On Stable Wall Boundary Conditions for the Hermite Discretization of the Linearised Boltzmann Equation

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Abstract

We define certain criteria, using the characteristic decomposition of the boundary conditions and energy estimates, which a set of stable boundary conditions for a linear initial boundary value problem, involving a symmetric hyperbolic system, must satisfy. We first use these stability criteria to show the instability of the Maxwell boundary conditions proposed by Grad[8]. We then recognise a special block structure of the moment equations which arises due to the recursion relations and the orthogonality of the Hermite polynomials; the block structure will help us in formulating stable boundary conditions for an arbitrary order Hermite discretization of the Boltzmann equation. The formulation of stable boundary conditions relies upon an Onsager matrix which will be constructed such that the newly proposed boundary conditions stay close to the Maxwell boundary conditions at least in the lower order moments.

1 Introduction

In gas dynamics, the rarefaction of a gas poses significant challenges. The ratio of the mean free path to the macroscopic length scale of the domain, known as the Knudsen number, helps us in describing the extent of rarefaction in a gas. Depending upon the range of the Knudsen number, the flow regime of a gas can be classified as: the hydrodynamic regime ($Kn \leq 0.001$), the slip flow regime ($0.001 \leq Kn < 0.01$), the transition regime ($0.01 \leq Kn < 10$) and the free molecular flow regime ($10 \leq Kn$). The evolution of the phase density function for all the flow regimes is appropriately described by the Boltzmann equation. There has been a significant amount of development in the past decades towards developing numerical methods for solving the Boltzmann equation. Direct Simulation Monte Carlo (DSMC) proves to be a method with high fidelity for solving the Boltzmann equation, an extensive discussion can be found in [2]. But DSMC methods have been found to be expensive for flow regimes with $Kn \leq 1$ due to the

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obvious presence of a large number of particles and therefore there is a need to come up with cheap solvers for flows in this regime.

The core idea of most of the methods, which appear as a substitute to Monte Carlo methods, lies in projecting the phase density function onto a finite dimensional space; the Grad's moment equations proposed in [8], where the phase density function is expanded in terms of the tensor valued Hermite polynomials, falls into this category. Since Grad discarded his own equations, not much attention was payed to them initially. But recently Grad's equations have been studied in detail since it has been found that properties like loss of hyperbolicity, presence of sub-shocks etc. can be overcome with the help of certain regularizations, see [3, 13, 25]. In the present work, we will focus upon low Mach rarefied gas flows. Therefore we will linearise the Boltzmann equation about a fixed ground state and then use a Hermite expansion, in the velocity space, to compute the deviations of the distribution function from this ground state; such an approximation will lead to set of linearised moment equations which are globally hyperbolic in nature [23].

Most realistic problems concerning gas dynamics involve an interaction between the gas and its surrounding environment; one of the crucial one being the interaction between a gas and a solid surface. Therefore one should endow a fluid model with appropriate boundary conditions. An initial step towards providing boundary conditions for moment equations was already taken in [8] where the Maxwell accommodation model was used to come up with Maxwell's boundary conditions(MBCs) for the Grad's-13 moment equations. In [32], the MBCs were also derived for the Regularized-13 equations(R13) which were then used to study certain benchmark problems. The MBCs for R13 equations were used in [27] to study a low Mach number flow over a sphere; the results were found to be promising as compared to those obtained from Stokes equations [1]. The use of MBCs was further extended to moment equations describing the flow of rarefied gas mixtures; see [10] for a detailed discussion and the results therein. In [20], the MBCs were used to compute a lid driven cavity flow using R13 equations and finite differences. In [9], the authors have studied a plane Coutte flow using R13 equations equipped with MBCs. See [29] and the references therein for a detailed discussion on boundary value problems arising from moment equations. Despite being physically intuitive, the studies conducted in [19, 21, 33] have brought out the physically inaccuracy of MBCs. In [31], the authors have discussed the instability of MBCs and its influence upon the convergence of Discontinuous Galerkin schemes for curved boundaries. The instability of MBCs motivates us to formulate stable boundary conditions for an arbitrary order Hermite discretization of the Boltzmann equation.

Stability of boundary conditions has a significant role to play in the well-posedness of IBVPs. The framework for well posedness of constant coefficient initial boundary value problems(IBVPs) has been developed in [7, 14, 15, 18]. The theoretical framework for well-posedness, for symmetric hyperbolic systems, usually relies upon the use of energy estimates which help in providing an upper bound for the solution, of an IBVP, in terms of the given data. These energy estimates were also used in [18] to formulate certain conditions which the boundary conditions must satisfy in order to be well posed. Apart from analysing the well-posedness of continuous problems, energy estimates have also been used in analysing the stability of numerical schemes; see [16, 31] and references therein for greater details. Therefore the stability of boundary conditions becomes crucial to obtain acceptable results both on the continuous and the discrete level.

From the previous works it is clear that the higher order moment methods are required in flow regimes which experience significant non-equilibrium; see [30] and [28] for a discussion regarding the derivation and the convergence of higher order moment methods for boundary value problems respectively. Moving along the same lines as [18], we will use energy estimates to define the notion of stable boundary conditions. We will then use our stability criteria to study the instability of MBCs. Further, we will recognise a special block structure for the moment equations which will help us to formulate stable boundary conditions for the same. Similar to [21] these boundary conditions will be given in terms of the Onsager matrix. Adopting the methodology proposed in [21], we will then use the MBCs to derive an explicit expression for the Onsager matrix.

2 Stability Criteria

Restricting ourselves to linear IBVPs, in the present section we will be defining the notion of stable boundary conditions along with the neccesary and the sufficient conditions for a set of boundary conditions to be stable. The energy estimate to be discussed in this section is closely related to the well-posedness of an IBVP; see [7, 11, 12, 18] for details. A linear IBVP can be given as

$$\partial_t \boldsymbol{\alpha}(\mathbf{x},t) + \sum_{i=1}^{d} \mathbf{A}^{(i)} \partial_{x_i} \boldsymbol{\alpha}(\mathbf{x},t) = \mathbf{P}\boldsymbol{\alpha}(\mathbf{x},t), \qquad \mathbf{x} \in \Omega, \quad t \geq 0 \tag{1a}$$

$$\boldsymbol{\alpha}(\mathbf{x},0) = \mathbf{f}(\mathbf{x}), \qquad \mathbf{x} \in \Omega, \quad t = 0 \tag{1b}$$

$$\mathbf{B}\boldsymbol{\alpha}(\mathbf{x},t) = \mathbf{g}(\mathbf{x},t), \qquad \mathbf{x} \in \partial\Omega, \quad t \geq 0 \tag{1c}$$

where $\boldsymbol{\alpha} \in \mathbb{R}^m$ is the solution vector, $\mathbf{A}^{(i)} \in \mathbb{R}^{m\times m}$ is a constant coefficient matrix which will be assumed to be symmetric and the domain $\Omega \subseteq \mathbb{R}^d$ is Lipschitz continuous and convex. The matrix $\mathbf{B} \in \mathbb{R}^{p\times m}$ prescribes the boundary conditions, the exact form of which will be discussed later and d is the total number of spatial dimensions. The initial condition $\mathbf{f}(\mathbf{x})$ and the inhomogeneity of the boundary conditions $\mathbf{g}(\mathbf{x},t)$ is the given data of the problem; both $\mathbf{f}$ and $\mathbf{g}$ will be considered to be infinitely differentiable i.e $\mathbf{f} \in [C^\infty(\Omega)]^m$ and $\mathbf{g} \in [C^\infty(\Omega)]^p$. To maintain coherence with the moment equations, which will be derived in the coming sections, we will assume $\mathbf{P} \in \mathbb{R}^{m\times m}$, which is also a constant coefficient matrix, to be negative semi-definite i.e.

$$\boldsymbol{\alpha}^T \mathbf{P} \boldsymbol{\alpha} \leq 0, \quad \boldsymbol{\alpha} \in \mathbb{R}^m. \tag{2}$$

Generically speaking, the IBVP in (1a)-(1c) is well-posed if there exists a unique solution which continuously depends upon the given data [7, 14]. Since the problem which we are considering is linear in nature hence, if the solution exists then the continuous dependence of it on the given data will ensure its uniqueness [18]. Thus, the IBVP given in (1a)-(1c) is well posed if (i) the solution to the IBVP exists and (ii) the solution is such that it is bounded by the given data of the problem in some suitable norm. For the existence of the solution it is necessary that we prescribe the correct number of boundary conditions which translates into the matrix $\mathbf{B}$, appearing in (1c), being of an appropriate size [7]. Let $\mathbf{n} = \mathbf{n}(\mathbf{x})$ be a unit vector which points out of the domain and is perpendicular to $\partial\Omega$ at the point $\mathbf{x}$, then we can define the flux matrix $\mathbf{A}^{(n)}$ as

$$\mathbf{A}^{(n)} = \sum_{i=1}^{d} n_i \mathbf{A}^{(i)} \tag{3}$$

which will be symmetric. We will assume that as $\mathbf{n}$ varies along the whole boundary, the eigenspectrum of $\mathbf{A}^{(n)}$ does not change, this is in accordance with the rotational invariance of the moment systems; see [17]. For the existence of a solution it is necessary that we only prescribe a boundary condition to those characteristics which come into the domain (see [7] for details); therefore, the number of rows of the matrix $\mathbf{B}$(i.e. p) should be equal to the number of negative eigenvalues of $\mathbf{A}^{(n)}$ and $rank(\mathbf{B}) = p$. Hence the assumption on the eigenspectrum of $\mathbf{A}^{(n)}$ ensures that the size of $\mathbf{B}$ remains the same for all the boundary points.

To ensure the uniqueness of the solution, we can now look into the following energy estimate which can be obtained by multiplying (1a) by $\boldsymbol{\alpha}^T$, integrating over the domain Ω and using Gauss-theorem

$$\frac{1}{2}\partial_t \int_{\Omega} \boldsymbol{\alpha}^T \boldsymbol{\alpha} d\mathbf{x} + \frac{1}{2} \oint_{\partial\Omega} \boldsymbol{\alpha}^T \mathbf{A}^{(n)} \boldsymbol{\alpha} ds = \int_{\Omega} \boldsymbol{\alpha}^T \mathbf{P} \boldsymbol{\alpha} d\mathbf{x} \leq 0, \quad (\because \mathbf{P} \leq 0). \tag{4}$$

Due to the symmetricity of $\mathbf{A}^{(i)}$, the entropy-entropy flux pair for (1a) can be recognised as $\boldsymbol{\alpha}^T\boldsymbol{\alpha}$ and $\boldsymbol{\alpha}^T\mathbf{A}^{(i)}\boldsymbol{\alpha}$ respectively. Under the assumption of $\mathbf{P}$ being semi-negative definite, the entropy flux across the boundary remains as the only source for the growth of the $L^2(\Omega)$ norm of the solution vector $\boldsymbol{\alpha}$ (or the growth of the entropy functional). Hence, we can bound the solution by the given data of the problem if we can bound the entropy flux as

$$\mathcal{H} = \boldsymbol{\alpha}^T \mathbf{A}^{(n)} \boldsymbol{\alpha} \geq -\lambda(t) \mathbf{g}(\mathbf{x}, t)^T \mathbf{g}(\mathbf{x}, t), \quad \mathbf{x} \in \partial\Omega \tag{5}$$

where $\lambda(t)$ is some scalar function independent of the solution and the given data of the problem. Assuming that we can somehow ensure an inequality of the form (5), then using (4) we have

$$\partial_t \|\boldsymbol{\alpha}\|^2 \leq \lambda(t) \oint_{\partial\Omega} \mathbf{g}(\mathbf{x}, t)^T \mathbf{g}(\mathbf{x}, t) ds, \tag{6}$$

where $\|.\|$ represents the standard $L^2(\Omega)$ norm, which ensures the uniqueness of the solution in case it exists. The afore-mentioned analysis shows that in order to obtain any reasonable results for our IBVP we need careful modelling of the boundary conditions. It can be shown that if we end up prescribing the wrong number of boundary conditions then the existence of the solution will be endangered and on the other hand if the boundary conditions do not lead to a bounded growth of the solution, in the sense of (6), then the uniqueness of the solution cannot be ensured. In the spirit of fulfilling the necessary conditions for the well-posedness of our IBVP, we have the definition

Definition 2.1. *A set of boundary conditions, $\mathbf{B}\boldsymbol{\alpha} = \mathbf{g}(\mathbf{x}, t)$, for our IBVP given in (1a)-(1c) will be called stable if it prescribes the correct number of boundary conditions and provides us with a bound of the following type for the $L^2(\Omega)$ norm of the solution $\boldsymbol{\alpha}$*

$$\partial_t \|\boldsymbol{\alpha}\|^2 \leq \lambda(t) \oint_{\partial\Omega} \mathbf{g}(\mathbf{x}, t)^T \mathbf{g}(\mathbf{x}, t) ds \tag{7}$$

where $\lambda(t)$ is some scalar function independent of the solution and the given data of the problem and $\mathbf{g}(\mathbf{x}, t)$ is the inhomogeneity arising from the boundary (see (1c)).

