profile of the effective viscosity of these models. Due to the convergence of the linearized HME, we take the solution the linearized HME with \( M = 200 \) as the reference solution. One can observe that Gu gives a relative larger effective viscosity \( \mu_{eff} \), while Lockerby gives a
relative smaller one. If one want to obtain a good approximation of the effective viscosity close to the wall, a lot of moments are needed.

We also take the solution of the linearized HME with \( M = 200 \) as the reference solution, and define the error as

\[
\text{err} = \mu_{\text{eff}}^{\text{reference}} - \mu_{\text{eff}}^{\text{model}}.
\]

Fig. 5.8 shows the error of Gu’s and Lockerby’s models and the linearized HME with \( M = 30 \). Gu’s model agrees with the reference very well away from the Knudsen layer and gives too large effective viscosity, while Lockerby’s model gives too small effective viscosity. For the linearized HME, by choosing a proper \( M \), the effective viscosity can be well captured.

6 Conclusion

In this paper, the globally hyperbolic moment equations (HME) is employed to study Kramers’ problem. Firstly, the set of linearized globally hyperbolic moment equations and their boundary conditions are built. The analytical solutions for the defect velocity and slip coefficient have been obtained for arbitrary order moment equations. In comparison with data from kinetic theory, it has been shown that they can accurately capture the Knudsen layer velocity profile over a wide range of accommodation coefficients, especially for the small accommodation coefficients case. The results indicate that the physics of non-equilibrium gas flow can be captured by high-order HME system.

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