From characteristic splitting, we know that $\mathbf{A}^{(n)} = \mathbf{X}\boldsymbol{\Lambda}\mathbf{X}^T$ where $\mathbf{X}$ and $\boldsymbol{\Lambda}$ contain the eigenvectors and the eigenvalues of $\mathbf{A}^{(n)}$ respectively. Using $\mathbf{X}$, we define

$$\mathbf{R}_0 = -\left(\mathbf{B}\mathbf{X}_-\right)^{-1} \mathbf{B}\mathbf{X}_0, \quad \mathbf{R}_+ = -\left(\mathbf{B}\mathbf{X}_-\right)^{-1} \mathbf{B}\mathbf{X}_+, \quad \hat{\mathbf{g}} = \left(\mathbf{B}\mathbf{X}_-\right)^{-1} \mathbf{g} \tag{8}$$

where $\mathbf{X}_{+/-/0}$ contain the eigenvectors corresponding to positive, negative and zero eigenvalues respectively. We now formulate the following conditions, which are both necessary and sufficient, for the stability of the boundary conditions in (1c)

Condition1 $rank(\mathbf{B}) = p$ and p should be equal to the number of negative eigenvalues of $\mathbf{A}^{(n)}$.

Condition2 $ker\{\mathbf{A}^{(n)}\} \subseteq ker\{\mathbf{B}\}$(or $\mathbf{R}_0 = 0$).

Condition3 $\mathbf{R}_+^T \boldsymbol{\Lambda}_- \mathbf{R}_+ + \boldsymbol{\Lambda}_+ \geq 0$.

Condition4 $\mathbf{R}_+^T \boldsymbol{\Lambda}_- \hat{\mathbf{g}} \in range(\boldsymbol{\Lambda}_+ + \mathbf{R}_+^T \boldsymbol{\Lambda}_- \mathbf{R}_+)$.

A detailed derivation of these conditions can be found in subsection 7.1. *Condition1* is a consequence of the definition of stability itself and ensures that we fulfil the necessary conditions for the existence of the solution. *Condition2* to *Condition4* ensure that we can bound the entropy flux at the boundary by the given data leading to the uniqueness of the solution to the IBVP.

As per *Condition4*, if we want to allow for any arbitrary inhomogeneity $\mathbf{g}$ then $range(\mathbf{R}_+^T) \subseteq range(\boldsymbol{\Lambda}_+ + \mathbf{R}_+^T \boldsymbol{\Lambda}_- \mathbf{R}_+)$, which is always satisfied if $\boldsymbol{\Lambda}_+ + \mathbf{R}_+^T \boldsymbol{\Lambda}_- \mathbf{R}_+$ is *s.p.d.* Therefore, in [18] the authors restrict $\boldsymbol{\Lambda}_+ + \mathbf{R}_+^T \boldsymbol{\Lambda}_- \mathbf{R}_+$ to be *s.p.d* for inhomogeneous boundary conditions ($\mathbf{g} \neq 0$) so as to obtain well-posedness of the IBVP. On the contrary, in the present work we only allow for those inhomogeneities which satisfy *Condition4* as a result of which $\mathbf{R}_+^T \boldsymbol{\Lambda}_- \mathbf{R}_+ + \boldsymbol{\Lambda}_+$ can even be semi-definite. As we will see in the coming sections, the matrix $\mathbf{B}$ in (1c) is modelled using some well defined physical process and remains the same for homogeneous($\mathbf{g} = 0$) and inhomogeneous($\mathbf{g} \neq 0$) boundaries; therefore, the allowable inhomogeneities depend upon the nature of the matrix $\mathbf{R}_+^T \boldsymbol{\Lambda}_- \mathbf{R}_+ + \boldsymbol{\Lambda}_+$(or $\mathbf{B}$).

Remark 1. An interesting question is whether the framework which will be developed in the present work can be easily extended to non-linear systems or not. Though even for non-linear systems it is crucial that we prescribe boundary conditions to only those characteristics which come into the domain but the bound in (7) does not guarantee the uniqueness of the solution. Therefore a formulation of boundary conditions, for non-linear problems, based upon the criteria presented in Definition 2.1 might not provide us with a unique solution.

3 The Boltzmann Equation

We will now restrict ourselves to a kinetic equation which is one dimensional in the physical and the velocity space. In the present setting, the Boltzmann equation, on a bounded position domain, is given as

$$\begin{aligned} &\partial_t f + \xi \partial_x f = Q(f,f), \quad (x,\xi,t) \in [x^{(-)}, x^{(+)}] \times \mathbb{R} \times [0,T] \\ &f(x,\xi,0) = f_I(x,\xi), \qquad x \in [x^{(-)}, x^{(+)}], t = 0 \end{aligned} \tag{9}$$

where $f = f(x,\xi,t)$ defines the phase density functional and f_I is some suitable initial condition; boundary conditions for (9) will be discussed later. The operator $Q(f,f)$ is such that it only vanishes under equilibrium i.e. $Q(f_{\mathcal{M}}, f_{\mathcal{M}}) = 0$ where $f_{\mathcal{M}}$ is the Maxwell-Boltzmann distribution function given as

$$f_{\mathcal{M}}(\xi;\rho,v,\theta) = \frac{\rho(t,x)}{\sqrt{2\pi\theta(t,x)}} \exp\left(-\frac{(\xi - v(t,x))^2}{2\theta(t,x)}\right) \tag{10}$$

with ρ, v and θ being the density, velocity and temperature (in energy units) respectively and are defined with respect to f as $\rho = \int_{\mathbb{R}} f d\xi$, $\rho v = \int_{\mathbb{R}} \xi f d\xi$ and $\rho v^2 + \rho\theta = \int_{\mathbb{R}} \xi^2 f d\xi$. In the present work, we are concerned with flow states which correspond to very low Mach number regimes. So, in terms of the distribution function, we are looking for perturbations of $f(x,\xi,t)$ around the global Maxwellian $f_0 = f_{\mathcal{M}}(\xi;\rho_0,0,\theta_0)$ where ρ_0 and θ_0 are ground states which are independent of x and t. To obtain an equation for the perturbation of f about f_0, we will linearise f through the relation $f \approx f_0 + \epsilon \tilde{f}$ with ϵ being some smallness parameter. Substituting the linearisation into the Boltzmann equation (9) and using $\partial_t f_0 = \partial_x f_0 = 0$, we obtain the linearised form of the Boltzmann equation upto $\mathcal{O}(\epsilon)$

$$\begin{aligned} &\partial_t \tilde{f} + \xi \partial_x \tilde{f} = \tilde{Q}(\tilde{f}), \quad (x,\xi,t) \in [x^{(-)}, x^{(+)}] \times \mathbb{R} \times [0,T] \\ &\tilde{f}(x,\xi,0) = \tilde{f}_I(x,\xi), \qquad x \in [x^{(-)}, x^{(+)}], t = 0 \end{aligned} \tag{11}$$

where $\tilde{Q}(\tilde{f})$ is the linearisation of $Q(f,f)$ about f_0 and has the property [6, 23]

$$\int_{\mathbb{R}} \tilde{f} f_0^{-1} \tilde{Q}(\tilde{f}) d\xi \leq 0 \tag{12}$$

which will prove to be helpful during the discussion of stable boundary conditions. The initial condition $\tilde{f}_I$ is the linearisation of f_I about f_0 upto $\mathcal{O}(\epsilon)$, we will assume $\tilde{f}_I$ to be in $L^2(\mathbb{R}, f_0^{-1})$.

3.1 The Maxwell Accommodation Model

Using the linearised Boltzmann equation given in (11), we would like to study a fluid flow inside a bounded position domain i.e. $x \in [x^{(-)}, x^{(+)}]$ such that at both $x = x^{(-)}$ and $x = x^{(+)}$ we have solid stationary impenetrable walls. Thus the gas in our bounded domain can only be excited through a temperature difference between the two confining walls. It is obvious that to study such a problem we need to equip our kinetic equation in (11) with appropriate boundary conditions.

As is clear from (11), the linearised Boltzmann equation is hyperbolic in nature with the advection speed being equal to the molecular velocity ξ. Therefore, we simply need to prescribe a value to the distribution function at the points in the phase space with positive and negative velocities at $x = x^{(-)}$ and $x = x^{(+)}$ respectively. Assuming the scattering at the boundary to be modelled by the Maxwell accommodation model, the boundary conditions are then given by

$$\tilde{f}(x^{(\pm)}, \xi, t) = \chi \tilde{f}_{\mathcal{M}}^{(\pm)}(\xi) + (1-\chi)\tilde{f}(x^{(\pm)}, -\xi, t), \quad \pm\xi < 0. \tag{13}$$

The functions $\tilde{f}_{\mathcal{M}}^{(\pm)}(\xi)$ appearing in the boundary conditions are the deviations of $f_{\mathcal{M}}$ from f_0, upto $\mathcal{O}(\epsilon)$, at the left and the right wall respectively and are given as

$$\tilde{f}_{\mathcal{M}}^{(\pm)}(\xi) = f_0 \left(\frac{\tilde{\rho}^{(\pm)}}{\rho_0} + \frac{\tilde{\theta}^{(\pm)}}{2\theta_0} \left(\frac{\xi^2}{\theta_0} - 1 \right) \right), \quad x = x^{(\pm)} \tag{14}$$

where $\tilde{\rho}^{(\pm)}$ and $\tilde{\theta}^{(\pm)}$ are the deviations of ρ and θ from the reference states ρ_0 and θ_0 upto $\mathcal{O}(\epsilon)$. The factor $\chi \in [0, 1]$ is the accommodation coefficient and determines the fraction of the molecules which are fully accommodated at the walls; the temperatures of the walls, $\tilde{\theta}^{(\pm)}$, are the given data of the problem but the densities, $\tilde{\rho}^{(\pm)}$, are determined such that the relative velocity of the gas in the direction normal to the wall remains zero.

3.2 Stability of the Maxwell Accommodation Model

It is crucial to discuss whether the Maxwell accommodation model given by (13) is stable or not for the linearised Boltzmann equation (11). Because if the Maxwell accommodation model is itself unstable then, we cannot expect to obtain a stable set of boundary conditions from it for our moment system. For the stability of the Maxwell accommodation model, we recall the following results from [23]; where for simplicity χ and $\tilde{\theta}^{(\pm)}$ were taken to be 1 and 0 respectively.

Multiplying the linearised Boltzmann equation (11) with $\tilde{f} f_0^{-1}$ and integrating with respect to ξ and x, we obtain

$$\frac{1}{2}\partial_t \int_{x^{(-)}}^{x^{(+)}} \int_{\mathbb{R}} \tilde{f}^2 f_0^{-1} d\xi dx + \frac{1}{2}\left[\int_{\mathbb{R}} \tilde{f}^2 f_0^{-1} \xi d\xi\right]_{x=x^{(+)}} - \frac{1}{2}\left[\int_{\mathbb{R}} \tilde{f}^2 f_0^{-1} \xi d\xi\right]_{x=x^{(-)}} = \int_{x^{(-)}}^{x^{(+)}} \int_{\mathbb{R}} \tilde{f} f_0^{-1} \tilde{Q}(\tilde{f}) d\xi dx \leq 0 \tag{15}$$

where we have used (12). For the linearised Boltzmann equation the inequality can be looked upon as an energy estimate, similar to (4), with $\int_{\mathbb{R}} \tilde{f}^2 f_0^{-1} d\xi$ and $\int_{\mathbb{R}} \tilde{f}^2 f_0^{-1} \xi d\xi$ corresponding to the entropy and the entropy flux respectively. Due to the temperatures of the walls being zero, the inhomogeneities arising from the walls are absent which is equivalent to $\mathbf{g} = 0$ in (1c). The Maxwell accommodation model will be stable, in the sense of Definition 2.1, if we can obtain ($\mathbf{g} = 0$ in (6))

$$\partial_t \int_{x^{(-)}}^{x^{(+)}} \int_{\mathbb{R}} \tilde{f}^2 f_0^{-1} d\xi dx \leq 0 \tag{16}$$

which is equivalent to requiring the positivity of the entropy flux across the boundary ($\mathcal{H} \geq 0$ in (5) with $\mathbf{g} = 0$) i.e.

$$\pm \int_{\mathbb{R}} \tilde{f}^2 f_0^{-1} \xi d\xi \geq 0, \quad x = x^{(\pm)}. \tag{17}$$

From the work done in [23], we know that both the above inequalities are satisfied which in turn provides us with the stability of the boundary conditions in (13).

4 Hermite discretization

Motivated from the work done in [8], in the present work we will discretize the linearised Boltzmann equation, in the velocity space, using the Hermite expansion in the following way

$$\tilde{f} \approx \tilde{f}_h = \sum_{i=0}^{m-1} \alpha_i(x,t) He_i\left(\frac{\xi}{\sqrt{\theta_0}}\right) f_0 \tag{18}$$

where, m can be looked upon as an indicator of our resolution in the velocity space. The Hermite approximation was shown to converge in [23], to the solution of the linearised Boltzmann equation, for the boundary value problem we are interested in. In all the coming sections

$$\langle f, g \rangle_\gamma = \int_\gamma f g d\xi, \quad \langle f, g \rangle_{(\gamma,w)} = \int_\gamma f g w d\xi \tag{19}$$

The Hermite polynomials, $He_i(\xi)$, appearing in our approximation enjoy the following well-known but crucial properties

$$\text{Orthogonality}: \int_{\mathbb{R}} He_i\left(\frac{\xi}{\sqrt{\theta_0}}\right) He_j\left(\frac{\xi}{\sqrt{\theta_0}}\right) f_0 d\xi = \delta_{ij}\rho_0 \tag{20a}$$

$$\text{Recursion}: \sqrt{i+1}He_{i+1}\left(\frac{\xi}{\sqrt{\theta_0}}\right) + \sqrt{i}He_{i-1}\left(\frac{\xi}{\sqrt{\theta_0}}\right) = \frac{\xi}{\sqrt{\theta_0}}He_i\left(\frac{\xi}{\sqrt{\theta_0}}\right) \tag{20b}$$

For all the coming discussions, we will define H_i as $H_i(\xi) = He_i\left(\xi/\sqrt{\theta_0}\right)$. Due to the orthogonality of the basis functions (20a), the coefficients α_i's appearing in our Hermite discretization (18) can be trivially given as

$$\rho_0\alpha_i = \left\langle H_i, \tilde{f}_h \right\rangle_{\mathbb{R}}. \tag{21}$$

The first few coefficients α_i's appearing in (18) are related to the deviations of the field variables($\tilde{\rho}, \tilde{v}$ and $\tilde{\theta}$), from their respective ground states(ρ_0, v_0 and θ_0), through the relations

$$\alpha_0 = \frac{\tilde{\rho}}{\rho_0}, \quad \alpha_1 = \frac{\tilde{v}}{\sqrt{\theta_0}}, \quad \alpha_2 = \frac{\tilde{\theta}}{\sqrt{2}\theta_0}. \tag{22}$$

In order to develop tools necessary to identify a special block structure of the moment equations, we would like to divide the set of expansion coefficients (or moments) into even, $\boldsymbol{\alpha}_o$, and odd, $\boldsymbol{\alpha}_e$, coefficients in the following way

$$\rho_0\left(\alpha_e\right)_i = \langle H_{2i}, \tilde{f}_h\rangle_{\mathbb{R}}, \quad i \in \{0, \dots (n^e-1)\} \tag{23a}$$

$$\rho_0\left(\alpha_o\right)_i = \langle H_{2i+1}, \tilde{f}_h\rangle_{\mathbb{R}}, \quad i \in \{0, \dots (n^o-1)\} \tag{23b}$$

where n^o and n^e represent the total number of odd and even moments respectively. The variables n^o and n^e depend upon the value of m (the total number of moments)

$$n^e = \begin{cases} \frac{m+1}{2}, & m \text{ is odd} \\ \frac{m}{2}, & m \text{ is even} \end{cases}, \quad n^o = \begin{cases} \frac{m-1}{2}, & m \text{ is odd} \\ \frac{m}{2}, & m \text{ is even.} \end{cases} \tag{24}$$

Clearly, n^o and n^e are such that $n^o + n^e = m$. From (24), one can see that the value of n^e is either equal to n^o or greater than n^o by one.

4.1 The Moment System

For convenience, we will non-dimensionalise x and t as $\hat{x} = \frac{x}{L}$ and $\hat{t} = \frac{t\sqrt{\theta_0}}{L}$ respectively where, L is some appropriately defined length scale and θ_0 is the reference temperature in energy units. In order to derive the linearised moment equations, we multiply the linearised Boltzmann equation by the scaled Hermite polynomials (H_i), integrate the resulting expression over the entire velocity space and replace $\tilde{f}$ by $\tilde{f}_h$ to obtain

$$
\partial_{\hat{t}} \underbrace{\begin{pmatrix} \boldsymbol{\alpha}_o \\ \boldsymbol{\alpha}_e \end{pmatrix}}_{\boldsymbol{\alpha}} + \underbrace{\begin{pmatrix} 0 & \mathbf{A}^{oe} \\ \mathbf{A}^{eo} & 0 \end{pmatrix}}_{\mathbf{A}^{(1)}} \partial_{\hat{x}} \begin{pmatrix} \boldsymbol{\alpha}_o \\ \boldsymbol{\alpha}_e \end{pmatrix} = \mathbf{P} \begin{pmatrix} \boldsymbol{\alpha}_o \\ \boldsymbol{\alpha}_e \end{pmatrix}, \quad (x,t) \in [x^{(-)}, x^{(+)}] \times [0,T]
$$

$$
\rho_0 \alpha_i(x,0) = \left\langle H_i, \tilde{f}_I \right\rangle_{\mathbb{R}}, \quad x \in [x^{(-)}, x^{(+)}], t = 0 \tag{25}
$$

where $\boldsymbol{\alpha}$ contains all the moments and has been assumed to be ordered as $\boldsymbol{\alpha} = (\boldsymbol{\alpha}_o, \boldsymbol{\alpha}_e)^T$ with the odd ($\boldsymbol{\alpha}_o$) and the even ($\boldsymbol{\alpha}_e$) moments defined in (23b) and (23a) respectively. A set of boundary conditions for the moment equations will be discussed later. The matrix block $\mathbf{A}^{oe} \in \mathbb{R}^{n^o \times n^e}$, appearing in the flux matrix, can be explicitly given as

$$
A^{oe}_{ij} = \frac{1}{\rho_0 \sqrt{\theta_0}} \left\langle H_{2i+1}, H_{2j} \xi \right\rangle_{(\mathbb{R}, f_0)} = \left(\delta_{i+1,j} \sqrt{2i+2} + \delta_{i,j} \sqrt{2i+1} \right). \tag{26}
$$

Additionally, $\mathbf{A}^{eo} = (\mathbf{A}^{oe})^T$ which implies that the moment system is symmetric hyperbolic. The block structure given in (25) has also been identified in [22] for semiconductor transport equation and shows that in the transport part of the moment equations (25), the odd moments are coupled with the even ones and vice versa. The matrix $\mathbf{P}$ appearing in (25) models the contribution from $\tilde{Q}(\tilde{f})$ and is given as

$$
P_{ij} = \frac{L}{\rho_0 \sqrt{\theta_0}} \left\langle H_i, \tilde{Q}\left(H_j f_0\right) \right\rangle_{\mathbb{R}}. \tag{27}
$$

Moreover, using (12) we have $\alpha_i P_{ij} \alpha_j \leq 0$ for all $\boldsymbol{\alpha} \in \mathbb{R}^m$ which shows the negative semi-definiteness of $\mathbf{P}$. The flux matrix $\mathbf{A}^{(n)}$, defined in (3), for our moment system is given as

$$
\mathbf{A}^{(n)} = \pm \mathbf{A}^{(1)} = \pm \begin{pmatrix} 0 & \mathbf{A}^{oe} \\ (\mathbf{A}^{oe})^T & 0 \end{pmatrix}, \quad x = x^{(\pm)} \tag{28}
$$

and shows a particular block structure which will be helpful in formulating boundary conditions. We would now like to find an equivalence between the moment system and the generic system introduced in (1a); this will help us in studying the stability of the boundary conditions to be discussed shortly. Let us first define the following for convenience

Definition 4.1. *A square matrix $\mathbf{A} \in \mathbb{R}^{m \times m}$ will be called Onsager compatible, if it has the following properties*

(i) The matrix $\mathbf{A}$ is structured as

$$
\mathbf{A} = \begin{pmatrix} \mathbf{0} & \mathbf{A}_1 \\ (\mathbf{A}_1)^T & 0 \end{pmatrix} \tag{29}
$$

with $\mathbf{A}_1 \in \mathbb{R}^{p \times q}$ such that $p + q = m$ and $p \leq q$. Note that in such a case, $\mathbf{A}$ will be symmetric.

(ii) All the rows of the matrix $\mathbf{A}_1$ are linearly independent or $rank(\mathbf{A}_1) = p$.

For all the *Onsager Compatible* matrices, we have

Lemma 4.1. *Let a matrix* $\mathbf{C}$ *be Onsager compatible with the same structure as that given in* (29), *then it has the following properties*

Property1 The $ker\{\mathbf{C}\}$ *is given as*

$$ker\{\mathbf{C}\} = span\left\{\begin{pmatrix}\mathbf{0}\\ ker\{\mathbf{C}_1\}\end{pmatrix}\right\}. \tag{30}$$

Property2 The eigenspectrum of $\mathbf{C}$ *is symmetric about the origin.*

Property3 The number of negative eigenvalues of $\mathbf{C}$ *are equal to* p.

Proof. See subsection 7.2. □

We will now show that $\mathbf{A}^{(1)}$ appearing in (25) is *Onsager Compatible*.

Lemma 4.2. *The flux matrix* $\mathbf{A}^{(1)}$ *appearing in* (25) *is Onsager compatible.*

Proof. See subsection 7.3. □

Due to Lemma 4.2 and (28), the flux matrix $\mathbf{A}^{(n)}$ is also *Onsager Compatible* and will have an eigenspectrum which will be the same at $x = x^{(\pm)}$ with the number of negative eigenvalues being equal to n^o. The symmetricity of $\mathbf{A}^{(1)}$, negative semi-definiteness of $\mathbf{P}$ and the nature of the eigenspectrum of $\mathbf{A}^{(n)}$ shows that our moment system is equivalent to the generic system introduced in (1a) and therefore *Condition1* to *Condition4* can be used to formulate stable boundary conditions for the same. Using the nature of the eigenspectrum of $\mathbf{A}^{(n)}$, we can complete our description of the IBVP by formally prescribing the boundary conditions through the relation

$$\boldsymbol{\alpha}_o = \mathbf{M}\boldsymbol{\alpha}_e + \mathbf{g} \quad \text{or} \quad \underbrace{(\mathbf{I}, -\mathbf{M})}_{\mathbf{B}}\boldsymbol{\alpha} = \mathbf{g}, \quad x = x^{(\pm)}, \tag{31}$$

where $\mathbf{M} \in \mathbb{R}^{n^o \times n^e}$, $\mathbf{B} \in \mathbb{R}^{n^o \times m}$ and $\mathbf{g} \in \mathbb{R}^{n^o}$ are unknown. It trivially follows that $rank(\mathbf{B}) = n^o$ which, along with the eigenspectrum of $\mathbf{A}^{(n)}$, shows that the boundary conditions in (31) satisfy *Condition1* required for stability. We note that due to the structure of $\mathbf{B}$ in (31) and *Property1* of $\mathbf{A}^{(n)}$, *Condition2* is equivalent to requiring

$$ker\{\mathbf{A}^{oe}\} \subseteq ker\{\mathbf{M}\} \tag{32}$$

where $\mathbf{A}^{oe}$ is as defined in (26). We would now like to find $\mathbf{M}$ and $\mathbf{g}$ such that we can have a bound of the type (7) for our IBVP given in (25) and (31).

4.2 Maxwell Boundary Conditions

We will first look into one of the ways of finding an explicit $\mathbf{M}$ and $\mathbf{g}$ appearing in (31). The derivation of MBCs for the moment equations, from the Maxwell accommodation model, is based upon the assumption of continuity of odd fluxes. The idea of assuming the continuity of all the odd fluxes near the wall was first developed by Grad[8] and was motivated by his study conducted on specular walls, $\chi = 0$ in (13). For this particular case he noticed that only the continuity of odd fluxes led to non-trivial boundary conditions; he then simply extended his observation to more general walls ($\chi \in [0,1]$). Unfortunately, as we will see in the coming discussion, the continuity of odd fluxes leads to unstable boundary conditions. The continuity of odd fluxes reads [8, 24]

$$\frac{1}{2}\langle H_{2i+1}, \tilde{f}_h^o\rangle_{\mathbb{R}} = \pm\,\beta\left[\langle H_{2i+1}, \tilde{f}_h^e\rangle_{\mathbb{R}^+} - \langle H_{2i+1}, \tilde{f}_{\mathcal{M}}^{(\pm)}\rangle_{\mathbb{R}^+}\right], \quad i \in \{0, \dots, n^o - 1\} \tag{33}$$

where $\tilde{f}_{\mathcal{M}}^{(\pm)}$ is as given in (13) with $\tilde{f}_h^o$ and $\tilde{f}_h^e$ representing the odd and the even parts of $\tilde{f}_h$, with respect to ξ, respectively. Using the definition of $\tilde{f}_{\mathcal{M}}^{(\pm)}$, we can further simplify (33)

$$\begin{aligned}\frac{1}{2}\langle H_{2i+1}, \tilde{f}_h^o\rangle_{\mathbb{R}} = \pm\,\beta\Bigg[&\langle H_{2i+1}, \tilde{f}_h^e\rangle_{\mathbb{R}^+} - \frac{\tilde{\rho}^{(\pm)}}{\rho_0}\langle H_{2i+1}, H_0\rangle_{(\mathbb{R}^+,f_0)}\\ &-\frac{\tilde{\theta}^{(\pm)}}{\sqrt{2}\theta_0}\langle H_{2i+1}, H_2\rangle_{(\mathbb{R}^+,f_0)}\Bigg], \quad \left(\text{with } \beta = \frac{\chi}{2-\chi}\right), \quad x = x^{(\pm)}\end{aligned} \tag{34}$$

As was discussed previously, the walls which bound the domain have been considered to be stationary and impenetrable which provides us with $\alpha_1 = 0$ at both the boundaries. Substituting $i = 0$ in (34) and using the restriction on α_1 for no penetration of the gas across the wall, we can obtain an expression for $\tilde{\rho}^{(\pm)}$

$$\frac{\tilde{\rho}^{(\pm)}}{\rho_0} = \frac{1}{\langle H_1, H_0\rangle_{(\mathbb{R}^+,f_0)}}\left[\langle H_1, \tilde{f}_h^e\rangle_{\mathbb{R}^+} - \langle H_1, H_2\rangle_{(\mathbb{R}^+,f_0)}\frac{\tilde{\theta}^{(\pm)}}{\sqrt{2}\theta_0}\right]. \tag{35}$$

By substituting the expression for $\tilde{\rho}^{(\pm)}$ into (34), we can write the MBCs in a matrix vector product form as

$$\boldsymbol{\alpha}_o = \pm 2\beta\mathbf{M}^{(mbc)}\boldsymbol{\alpha}_e \pm \mathbf{g}^{(\pm)}, \quad x = x^{(\pm)} \tag{36}$$

where the matrix $\mathbf{M}^{(mbc)} \in \mathbb{R}^{n^o \times n^e}$ and is independent of the accommodation coefficient χ. In tensorial form, $\mathbf{M}^{(mbc)}$ is given as

$$M_{ij}^{(mbc)} = \frac{1}{\rho_0}\left[\langle H_{2i+1}, H_{2j}\rangle_{(\mathbb{R}^+,f_0)} - \langle H_{2i+1}, H_0\rangle_{(\mathbb{R}^+,f_0)}\frac{\langle H_1, H_{2j}\rangle_{(\mathbb{R}^+,f_0)}}{\langle H_1, H_0\rangle_{(\mathbb{R}^+,f_0)}}\right]. \tag{37}$$

The vectors $\mathbf{g}^{(\pm)} \in \mathbb{R}^{n^o}$ are the inhomogeneities arising from the walls and are given as

$$g_i^{(\pm)} = \begin{cases} 0, & i = 0 \\ \left(\frac{\sqrt{2}\beta\tilde{\theta}^{(\pm)}}{\theta_0\rho_0}\right)\left[\frac{\langle H_{2i+1},H_0\rangle_{(\mathbb{R}^+,f_0)}\langle H_1,H_2\rangle_{(\mathbb{R}^+,f_0)}}{\langle H_1,H_0\rangle_{(\mathbb{R}^+,f_0)}} - \langle H_{2i+1},H_2\rangle_{(\mathbb{R}^+,f_0)}\right], & i \geq 1 \end{cases}. \tag{38}$$

From (36), the boundary matrix $\mathbf{B}$ and $\mathbf{M}$ and the inhomogeneity $\mathbf{g}$ appearing in (31) can be identified as

$$\mathbf{M} = \pm 2\beta\mathbf{M}^{(mbc)}, \quad \mathbf{B}^{(mbc)} = \left(\mathbf{I}, \mp 2\beta\mathbf{M}^{(mbc)}\right), \quad \mathbf{g} = \pm\mathbf{g}^{(\pm)}, \quad x = x^{(\pm)} \tag{39}$$

which provides us with an explicit set of boundary conditions for our moment system. Similar to the stability analysis of the Maxwell accommodation model, discussed earlier, we would like to know whether the MBCs are stable in the sense of Definition 2.1; we will discuss this now in more detail.

4.3 Instability of MBCs

As was discussed previously, a set of boundary conditions of the form (31) satisfy *Condition1*; therefore, MBCs in (36) fulfil *Condition1*. From numerical investigation we have found that for all the moment systems, upto $m = 50$, in which $n^e \neq n^o$, the MBCs do not satisfy *Condition2* and are thus unstable; whereas for systems in which $n^e = n^o$, MBCs are stable. The reason for MBCs being stable for moment systems with $n^o = n^e$ will become apparent in the coming sections. A proof for the instability of the MBCs in the case of $n^e \neq n^o$ is beyond the scope of the present article but we will provide the following example to demonstrate our claim.

Example 1. Let us consider a case which corresponds to $m = 5$ in (18). For such a system, the list of variables and the flux matrix ($\mathbf{A}^{(1)}$) can be given as

$$\boldsymbol{\alpha}_5 = (\alpha_1, \alpha_3, \alpha_0, \alpha_2, \alpha_4), \quad \mathbf{A}_5^{(1)} = \begin{pmatrix} 0 & 0 & 1 & \sqrt{2} & 0 \\ 0 & 0 & 0 & \sqrt{3} & 2 \\ 1 & 0 & 0 & 0 & 0 \\ \sqrt{2} & \sqrt{3} & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 & 0 \end{pmatrix}. \tag{40}$$

The kernel of the flux matrix and its eigenspectrum are given as

$$ker\{\mathbf{A}_5^{(1)}\} = \kappa\left(0, 0, 2\sqrt{\frac{2}{3}}, -\frac{2}{\sqrt{3}}, 1\right)^T \quad (\text{with } \kappa \in \mathbb{R}) \tag{41}$$

$$\lambda(\mathbf{A}_5^{(1)}) = \left(\pm\sqrt{\sqrt{10}+5}, \pm\sqrt{\sqrt{10}+5}, 0\right). \tag{42}$$

The MBCs for this particular system are given by

$$\underbrace{\begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & \mp 2\beta\sqrt{\frac{2}{3\pi}} & \mp\frac{2\beta}{3}\sqrt{\frac{2}{\pi}} \end{pmatrix}}_{\mathbf{B}_5^{(mbc)}} \boldsymbol{\alpha}_5 = \pm \underbrace{\begin{pmatrix} 0 \\ 2\beta\sqrt{\frac{1}{3\pi}}\frac{\tilde{\theta}^{(\pm)}}{\theta_0} \end{pmatrix}}_{\mathbf{g}_5^{(\pm)}}, \quad x = x^{(\pm)}. \tag{43}$$

Considering the eigenspectrum of the flux matrix given in (42) and the entries of the boundary matrix $\mathbf{B}_5^{(mbc)}$, it is clear that the MBCs for the present moment system satisfy *Condition1*. Checking for *Condition2*, we find

$$\|\mathbf{B}_5^{(mbc)} ker\{\mathbf{A}_5^{(1)}\}\|_{l^2} = \frac{2\sqrt{2}|\kappa|}{3\sqrt{\pi}}, \quad \kappa \neq 0, \quad x = x^{(\pm)}. \tag{44}$$

Clearly, $\|\mathbf{B}_5^{(mbc)} ker\{\mathbf{A}_5^{(1)}\}\|_{l^2} \neq 0$ for $x = x^{(\pm)}$ which shows the instability of the MBCs.

Remark 2. Considering the instability of MBCs it seems reasonable to only consider those moment systems in which $n^o = n^e$ but it is crucial to remind oneself that such a moment system does not exist in multi-dimensions and therefore it is important to fix the boundary conditions for moment systems with $n^o \neq n^e$.

5 Onsager Boundary Conditions

After the discussion of the previous section, we concluded that the matrix $\mathbf{M}^{(mbc)}$ does not satisfy (32) and thus the MBCs are unstable for a large variety of moment equations. This motivates us to come up with a set of stable boundary conditions for which we will exploit the *Onsager Compatibility* of the flux matrix $\mathbf{A}^{(n)}$ given in (28); similar to the work done in [21, 26], we will call these the Onsager boundary conditions (OBCs). Before looking into the moment equations specifically, we would like to develop a set of general OBCs for all those symmetric hyperbolic systems which have an *Onsager Compatible* flux matrix; an extension to moment equations will then follow in a straightforward fashion.

Theorem 5.1. *Let the flux matrix, corresponding to a general symmetric hyperbolic system (1a), $\mathbf{A}^{(n)} \in \mathbb{R}^{m\times m}$ defined in (3) be Onsager compatible along the whole boundary with*

$$\mathbf{A}^{(n)} = \begin{pmatrix} \mathbf{0} & \mathbf{A}_n^* \\ (\mathbf{A}_n^*)^T & 0 \end{pmatrix}, \quad \mathbf{x} \in \partial\Omega \tag{45}$$

where $\mathbf{A}_n^* \in \mathbb{R}^{p\times q}$ and $p \leq q$. Also, let the solution vector $\boldsymbol{\alpha}$ to be structured as

$$\boldsymbol{\alpha} = \begin{pmatrix} \boldsymbol{\alpha}_p \\ \boldsymbol{\alpha}_q \end{pmatrix} \tag{46}$$

where $\boldsymbol{\alpha}_p \in \mathbb{R}^p$ and $\boldsymbol{\alpha}_q \in \mathbb{R}^q$. At the boundary, let $\boldsymbol{\alpha}_p$ and $\boldsymbol{\alpha}_q$ be related as

$$\boldsymbol{\alpha}_p = \mathbf{M}\boldsymbol{\alpha}_q + \mathbf{g} = \mathbf{L}\mathbf{A}_n^*\boldsymbol{\alpha}_q + \mathbf{g} \quad \textit{or} \quad \underbrace{(\mathbf{I}, -\mathbf{M})}_{\mathbf{B}}\boldsymbol{\alpha} = \mathbf{g}, \quad \mathbf{x} \in \partial\Omega \tag{47}$$

where $\mathbf{L} \in \mathbb{R}^{p\times p}$ *is a constant symmetric positive semi-definite matrix,* $\mathbf{M} \in \mathbb{R}^{p\times q}$ *and* $\mathbf{g} \in$ *range*$(\mathbf{L})$ *is the inhomogeneity arising from the boundary. Then, the boundary conditions in* (47) *are stable in the sense of Definition 2.1.*

Proof. See subsection 7.4. □

We showed previously that *Condition1* to *Condition4* are both necessary and sufficient for a set of boundary conditions to be stable. Since, the general OBCs given by (47) are stable this immediately implies that they satisfy the stability conditions for hyperbolic systems which have an *Onsager Compatible* flux matrix.

5.1 OBCs for Moment Equations

The flux matrix $\mathbf{A}^{(n)}$ given in (28) is *Onsager Compatible* at $x = x^{(\pm)}$ and therefore we can use the framework developed in Theorem 5.1 to formulate the OBCs for our moment system. By comparing the moment system and the flux matrix $\mathbf{A}^{(n)}$, given in (25) and (28) respectively, with the general formulation developed in Theorem 5.1 we find

$$\mathbf{A}_n^* = \pm\mathbf{A}^{oe}, \quad \boldsymbol{\alpha}_p = \boldsymbol{\alpha}_o, \quad \boldsymbol{\alpha}_q = \boldsymbol{\alpha}_e, \quad \mathbf{g} = \pm\mathbf{g}^{(\pm)}, \quad x = x^{(\pm)} \tag{48}$$

where $\boldsymbol{\alpha}_o$ and $\boldsymbol{\alpha}_e$ are the odd and the even moments defined in (23b) and (23a) respectively and $\mathbf{g}^{(\pm)}$ is as defined in (38). Using (48) in the general formulation (47), the OBCs for our moment system are given as

$$\boldsymbol{\alpha}_o = \pm\mathbf{L}\mathbf{A}^{oe}\boldsymbol{\alpha}_e \pm \mathbf{g}^{(\pm)}, \quad x = x^{(\pm)} \tag{49}$$

where $\mathbf{L}$ is an unknown symmetric positive semi definite matrix; similar to [21, 26], we will call this matrix the Onsager matrix. We note that for (49) to be stable we require $\mathbf{g}^{(\pm)} \in$ *range*$(\mathbf{L})$, this can only be shown after we have formulated an explicit expression for $\mathbf{L}$. The whole methodology which follows can be summarised as

Step1 We know that the MBCs satisfy *Condition1* but not *Condition2*; therefore, we will first transform $\mathbf{M}^{(mbc)}$ into $\mathbf{M}^{(mbc,*)}$ such that $\mathbf{M}^{(mbc,*)}$ satisfies (32). Then, $\mathbf{M}^{(mbc,*)}$ will be row equivalent with $\mathbf{A}^{oe}$ i.e. it could be expressed as

$$2\beta\mathbf{M}^{(mbc,*)} = \mathbf{L}\mathbf{A}^{oe} \tag{50}$$

where $\mathbf{L}$ could be any matrix not necessarily symmetric positive definite.

Step2 We will then show that $\mathbf{L}$ obtained through *Step1* is indeed symmetric positive semi-definite and is therefore the required Onsager matrix.

Step3 From the Onsager matrix obtained from *Step2*, we will show that $\mathbf{g}^{(\pm)} \in range(\mathbf{L})$.

We will now discuss the above steps in more technical details. For further analysis, we will split $\mathbf{A}^{oe}$ and $\mathbf{M}^{(mbc)}$ as

$$\mathbf{A}^{oe} = \left(\hat{\mathbf{A}}^{oe}, \tilde{\mathbf{A}}^{oe}\right), \quad \mathbf{M}^{(mbc)} = \left(\hat{\mathbf{M}}^{(mbc)}, \tilde{\mathbf{M}}^{(mbc)}\right) \tag{51}$$

where $\hat{\mathbf{A}}^{oe}, \hat{\mathbf{M}}^{(mbc)} \in \mathbb{R}^{n^o \times (n^e-1)}$ and $\tilde{\mathbf{A}}^{oe}, \tilde{\mathbf{M}}^{(mbc)} \in \mathbb{R}^{n^o}$. The invertibility of $\hat{\mathbf{A}}^{oe}$, which follows from (80), shows that $ker\{\mathbf{A}^{oe}\} = span\{\mathbf{a}^{oe}\}$ where

$$\mathbf{a}^{oe} = \begin{pmatrix} \left(\hat{\mathbf{A}}^{oe}\right)^{-1} \tilde{\mathbf{A}}^{oe} \\ -1 \end{pmatrix}. \tag{52}$$

From the null-space of $\mathbf{A}^{oe}$ it is clear that a transformation of $\tilde{\mathbf{M}}^{(mbc)}$ will be enough to ensure that $\mathbf{a}^{oe}$ will belong to $ker\{\mathbf{M}^{(mbc,*)}\}$ and we do not need to disturb the coefficients of $\hat{\mathbf{M}}^{(mbc)}$; therefore, the following structure for $\mathbf{M}^{(mbc,*)}$ will be sufficient to proceed with our construction of the Onsager matrix

$$\mathbf{M}^{(mbc,*)} = \left(\hat{\mathbf{M}}^{(mbc)}, \tilde{\mathbf{M}}^{(mbc,*)}\right) \tag{53}$$

where $\tilde{\mathbf{M}}^{(mbc,*)} = \hat{\mathbf{M}}^{(mbc)} \left(\hat{\mathbf{A}}^{oe}\right)^{-1} \tilde{\mathbf{A}}^{oe}$ which can be obtained by requiring $\mathbf{M}^{(mbc,*)}\mathbf{a}^{oe} = 0$. Using $\tilde{\mathbf{M}}^{(mbc,*)}$ we obtain $\mathbf{M}^{(mbc,*)} = \hat{\mathbf{M}}^{(mbc)} \left(\hat{\mathbf{A}}^{oe}\right)^{-1} \mathbf{A}^{oe}$ which leads to

$$\mathbf{L} = 2\beta \hat{\mathbf{M}}^{(mbc)} \left(\hat{\mathbf{A}}^{oe}\right)^{-1}. \tag{54}$$

with the help of (50). We will now show that $\mathbf{L}$ is indeed symmetric positive semi definite .

Theorem 5.2. *The matrix $\mathbf{L}$ given by (54) is symmetric positive semi-definite.*

Proof. See subsection 7.5. □

With the Onsager matrix $\mathbf{L}$ given by (54), we have an explicit set of OBCs from (49). But the stability of the OBCs can only be assured once we have completed *Step3*; hence, we have the result

Lemma 5.1. *The inhomogeneity $\mathbf{g}^{(\pm)}$ given by (38) is such that $\mathbf{g}^{(\pm)} \in range(\mathbf{L})$ where $\mathbf{L}$ is given by (54).*

Proof. See subsection 7.6. □

With Lemma 5.1, we have completed our formulation of the OBCs. By replacing $\mathbf{L}$ from (54) into (49), we summarise the OBCs for the moment system through the relation

$$\boldsymbol{\alpha}_o = \pm 2\beta \mathbf{M}^{(obc)} \boldsymbol{\alpha}_e \pm \mathbf{g}^{(\pm)}, \quad x = x^{(\pm)} \tag{55}$$

with $\mathbf{M}^{(obc)}$ given by

$$\mathbf{M}^{(obc)} = \hat{\mathbf{M}}^{(mbc)} \left(\hat{\mathbf{A}}^{oe} \right)^{-1} \mathbf{A}^{oe}. \tag{56}$$

The matrix $\mathbf{M}$ and $\mathbf{B}^{(obc)}$, appearing in (31), can now be identified as

$$\mathbf{M} = \pm 2\beta \mathbf{M}^{(obc)}, \quad \mathbf{B}^{(obc)} = \left(\mathbf{I}, \mp 2\beta \mathbf{M}^{(obc)} \right), \quad x = x^{(\pm)}. \tag{57}$$

The explicit formulation of boundary conditions is similar for different values of m (18). Hence, we present the OBCs corresponding to $m = 5$ by revisiting the example presented in subsection 4.3.

Example 2. Consider the moment system corresponding to $m = 5$ in (18). The solution vector $\boldsymbol{\alpha}_5$, the flux matrix $\mathbf{A}_5^{(1)}$ and the boundary matrix $\mathbf{B}_5^{(mbc)}$ corresponding to this system have been given in (40) and (43); it is trivial to see that the flux matrix $\mathbf{A}_5^{(1)}$ is *Onsager compatible* and hence we can formulate a set of stable OBCs for the present moment system. Following the splitting of the boundary matrix and the flux matrix given in (51), we obtain the following expression for $\hat{\mathbf{M}}_5^{(mbc)}$ and $\hat{\mathbf{A}}_5^{oe}$

$$\hat{\mathbf{M}}_5^{(mbc)} = \begin{pmatrix} 0 & 0 \\ 0 & 2\sqrt{\frac{2}{3\pi}} \end{pmatrix}, \quad \hat{\mathbf{A}}_5^{oe} = \begin{pmatrix} 1 & \sqrt{2} \\ 0 & \sqrt{3} \end{pmatrix}. \tag{58}$$

Using the formulae for the Onsager matrix $\mathbf{L}$ from (54), we obtain

$$\mathbf{L}_5 = \hat{\mathbf{M}}_5^{(mbc)} \left(\hat{\mathbf{A}}_5^{oe} \right)^{-1} = \begin{pmatrix} 0 & 0 \\ 0 & \frac{2\beta\sqrt{\frac{2}{\pi}}}{3} \end{pmatrix}. \tag{59}$$

One can now check that $\mathbf{L}_5$ is symmetric positive semi-definite and $\mathbf{g}_5^{(\pm)}$, defined in (43), is in the range of $\mathbf{L}_5$. Therefore, the following set of boundary conditions are stable for the present moment system

$$\boldsymbol{\alpha}_o^5 = \pm \mathbf{L}_5 \mathbf{A}_5^{oe} \boldsymbol{\alpha}_e^5 \pm \mathbf{g}_5^{(\pm)}, \quad x = x^{(\pm)} \tag{60}$$

where $\boldsymbol{\alpha}_o^5 \in \mathbb{R}^2$ and $\boldsymbol{\alpha}_e^5 \in \mathbb{R}^3$ are given as $\boldsymbol{\alpha}_o^5 = (\alpha_1, \alpha_3)$, $\boldsymbol{\alpha}_e^5 = (\alpha_0, \alpha_2, \alpha_4)$ and the matrix $\mathbf{A}_5^{oe} \in \mathbb{R}^{2\times 3}$ is the upper right block of $\mathbf{A}_5^{(1)}$ defined in (40). The set of OBCs given in (60) can also be written as

$$\underbrace{\begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & \mp 2\beta\sqrt{\frac{2}{3\pi}} & \underline{\mp \frac{4\beta}{3}\sqrt{\frac{2}{\pi}}} \end{pmatrix}}_{\mathbf{B}_5^{(obc)}} \boldsymbol{\alpha}_5 = \pm \mathbf{g}_5^{(\pm)}, \quad x = x^{(\pm)}. \tag{61}$$

Comparing the Onsager boundary matrix $\mathbf{B}_5^{(obc)}$ with $\mathbf{B}_5^{(mbc)}$ given in (43), we find that the underlined term, which corresponds to the highest moment in the system, is the one which differs between the two. Thus, by using the formulation presented in the earlier sections, we have stabilised the boundary conditions given in (43) by altering just the coefficient of the highest order moment appearing in the boundary conditions.

Remark 3. For the case when $n^o = n^e$, we will have

$$\mathbf{A}^{oe} = \hat{\mathbf{A}}^{oe}, \quad \mathbf{M}^{(mbc)} = \hat{\mathbf{M}}^{(mbc)} \tag{62}$$

and therefore $ker\{\mathbf{A}^{oe}\} = \emptyset$. Which means that *Condition2* will be automatically satisfied since the empty set is a subset of every set. Using (62) in (56) we obtain $\mathbf{M}^{(obc)} = \mathbf{M}^{(mbc)}$. which shows that the MBCs are stable for all moment systems which have $n^o = n^e$.

Remark 4. A non-trivial normal velocity of the walls changes the number of characteristics which come into the domain; see [5]. Therefore we cannot simply extend the boundary conditions presented in (55), for moving walls, by replacing $g_0^{(\pm)}$ in (38) by $v^{(\pm)}$, with $v^{(\pm)}$ representing the normal velocity of the wall. If we do so then we will end up prescribing the incorrect number of boundary conditions. We leave the formulation of stable boundary conditions for moving walls as a part of the future work.

5.2 Relation to Discrete Velocity Models

We will now compare the OBCs to the boundary implementation presented in [23] where the authors diagonalize the flux matrix appearing in (25) ($\mathbf{A}^{(1)}$) with the help of m Gauss-Hermite quadrature points in the velocity space, $\{z_i\}$, using which the moment system in (25) can be written as

$$\partial_t \tilde{f}_h(x, z_i, t) + z_i \partial_x \tilde{f}_h(x, z_i, t) = \tilde{Q}_h(\tilde{f}_h(x, z_i, t), \tilde{f}_h(x, z_i, t)), \quad i \in \{0, \dots m-1\} \tag{63}$$

where $\tilde{Q}_h$ represents the discrete version of the linearised collision operator $\tilde{Q}$ computed with the help of a quadrature defined on the grid points $\{z_i\}$. Writing the moment system as a discrete velocity scheme makes the implementation of the boundary conditions very straightforward due to the following reasons. Consider the boundary $x = x^{(\pm)}$, then, similar to the boundary conditions for the Boltzmann equation (13), we need to prescribe a value to the distribution function for all those grid points(z_i) which lie in the half space $\pm\xi < 0$. This translates into

$$\tilde{f}_h(x^{(\pm)}, z_i, t) = \chi f_{\mathcal{M}}^{(\pm)}(z_i) + (1-\chi)\tilde{f}_h(x^{(\pm)}, -z_i, t), \quad \pm z_i < 0 \tag{64}$$

with $f_{\mathcal{M}}^{(\pm)}$ as defined in (14). Plugging in the Hermite discretization from (18) into the above relation, we can come up with the desired number of relations for the coefficients (α_i); the boundary conditions given by (64) were also shown to be stable in [23].

From the discussion done in section 2, it is clear that a boundary implementation of the type (64), for the moment system, is only possible if the values of the distribution function at the gauss points corresponding to $\pm z_i < 0$ have a one-to-one mapping to the characteristic variables which come into the domain ($\mathbf{W}_-$). Such a mapping, for moment systems arising from a multi-dimensional velocity space and based upon Gauss-Hermite grid points, exists [23]. But for the approximation of the distribution function based upon spherical harmonics, see [3, 5, 8, 28], the existence of such a mapping is not very clear due to the following reasons (i) the maximum degree of the Hermite polynomials in each of the spatial directions is equal, as a result of which, we atleast need n^3 ($n \in \mathbb{N}$) Gauss-Hermite quadrature points in the velocity space to perform all the velocity space integrals appearing in the moment system exactly. But the number of moment variables (and the characteristic variables) for these moment equations are not equal to n^3 [30]and (ii) the rotational invariance of the moment systems prohibits the existence of an underlying discrete velocity grid; for the Grad's-20 moment system, a possible reason why (64) cannot be used for prescribing boundary conditions has been shown in subsection 7.7.

On the other hand, the formulation presented in the present work is completely independent of the underlying discrete velocity grid. Moreover, a preliminary computational analysis shows that even for moment systems which are based upon a spherical harmonic approximation of the distribution function, the flux matrix is *Onsager compatible*. Therefore, the framework presented in this article can be easily extended to include multi-dimensional moment systems.

5.3 Discussion

We find the following similarities between the entropy flux at the boundary corresponding to the true solution of the Boltzmann equation and the one we obtain through the approximation $\tilde{f}_h$. For $\mathbf{g}^{(\pm)} = 0$ in (55), the entropy flux across the boundary for our moment system is given by

$$\begin{aligned} \pm\boldsymbol{\alpha}^T\mathbf{A}^{(1)}\boldsymbol{\alpha} &= \pm\int \xi \tilde{f}_h^2 f_0^{-1} d\xi, \quad x = x^{(\pm)} \\ &= \pm\, 2\boldsymbol{\alpha}_o^T\mathbf{A}^{oe}\boldsymbol{\alpha}_e = 2\left(\mathbf{A}^{oe}\boldsymbol{\alpha}_e\right)^T\mathbf{L}\mathbf{A}^{oe}\boldsymbol{\alpha}_e \geq 0, \quad (\because \mathbf{L} \geq 0) \end{aligned} \tag{65}$$

which can be looked upon as the discretized version of (17), in the velocity space, with $\tilde{f}$ replaced by its approximation $\tilde{f}_h$. Therefore by constructing OBCs we have mimicked the behaviour of the true entropy flux of the linearised Boltzmann equation at the boundary, though in doing so we had to give up the MBCs.

Using the OBCs, we can better understand the instability which arises due to the MBCs. The MBCs in (36), assuming $\mathbf{g}^{(\pm)} = 0$ and $(\alpha_e)_{n^e-1}$ begin the last component of $\boldsymbol{\alpha}_e$, can be written as

$$\begin{aligned}\boldsymbol{\alpha}_o &= \pm\left[\mathbf{L}\mathbf{A}^{oe}\boldsymbol{\alpha}_e + 2\beta\left(\tilde{\mathbf{M}}^{(mbc)} - \tilde{\mathbf{M}}^{(mbc,*)}\right)(\alpha_e)_{n^e-1}\right], \quad x = x^{(\pm)} \\ &= \pm\left[\mathbf{L}\mathbf{A}^{oe}\boldsymbol{\alpha}_e + \Delta\tilde{\mathbf{M}}^{(mbc)}(\alpha_e)_{n^e-1}\right], \quad \left(\text{with } \Delta\tilde{\mathbf{M}}^{(mbc)} = 2\beta\left(\tilde{\mathbf{M}}^{(mbc)} - \tilde{\mathbf{M}}^{(mbc,*)}\right)\right)\end{aligned} \tag{66}$$

where $\mathbf{L}$ is given by (54), $\tilde{\mathbf{M}}^{(mbc)}$ and $\tilde{\mathbf{M}}^{(mbc,*)}$ are the vectors appearing in (51) and (50) respectively. The fact that $\Delta\tilde{\mathbf{M}}^{(mbc)} \neq 0$ is the reason why the MBCs do not satisfy *Condition2*. Using (66), the entropy flux across the boundary, $\mathcal{H}$, corresponding to the moment system can be written as

$$\begin{aligned}\frac{1}{2}\mathcal{H} = \frac{1}{2}\boldsymbol{\alpha}^T\mathbf{A}^{(n)}\boldsymbol{\alpha} &= \pm\,\boldsymbol{\alpha}_o^T\mathbf{A}^{oe}\boldsymbol{\alpha}_e, \quad x = x^{(\pm)} \\ &= \left(\mathbf{A}^{oe}\boldsymbol{\alpha}_e\right)^T\mathbf{L}\mathbf{A}^{oe}\boldsymbol{\alpha}_e + (\alpha_e)_{n^e-1}\left(\Delta\mathbf{M}^{(mbc)}\right)^T\mathbf{A}^{oe}\boldsymbol{\alpha}_e \\ &\geq (\alpha_e)_{n^e-1}\left(\Delta\mathbf{M}^{(mbc)}\right)^T\mathbf{A}^{oe}\boldsymbol{\alpha}_e, \quad (\because \mathbf{L} \geq 0)\end{aligned} \tag{67}$$

Replacing the bound on the entropy flux into the energy estimate (4), we obtain

$$\partial_t\|\boldsymbol{\alpha}\|^2 \leq -2\,(\alpha_e)_{n^e-1}\left(\Delta\mathbf{M}^{(mbc)}\right)^T\mathbf{A}^{oe}\boldsymbol{\alpha}_e \tag{68}$$

which shows that the growth of the $L^2(\Omega)$ norm of the solution can only be bounded by the solution itself implying that the uniqueness of the solutions obtained through MBCs cannot be ensured.

The construction of the Onsager matrix shows the importance of *Condition2* in formulating the OBCs for the moment system. We will now present an intuitive understanding of this condition. The entropy flux $\boldsymbol{\alpha}^T\mathbf{A}^{(n)}\boldsymbol{\alpha}$ represents the transport of entropy across $\partial\Omega$ and therefore it should not depend upon that part of the solution which does not have any velocity in the normal direction i.e. it should be independent of $\mathbf{W}_0$ which represent the resting waves(see (69)). This statement is also justified by (71) where $\mathcal{H}$ only depends upon $\mathbf{W}_+$ and $\mathbf{W}_-$. But if *Condition2* is not satisfied then $\mathbf{R}_0 \neq 0$ in (69), which is the case for the MBCs, leading to an artificial contribution from $\mathbf{W}_0$ into $\mathcal{H}$ through the boundary conditions. This leads to a non-physical entropy flux at the boundary which is responsible for instabilities.

The construction of the matrix $\mathbf{L}$ discussed in the above sections is one of the various methods which are possible to construct a symmetric positive semi-definite $\mathbf{L}$ and is based upon our hypothesis that the coefficients for the lower order moments arising from MBCs should not be disturbed which complies with the methodology developed recently in [26] and [21]. Contrary to the methodology suggested in the present work, one might choose to transform both the coefficients of the higher and the lower oder moments in the MBCs to obtain an Onsager matrix; therefore, there could be various ways to obtain a desirable Onsager matrix. The extent to which different $\mathbf{L}$ influence the physical accuracy of our Hermite discretization in (18) is an intriguing question in itself. It might be very much possible that an Onsager matrix constructed in a different way will lead to more physically accurate results. An attempt towards this direction was already made in [21] where the authors altered the coefficients of the initially obtained Onsager matrix to obtain physically more accurate results; on the other hand it seems most reasonable to stay as close to MBCs as possible. Despite of the fact that there might exist a physically more accurate Onsager matrix, the importance of stable boundary conditions cannot be underestimated. It has been shown in many studies (see [16, 31] and references therein for a detailed discussion) that numerical schemes fail to converge, specially for curved boundaries, if one does not provide stable boundary conditions; therefore in order to obtain convergent numerical results it is crucial that one uses OBCs over MBCs.

From (54) it is clear that our model for $\mathbf{L}$ relies on the invertibility of $\hat{\mathbf{A}}^{oe}$. The requirement for the invertibility of $\hat{\mathbf{A}}^{oe}$ is nicely met in the one dimensional case; but whether such an invertibility exists for a multi-dimensional case is not very clear. Though a premature computational analysis shows that $\hat{\mathbf{A}}^{oe}$ is invertible even for multi-dimensional systems, atleast in general. If the invertibility of $\hat{\mathbf{A}}^{oe}$ can be shown for an arbitrary order moment system or can be assumed due to certain arguments then $\mathbf{L}$ can be modelled similar to (54) and a proof for the symmetric positive semi definiteness of $\mathbf{L}$ in the multi-dimensional case could be constructed along the same lines as in Theorem 5.2.

6 Conclusion

In the present work we have discussed a methodology to construct stable boundary conditions for a moment system arising from one-dimensional kinetic equation. We have first discussed the computation of boundary conditions using the Maxwell accommodation model which is well-known in the literature. Then by studying the kernel of the various matrices involved, we proposed a model for the Onsager matrix; this model was then shown to be symmetric positive semi-definite with the help of recursion relations of the Hermite polynomials. The model for the Onsager matrix was such that the coefficients of the lower order moments appearing in the Maxwell boundary conditions were not disturbed; such a model complied with the earlier proposed methodologies to construct the Onsager matrix.

7 Appendix

7.1 Analysis using characteristic splitting

A well-known methodology to study the stability of the boundary conditions is through their characteristic decomposition; see [7, 18] for a detailed discussion of this framework. Let the eigenvalue decomposition of $\mathbf{A}^{(n)}$ be $\mathbf{X}\mathbf{\Lambda}\mathbf{X}^T$ with $\mathbf{X}$ and $\mathbf{\Lambda}$ being the matrices containing the eigenvectors and the eigenvalues respectively. Then by introducing the characteristic variables

$\mathbf{W} = \mathbf{X}^T\boldsymbol{\alpha}$ into (1c) we can split the boundary conditions as

$$\mathbf{W}_- = \hat{\mathbf{R}}\hat{\mathbf{W}} + \hat{\mathbf{g}}, \quad \left(\text{with } \hat{\mathbf{W}} = \begin{pmatrix} \mathbf{W}_+ \\ \mathbf{W}_- \end{pmatrix}, \hat{\mathbf{R}} = (\mathbf{R}_+, \mathbf{R}_0), \hat{\mathbf{g}} = (\mathbf{B}\mathbf{X}_-)^{-1}\mathbf{g}\right) \tag{69}$$

where $\mathbf{W}_{-/+/0}$ are the characteristic variables which move with negative, positive and zero characteristic speeds respectively. The matrices $\mathbf{X}_{-/+/0}$ contain those eigenvectors which correspond to negative, positive and zero eigenvalues. We note that the unit vector $\mathbf{n}$ points out of the domain and therefore $\mathbf{W}_-$ represents those variables which bring information into the domain. The matrices $\mathbf{R}_+$ and $\mathbf{R}_0$ are given as

$$\mathbf{R}_0 = -(\mathbf{B}\mathbf{X}_-)^{-1}\mathbf{B}\mathbf{X}_0, \quad \mathbf{R}_+ = -(\mathbf{B}\mathbf{X}_-)^{-1}\mathbf{B}\mathbf{X}_+. \tag{70}$$

Using the characteristic variables and the boundary conditions in (69), we can simplify the entropy flux at the boundary, $\mathcal{H}$, as

$$\mathcal{H} = \boldsymbol{\alpha}^T\mathbf{A}^{(n)}\boldsymbol{\alpha} = \mathbf{W}^T\boldsymbol{\Lambda}\mathbf{W} = \underbrace{\hat{\mathbf{W}}^T\left(\hat{\boldsymbol{\Lambda}} + \hat{\mathbf{R}}^T\boldsymbol{\Lambda}_-\hat{\mathbf{R}}\right)\hat{\mathbf{W}} + 2\hat{\mathbf{W}}^T\hat{\mathbf{R}}^T\boldsymbol{\Lambda}_-\hat{\mathbf{g}}}_{\tilde{\mathcal{H}}} + \hat{\mathbf{g}}^T\boldsymbol{\Lambda}_-\hat{\mathbf{g}}. \tag{71}$$

where $\boldsymbol{\Lambda}_+$ and $\boldsymbol{\Lambda}_-$ are diagonal matrices which contain positive and negative eigenvalues of $\mathbf{A}^{(n)}$ on their diagonals respectively. The matrix $\hat{\boldsymbol{\Lambda}}$ is a block diagonal matrix with the first block being $\boldsymbol{\Lambda}_+$ and all the other entries being zero. In order to study $\mathcal{H}$, we have a crucial result which follows from elementary linear algebra

Lemma 7.1. *Let $\mathbf{x} \in \mathbb{R}^n$ and $\mathbf{C} \in \mathbb{R}^{n\times n}$ be a symmetric positive semi-definite matrix. Let $\mathcal{M} = \mathbf{x}^T\mathbf{C}\mathbf{x} + 2\mathbf{x}^T\mathbf{h}$ where $\mathbf{h} \in range(\mathbf{C})$ and is independent of $\mathbf{x}$. Then, $\mathcal{M}$ can be bounded as $\mathcal{M} \geq -\mathbf{h}^T\mathbf{C}^\dagger\mathbf{h}$ where $\mathbf{C}^\dagger$ is the pseudo-inverse of $\mathbf{C}$.*

Proof. The quadratic form $\mathcal{M}$ can be expressed as

$$\mathcal{M} = (\mathbf{x} + \tilde{\mathbf{h}})^T\mathbf{C}(\mathbf{x} + \tilde{\mathbf{h}}) - \tilde{\mathbf{h}}^T\mathbf{C}\tilde{\mathbf{h}}, \quad (\text{with } \tilde{\mathbf{h}} = \mathbf{C}^\dagger\mathbf{h}). \tag{72}$$

where $\mathbf{C}^\dagger$ represents the pseudo-inverse of $\mathbf{C}$. Since $\mathbf{C} \geq 0$, we then have $\mathcal{M} \geq -\tilde{\mathbf{h}}^T\mathbf{C}\tilde{\mathbf{h}} = -\mathbf{h}^T\mathbf{C}^\dagger\mathbf{h}$. □

Comparing the general formulation presented in Lemma 7.1 with $\tilde{\mathcal{H}}$, we can identify $\mathbf{C}$ and $\mathbf{h}$ as

$$\mathbf{C} = \hat{\boldsymbol{\Lambda}} + \hat{\mathbf{R}}^T\boldsymbol{\Lambda}_-\hat{\mathbf{R}}, \quad \mathbf{h} = \hat{\mathbf{R}}^T\boldsymbol{\Lambda}_-\hat{\mathbf{g}} \tag{73}$$

Therefore, if we can somehow ensure the positive semi-definiteness of $\mathbf{C}$ then we will be able to bound $\tilde{\mathcal{H}}$ solely in terms of $\mathbf{h}$ which will provide us with a bound of the type (5) for the entropy flux, $\mathcal{H}$, leading to the stability of the boundary conditions. By choosing $\hat{\mathbf{W}} = (\mathbf{0}, \mathbf{W}_0)$, with $\mathbf{W}_0$ being arbitrary, and then by choosing $\hat{\mathbf{W}} = (\mathbf{W}_+, \mathbf{0})$, with $\mathbf{W}_+$ being arbitrary, in the quadratic form of $\mathbf{C}$ ($\hat{\mathbf{W}}^T\mathbf{C}\hat{\mathbf{W}}$), we can find the conditions such that $\mathbf{C} \geq 0$

$$\mathbf{R}_0 = 0 \quad \Leftrightarrow \quad ker\{\mathbf{A}^n\} \subseteq ker\{\mathbf{B}\} \tag{74a}$$

$$\mathbf{R}_+^T\boldsymbol{\Lambda}_-\mathbf{R}_+ + \boldsymbol{\Lambda}_+ \geq 0 \tag{74b}$$

If the above two conditions are satisfied along with $\mathbf{h} \in range(\mathbf{C})$, then due to Lemma 7.1 $\mathcal{H}$ in (71) can be bounded as

$$\mathcal{H} \geq -\mathbf{h}^T\mathbf{C}^\dagger\mathbf{h} + \hat{\mathbf{g}}^T\boldsymbol{\Lambda}_-\hat{\mathbf{g}} \tag{75}$$

which provides us with a bound of the type (5) and hence stability in the sense of Definition 2.1. The above analysis can be summarised in the form of the following conditions

Condition1 $rank(\mathbf{B}) = p$ and p should be equal to the number of negative eigenvalues of $\mathbf{A}^{(n)}$.

Condition2 $ker\{\mathbf{A}^{(n)}\} \subseteq ker\{\mathbf{B}\}$(or $\mathbf{R}_0 = 0$).

Condition3 $\mathbf{R}_+^T\boldsymbol{\Lambda}_-\mathbf{R}_+ + \boldsymbol{\Lambda}_+ \geq 0$.

Condition4 $\mathbf{R}_+^T\boldsymbol{\Lambda}_-\hat{\mathbf{g}} \in range(\boldsymbol{\Lambda}_+ + \mathbf{R}_+^T\boldsymbol{\Lambda}_-\mathbf{R}_+)$.

7.2 Proof of Lemma-4.1

Lemma 7.2. *Let a matrix* $\mathbf{C}$ *be Onsager compatible with the same structure as that given in* (29)*, then it has the following properties*

Property1 The $ker\{\mathbf{C}\}$ *is given as*

$$ker\{\mathbf{C}\} = span\left\{\begin{pmatrix}\mathbf{0}\\ ker\{\mathbf{C}_1\}\end{pmatrix}\right\}. \tag{76}$$

Property2 The eigenspectrum of $\mathbf{C}$ *is symmetric about the origin.*

Property3 The number of negative eigenvalues of $\mathbf{C}$ *are equal to* p.

Proof. The proof for *Property1* immediately follows from the second condition required for *Onsager Compatibility* as per which $ker\{\mathbf{C}_1^T\} = \emptyset$. For the proof of *Property2*, we have the following. Let $\mathbf{x}$ be an eigenvector of $\mathbf{C}$ with the eigenvalue λ, then

$$\mathbf{C}\mathbf{x} = \begin{pmatrix}\mathbf{0} & \mathbf{C}_1\\ \mathbf{C}_1^T & 0\end{pmatrix}\begin{pmatrix}\mathbf{x}_1\\ \mathbf{x}_2\end{pmatrix} = \begin{pmatrix}\mathbf{C}_1\mathbf{x}_2\\ \mathbf{C}_1^T\mathbf{x}_1\end{pmatrix} = \lambda\begin{pmatrix}\mathbf{x}_1\\ \mathbf{x}_2\end{pmatrix} \tag{77}$$

where $\mathbf{x}_1 \in \mathbb{R}^p$ and $\mathbf{x}_2 \in \mathbb{R}^q$. Using the above we obtain

$$\begin{pmatrix}\mathbf{0} & \mathbf{C}_1\\ \mathbf{C}_1^T & 0\end{pmatrix}\begin{pmatrix}-\mathbf{x}_1\\ \mathbf{x}_2\end{pmatrix} = \begin{pmatrix}\mathbf{C}_1\mathbf{x}_2\\ -\mathbf{C}_1^T\mathbf{x}_1\end{pmatrix} = -\lambda\begin{pmatrix}-\mathbf{x}_1\\ \mathbf{x}_2\end{pmatrix} \tag{78}$$

which shows that $-\lambda$ is also an eigenvalue of $\mathbf{C}$ and proves *Property2*. Due to *Property1* the matrix $\mathbf{C}$ has a zero eigenvalue with a multiplicity of $q-p$. Thus the number of negative eigenvalues of $\mathbf{C}$ are equal to $\frac{m-(q-p)}{2} = \frac{p+q-(q-p)}{2} = p$, which proves our claim. □

7.3 Proof of Lemma-4.2

Lemma 7.3. *The flux matrix* $\mathbf{A}^{(1)}$ *appearing in* (25) *is Onsager compatible.*

Proof. From (25) it is clear that $\mathbf{A}^{(1)}$ has the structure

$$\mathbf{A}^{(1)} = \begin{pmatrix} 0 & \mathbf{A}^{oe} \\ (\mathbf{A}^{oe})^T & 0 \end{pmatrix} \tag{79}$$

with $\mathbf{A}^{oe} \in \mathbb{R}^{n^o \times n^e}$; moreover due to (24) $n^o \leq n^e$. From the tensorial structure of $\mathbf{A}^{oe}$ given in (26), we know that it will have the form

$$\mathbf{A}^{oe} = \begin{bmatrix} 1 & \sqrt{2} & 0 & \cdots & \cdots & \cdots & \cdots & 0 \\ 0 & \sqrt{3} & 2 & \ddots & & & & \vdots \\ 0 & 0 & \sqrt{5} & \sqrt{6} & \ddots & & & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & & \vdots \end{bmatrix} \tag{80}$$

which shows the linear independence of all of its rows and thus $rank(\mathbf{A}^{oe}) = n^o$. This proves our claim. □

7.4 Proof of Theorem-5.1

Theorem 7.1. *Let the flux matrix, corresponding to a general symmetric hyperbolic system* (1a), $\mathbf{A}^{(n)} \in \mathbb{R}^{m\times m}$ *defined in* (3) *be Onsager compatible with*

$$\mathbf{A}^{(n)} = \begin{pmatrix} \mathbf{0} & \mathbf{A}_n^* \\ (\mathbf{A}_n^*)^T & 0 \end{pmatrix}, \quad \mathbf{x} \in \partial\Omega \tag{81}$$

where $\mathbf{A}_n^* \in \mathbb{R}^{p\times q}$ *and* $p \leq q$. *Also, assume the solution vector* $\boldsymbol{\alpha}$ *to be structured as* $\boldsymbol{\alpha} = (\boldsymbol{\alpha}_p, \boldsymbol{\alpha}_q)^T$ *where* $\boldsymbol{\alpha}_p \in \mathbb{R}^p$ *and* $\boldsymbol{\alpha}_q \in \mathbb{R}^q$. *At the boundary, let* $\boldsymbol{\alpha}_p$ *and* $\boldsymbol{\alpha}_q$ *be related as*

$$\boldsymbol{\alpha}_p = \mathbf{M}\boldsymbol{\alpha}_q + \mathbf{g} = \mathbf{L}\mathbf{A}_n^*\boldsymbol{\alpha}_q + \mathbf{g} \quad \textit{or} \quad \underbrace{(\mathbf{I}, -\mathbf{M})}_{\mathbf{B}}\boldsymbol{\alpha} = \mathbf{g}, \quad \mathbf{x} \in \partial\Omega \tag{82}$$

where $\mathbf{L} \in \mathbb{R}^{p\times p}$ *is a constant symmetric positive semi-definite matrix,* $\mathbf{M} \in \mathbb{R}^{p\times q}$ *and* $\mathbf{g} \in$ *range*$(\mathbf{L})$ *is the inhomogeneity arising from the boundary. Then, the boundary conditions in* (82) *are stable in the sense of Definition 2.1.*

Proof. Since $\mathbf{A}^{(n)}$ is *Onsager compatible* then due to Lemma 4.1 the matrix $\mathbf{A}^{(n)}$ also possesses *Property1* to *Property3*. From *Property3* of the flux matrix $\mathbf{A}^{(n)}$, we know that the OBCs in (82) prescribe the correct number of boundary conditions. In order to see whether we can reproduce a bound of the type (7) with (82), we recall the entropy flux across the boundary (5) corresponding to (1a)

$$\mathcal{H} = \boldsymbol{\alpha}^T \mathbf{A}^{(n)} \boldsymbol{\alpha} = 2\boldsymbol{\alpha}_p^T \mathbf{A}_n^* \boldsymbol{\alpha}_q = 2\left[\hat{\boldsymbol{\alpha}}_q^T \mathbf{L} \hat{\boldsymbol{\alpha}}_q + \hat{\boldsymbol{\alpha}}_q^T \mathbf{g}\right], \quad (\text{with } \hat{\boldsymbol{\alpha}}_q = \mathbf{A}_n^* \boldsymbol{\alpha}_q) \tag{83}$$

where we have used (81) and (82). Since $\mathbf{g} \in range(\mathbf{L})$ and $\mathbf{L}$ has been assumed to be symmetric positive semi-definite, we can use the result of Lemma 7.1 to bound $\mathcal{H}$ as $\mathcal{H} \geq -\frac{1}{2}\mathbf{g}^T \mathbf{L}^\dagger \mathbf{g}$, with $\mathbf{L}^\dagger$ begin the pseudo-inverse of $\mathbf{L}$. Replacing the bound for $\mathcal{H}$ in (4), we find

$$\partial_t \int_\Omega \boldsymbol{\alpha}^T \boldsymbol{\alpha} d\mathbf{x} \leq \frac{1}{2} \oint_{\partial\Omega} \mathbf{g}^T \mathbf{L}^\dagger \mathbf{g} ds \tag{84}$$

which shows the stability of the boundary conditions in (82). □

7.5 Proof of Theorem-5.2

Theorem 7.2. *The matrix* $\mathbf{L}$ *given by* (54) *is symmetric positive semi-definite.*

Proof. If $\mathbf{L}$ is symmetric positive semi-definite then $\hat{\mathbf{P}} = \frac{1}{2\beta}\left(\hat{\mathbf{A}}^{oe}\right)^T \mathbf{L}\hat{\mathbf{A}}^{oe} = \left(\hat{\mathbf{A}}^{oe}\right)^T \hat{\mathbf{M}}^{(mbc)}$ should also be symmetric positive semi-definite due to the invertibility of $\hat{\mathbf{A}}^{oe}$.

- Symmetricity: Using the expression for $\hat{\mathbf{M}}^{(mbc)}$ from (37), $\mathbf{P}$ can be written in tensorial form as

$$\hat{P_{ik}} = \hat{A}_{ji}^{oe} \hat{M}_{jk}^{(mbc)} \tag{85a}$$

$$= \underbrace{\frac{1}{\rho_0}\hat{A}_{ji}^{oe}\langle H_{2j+1}, H_{2k}\rangle_{(\mathbb{R}^+,f_0)}}_{P_{ik}^{(1)}} - \underbrace{\frac{1}{\rho_0}\hat{A}_{ji}^{oe}\langle H_{2j+1}, H_0\rangle_{(\mathbb{R}^+,f_0)} \frac{\langle H_1, H_{2k}\rangle_{(\mathbb{R}^+,f_0)}}{\langle H_1, H_0\rangle_{(\mathbb{R}^+,f_0)}}}_{P_{ik}^{(2)}}. \tag{85b}$$

Using the definition of $\hat{\mathbf{A}}^{oe}$ from (26), the above expression can be simplified as

$$\begin{aligned}
\sqrt{\theta_0}\rho_0^2 P_{ik}^{(1)} &= \langle H_{2j+1}, H_{2i}\xi\rangle_{(\mathbb{R},f_0)} \langle H_{2j+1}, H_{2k}\rangle_{(\mathbb{R}^+,f_0)} \\
&= \rho_0\sqrt{\theta_0}\sqrt{2i+1}\,\langle H_{2i+1}, H_{2k}\rangle_{(\mathbb{R}^+,f_0)} + \rho_0\sqrt{\theta_0}\sqrt{2i}\,\langle H_{2i-1}, H_{2k}\rangle_{(\mathbb{R}^+,f_0)} \\
&= \rho_0\,\langle H_{2i}, H_{2k}\xi\rangle_{(\mathbb{R}^+,f_0)}.
\end{aligned} \tag{86}$$

Now doing the same for $P_{ik}^{(2)}$ we have

$$\begin{aligned}
\sqrt{\theta_0}\rho_0^2 P_{ik}^{(2)} &= \langle H_{2j+1}, H_{2i}\xi\rangle_{(\mathbb{R},f_0)} \langle H_{2j+1}, H_0\rangle_{(\mathbb{R}^+,f_0)} \frac{\langle H_1, H_{2k}\rangle_{(\mathbb{R}^+,f_0)}}{\langle H_1, H_0\rangle_{(\mathbb{R}^+,f_0)}} \\
&= \rho_0\sqrt{\theta_0}\left(\sqrt{2i+1}\,\langle H_{2i+1}, H_0\rangle_{(\mathbb{R}^+,f_0)} + \sqrt{2i}\,\langle H_{2i-1}, H_0\rangle_{(\mathbb{R}^+,f_0)}\right) \\
&\quad \times \frac{\langle H_1, H_{2k}\rangle_{(\mathbb{R}^+,f_0)}}{\langle H_1, H_0\rangle_{(\mathbb{R}^+,f_0)}} \\
&= \rho_0 \frac{\langle \xi H_0, H_{2i}\rangle_{(\mathbb{R}^+,f_0)}\langle H_1, H_{2k}\rangle_{(\mathbb{R}^+,f_0)}}{\langle H_1, H_0\rangle_{(\mathbb{R}^+,f_0)}} \\
&= \rho_0\sqrt{\theta_0}\frac{\langle H_1, H_{2i}\rangle_{(\mathbb{R}^+,f_0)}\langle H_1, H_{2k}\rangle_{(\mathbb{R}^+,f_0)}}{\langle H_1, H_0\rangle_{(\mathbb{R}^+,f_0)}} \qquad (\because \frac{\xi}{\sqrt{\theta_0}}H_0 = H_1).
\end{aligned} \tag{87}$$

The expressions (86) and (87) are now symmetric with respect to i and k which implies that $\mathbf{P}$ is symmetric and so is $\mathbf{L}$. In writing the above relation we have used the orthogonality (20a) and the recursion relation (20b) of the Hermite polynomials.

- Positive Semi-Definiteness: Let the quadratic form of $\mathbf{P}$ be represented by κ then,

$$\kappa = x_i P_{ik}^{(1)} x_k - x_i P_{ik}^{(2)} x_k. \tag{88}$$

Let $\bar{f}$ be a function such that

$$\bar{f}(\xi) = \sum_{i=0}^{n^e-1} x_i H_{2i}(\xi) f_0(\xi), \quad \xi \in \mathbb{R}^+. \tag{89}$$

Then κ reads

$$\begin{aligned}
\rho_0\kappa &= \frac{1}{\sqrt{\theta_0}}\left\langle x_i H_{2i} f_0 f_0^{-1}, x_k H_{2k}\xi f_0\right\rangle_{\mathbb{R}^+} - \frac{\langle H_1, x_i H_{2i} f_0\rangle_{\mathbb{R}^+}\langle H_1, x_k H_{2k} f_0\rangle_{\mathbb{R}^+}}{\langle H_1, H_0\rangle_{(\mathbb{R}^+,f_0)}} \\
&= \left\langle \bar{f}^2, H_1 f_0^{-1}\right\rangle_{\mathbb{R}^+} - \frac{\langle H_1, \bar{f}\rangle_{\mathbb{R}^+}^2}{\langle H_1, H_0\rangle_{(f_0,\mathbb{R}^+)}} \qquad (\because H_1 = \frac{\xi}{\sqrt{\theta_0}}).
\end{aligned} \tag{90}$$

The integrals in the above expression will be bounded because $\bar{f} \in L^2(\mathbb{R}^+, f_0^{-1})$. Let

$$\hat{x}_1(\xi) = \bar{f}\sqrt{H_1 f_0^{-1}}, \quad \hat{x}_2(\xi) = H_0\sqrt{H_1 f_0} \quad \forall \quad \xi \in \mathbb{R}^+. \tag{91}$$

Then by Cauchy-Schwartz inequality we have

$$|\langle \hat{x}_1, \hat{x}_2\rangle_{\mathbb{R}^+}|^2 \leq \langle \hat{x}_1, \hat{x}_1\rangle_{\mathbb{R}^+}\langle \hat{x}_2, \hat{x}_2\rangle_{\mathbb{R}^+}. \tag{92}$$

Substituting the expression for $\hat{x}_1$ and $\hat{x}_2$ in the relation above we obtain

$$\begin{aligned}
\langle \bar{f}\sqrt{H_1 f_0^{-1}}, H_0\sqrt{H_1 f_0}\rangle_{\mathbb{R}^+}^2 \leq &\langle \bar{f}\sqrt{H_1 f_0^{-1}}, \bar{f}\sqrt{H_1 f_0^{-1}}\rangle_{\mathbb{R}^+} \\
&\times \langle H_0\sqrt{H_1 f_0}, H_0\sqrt{H_1 f_0}\rangle_{\mathbb{R}^+}.
\end{aligned} \tag{93}$$

The above expression can be further simplified to

$$\langle H_1, H_0 f_0\rangle_{\mathbb{R}^+} \left\langle \bar{f}^2, H_1 f_0^{-1}\right\rangle_{\mathbb{R}^+} \geq \langle H_1, \bar{f}\rangle_{\mathbb{R}^+}^2. \tag{94}$$

Since $\langle H_1, H_0 f_0\rangle_{\mathbb{R}^+} > 0$, the above inequality immediately implies

$$\kappa \geq 0 \tag{95}$$

with equality in the above expression if and only if

$$\hat{x}_1 = \gamma \hat{x}_2 \quad \Rightarrow \bar{f} = \gamma f_0 \tag{96}$$

where $\gamma \in \mathbb{R}$.

The symmetric positive semi-definiteness of $\hat{\mathbf{P}}$ implies the same for $\mathbf{L}$. □

7.6 Proof of Lemma-5.1

Lemma 7.4. *The inhomogeneity $\mathbf{g}^{(\pm)}$ given by (38) is such that $\mathbf{g}^{(\pm)} \in range(\mathbf{L})$ where $\mathbf{L}$ is given by (54).*

Proof. From (37), we can trivially conclude for $\mathbf{M}^{(mbc)}$ that

$$\mathbf{M}^{(mbc)} = \begin{pmatrix} 0 & \mathbf{0} \\ \mathbf{0} & \tilde{\mathbf{M}}^{(mbc)} \end{pmatrix} \tag{97}$$

where $\tilde{\mathbf{M}}^{(mbc)} \in \mathbb{R}^{(n^o-1)\times(n^o-1)}$. The first row of $\mathbf{M}^{(mbc)}$ being zero captures the no penetration boundary condition of the fluid and the first column begin zero shows us that α_0, which corresponds to the deviation of density(see (22)), has no role to play in any of the boundary conditions. Using the above properties of $\mathbf{M}^{(mbc)}$ in our model for the Onsager matrix (54), we have

$$\mathbf{L} = \begin{pmatrix} 0 & \mathbf{0} \\ \mathbf{0} & \tilde{\mathbf{L}} \end{pmatrix} \tag{98}$$

where $\tilde{\mathbf{L}} \in \mathbb{R}^{(n^o-1)\times(n^o-1)}$. Since the equality in the Cauchy-Schwartz inequality (95) exists if and only if (96) holds so $\tilde{\mathbf{L}}$ will be a $s.p.d$ matrix. The temperatures of the walls, $\tilde{\theta}^{(\pm)}$ in (14), can be arbitrary chosen therefore the inhomogeneity $\mathbf{g}^{(\pm)}$, given in (38), can be structured as

$$\mathbf{g}^{(\pm)} = \begin{pmatrix} 0 \\ \tilde{\mathbf{g}}^{(\pm)} \end{pmatrix} \tag{99}$$

where $\tilde{\mathbf{g}}^{(\pm)} \in \mathbb{R}^{n^o-1}$ and is arbitrary. Comparing the structure of $\mathbf{g}^{(\pm)}$ with that of $\mathbf{L}$ and using the $s.p.d$ nature of $\tilde{\mathbf{L}}$, we immediately find $\mathbf{g}^{(\pm)} \in range(\mathbf{L})$. □

7.7 Relation of the Grad's-20 moment system to Discrete Velocity Models

Let us consider the following distribution function for a multi-dimensional velocity space which corresponds to the Grad's-20 moment system [4]

$$f_M(\mathbf{x}, \boldsymbol{\xi}, t) = \sum_{|\beta^{(i)}| \le M} \alpha_{\beta^{(i)}}(\mathbf{x}, t)\psi_{\beta^{(i)}}(\boldsymbol{\xi}) f_0 \tag{100}$$

where $\beta^{(i)} = \left(m_1^{(i)}, \ldots, m_d^{(i)}\right)$ is a multi-index, $M = 3$ and

$$\psi_{\beta^{(i)}}(\boldsymbol{\xi}) = \prod_{p=1}^{d} He_{m_p^{(i)}}\left(\frac{\xi_p}{\sqrt{\theta_0}}\right). \tag{101}$$

The total number of moment variables, $\alpha_{\beta^{(i)}}$, will be $m = 20$. Assuming the normal to the wall boundary to be pointing in the positive x-direction, we are only concerned about the characteristic variables arising from the flux matrix corresponding to the positive x-direction, which is given by

$$A_{ij}^{(1)} = \int_{\mathbb{R}^d} \psi_{\beta^{(i)}} \xi_1 \psi_{\beta^{(j)}} f_0 d\boldsymbol{\xi} \tag{102}$$

The maximum possible degree of the Hermite polynomials, in each direction, is $M = 3$. Therefore the minimum number of Gauss-Hermite grid points (in the 3D velocity space) required to perform the integral appearing in $\mathbf{A}^{(1)}$ exactly are $G = 4 \times 4 \times 4$ ($L + 1$ gauss points provide exact integration for polynomials upto $2L + 1$ degree). Let $\{d_i\}$ and $\{\mathbf{z}_i\}$ denote the weights and the locations of all of these G number of quadrature points (we implicitly assume some ordering for the Gauss points in different directions). Then

$$A_{ij}^{(1)} = \int_{\mathbb{R}^d} \psi_{\beta^{(i)}} \xi_1 \psi_{\beta^{(j)}} f_0 d\boldsymbol{\xi} = \sum_{m=0}^{G-1} \psi_{\beta^{(i)}}(\mathbf{z}_m) z_m^{(1)} \psi_{\beta^{(j)}}(\mathbf{z}_m) f_0(\mathbf{z}_m) d_m \tag{103}$$

where $z_m^{(1)}$ is the x-component of the m-the quadrature point location. Then $\mathbf{A}^{(1)}$ can be decomposed as

$$\mathbf{A}^{(1)} = \mathbf{R}\boldsymbol{\Lambda}\mathbf{R}^T \tag{104}$$

where

$$R_{ij} = \psi_{\beta^{(i)}}(\mathbf{z}_j)\sqrt{f_0(\mathbf{z}_j) d_j}, \quad \Lambda_{ij} = \delta_{ij} z_i^{(1)}. \tag{105}$$

Clearly $\mathbf{R} \in \mathbb{R}^{m \times G}$ and $\boldsymbol{\Lambda} \in \mathbb{R}^{G \times G}$. Though $R_{ij} R_{kj} = \delta_{ik}$, the expression in (104) is not the eigenvalue decomposition of $\mathbf{A}^{(1)}$. Let $\boldsymbol{\alpha} \in \mathbb{R}^m$ represent a vector containing all the moments $\alpha_{\beta^{(i)}}$ and let the eigenvalue decomposition of $\mathbf{A}^{(1)}$ be given as $\mathbf{A}^{(1)} = \mathbf{X}\boldsymbol{\Lambda}\mathbf{X}^T$, then

$$\boldsymbol{\alpha} = \mathbf{R}\mathbf{F} = \mathbf{X}\mathbf{W} \Rightarrow \mathbf{W} = \tilde{\mathbf{R}}\mathbf{F} \quad (\tilde{\mathbf{R}} = \mathbf{X}^T\mathbf{R}) \tag{106}$$

where $\mathbf{W}$ are the characteristic variables and $F_i = \sqrt{\frac{d_i}{f_0(\mathbf{z}_i)}} f(\mathbf{x}, \mathbf{z}_i, t)$. Let us assume $\mathbf{F}$ to be ordered as

$$\mathbf{F} = \begin{pmatrix} \mathbf{F}^- \\ \mathbf{F}^+ \end{pmatrix} \quad \text{where} \quad F_i^{\pm} = \sqrt{\frac{d_i}{f_0(\mathbf{z}_i)}} f(\mathbf{x}, \mathbf{z}_i, t) \quad \pm z_i^{(1)} > 0, \tag{107}$$

using which the relation in (106) becomes

$$\mathbf{W} = \tilde{\mathbf{R}}\mathbf{F} = \tilde{\mathbf{R}}^-\mathbf{F}^- + \tilde{\mathbf{R}}^+\mathbf{F}^+. \tag{108}$$

By prescribing a value to $\mathbf{F}^-$, we provide a value to the incoming part of the distribution function which will be similar to (64). A computational study of the matrix $\tilde{\mathbf{R}}^-$ shows that its structure is such that a prescribed value for $\mathbf{F}^-$, influences all the components of $\mathbf{W}$, which is undesirable. Therefore, we cannot use (64) to prescribe boundary conditions for the Grad's-20 moment system.

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