Half-range Orthogonality Relations Basic to the Solution of Time-dependent Boundary Value Problems in the Kinetic Theory of Gases

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1. Introduction

We wish to consider here the linearized BGK model of the Boltzmann equation expressed as [1]

$$\left(\frac{\partial}{\partial t} + c_x \frac{\partial}{\partial x} + 1\right) h(x, \mathbf{c}, t) = (\pi)^{-3/2} \int h(x, \mathbf{c}', t) K(\mathbf{c}'; \mathbf{c}) e^{-c'^2} d^3 c',$$
(1)

with

$$K(\mathbf{c}':\mathbf{c}) = 1 + 2\mathbf{c} \cdot \mathbf{c}' + \frac{2}{3}({c'}^2 - \frac{3}{2})(c^2 - \frac{3}{2}).$$
(2)

Here $h(x, \mathbf{c}, t)$ represents the perturbation of the particle distribution function from the Maxwellian distribution, \mathbf{c} , with components c_x , c_y , and c_z and magnitude c, is the velocity, t is the time and x is the space variable. Since we are interested here in temperature-density effects, we can take 'moments' of Eqn. (1), in the manner of Cercignani [1], to obtain equations dependent only on x, c_x and t. Thus we let

$$\psi_1(x, c_x, t) = (\pi)^{-1/2} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \exp\left[-(c_y^2 + c_z^2)\right] h(x, \mathbf{c}, t) \, dc_y \, dc_z \tag{3a}$$

and

$$\psi_2(x, c_x, t) = (\pi)^{-1/2} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \exp\left[-(c_y^2 + c_z^2)\right] h(x, \mathbf{c}, t) (c_y^2 + c_z^2 - 1) \, dc_y \, dc_z$$
(3b)

so that the density perturbation

$$\Delta N(x,t) = (\pi)^{-3/2} \int h(x,\mathbf{c},t) \, e^{-c^2} \, d^3c \tag{4}$$

and the temperature perturbation

$$\Delta T(x,t) = \frac{2}{3}(\pi)^{-3/2} \int h(x,\mathbf{c},t)(c^2 - \frac{3}{2}) e^{-c^2} d^3c$$
(5)

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can be expressed as

$$\Delta N(x,t) = \frac{1}{\pi} \int_{-\infty}^{\infty} \psi_1(x,\mu,t) \, e^{-\mu^2} \, d\mu \tag{6}$$

and

$$\Delta T(x,t) = \frac{2}{3\pi} \int_{-\infty}^{\infty} \left[(\mu^2 - \frac{1}{2}) \psi_1(x,\mu,t) + \psi_2(x,\mu,t) \right] e^{-\mu^2} d\mu.$$
(7)

If we multiply Eqn. (1) by $\exp(-c_y^2 - c_z^2)$ and integrate from $-\infty$ to ∞ over both c_y and c_z and then multiply Eqn. (1) by $(c_y^2 + c_z^2 - 1) \exp(-c_y^2 - c_z^2)$ and integrate similarly, we find that we write the two resulting equations as

$$\left(\frac{\partial}{\partial t} + \mu \frac{\partial}{\partial x} + 1\right) \Psi(x, \mu, t) = (\pi)^{-1/2} \int_{-\infty}^{\infty} \left[\mathbf{Q}(\mu)\mathbf{Q}^{T}(\mu') + 2\mu\mu'\mathbf{P}\right] \Psi(x, \mu', t) e^{-\mu'^{2}} d\mu',$$
(8)

where we now use μ for c_x . Here $\Psi(x, \mu, t)$ is a two vector, with elements $\psi_1(x, \mu, t)$ and $\psi_2(x, \mu, t)$. Also

$$\mathbf{Q}(\mu) = \begin{vmatrix} \frac{(\frac{2}{3})^{1/2}(\mu^2 - \frac{1}{2}) & 1\\ \frac{(\frac{2}{3})^{1/2}}{2} & 0 \end{vmatrix}$$
(9a)

and

$$\mathbf{P} = \begin{vmatrix} 1 & 0 \\ 0 & 0 \end{vmatrix}. \tag{9b}$$

Equations (6) and (7) give the density and temperature perturbations in terms of $\Psi(x, \mu, t)$; we note that the xx component of the perturbed pressure tensor

$$\Delta P_{xx}(x,t) = (\pi)^{-3/2} \int h(x,\mathbf{c},t) c_x^2 e^{-c^2} d^3 c$$
(10)

can also be expressed in terms of $\Psi(x, \mu, t)$:

$$\Delta P_{xx}(x,t) = (\pi)^{-1} \left| \begin{matrix} 1 \\ 0 \end{matrix} \right|^T \int_{-\infty}^{\infty} \Psi(x,\mu,t) \, e^{-\mu^2} \mu^2 \, d\mu.$$
(11)

From the work of Cercignani [1], we note that the solutions to three scalar equations would be required, in addition to $\Psi(x, \mu, t)$, in order to construct h(x, c, t); however, the scalar equations can be solved generally with limited difficulty. We thus focus our attention here on solving Eqn. (8) subject to appropriate constraints.

2. Elementary Solutions

In a recent paper [2], hereafter referred to as SB, a set of elementary solutions to Eqn. (8) was found by proposing the separation *Ansatz*

$$\Psi(x,\mu,t) = e^{st} \Phi(v,\mu;s) e^{-(s+1)x/v},$$
(12)

where s is, in general, a complex parameter. Since we intend to develop here a collection of orthogonality relations that is useful for solving boundary value problems in terms of the elementary solutions of Eqn. (8), we first wish to summarize some of the basic results of SB. In terms of the arbitrary parameter s, a solution of Eqn. (8) can be written as

$$\Psi(x, \mu, t) = e^{st} \left\{ \sum_{\alpha=1}^{\kappa} \left[A(v_{\alpha}) \Phi(v_{\alpha}, \mu; s) \exp\left[-(s+1)x/v_{\alpha}\right] + A(-v_{\alpha}) \Phi(-v_{\alpha}, \mu; s) \exp\left[(s+1)x/v_{\alpha}\right] \right] + \int_{-\infty}^{\infty} \Phi(v, \mu; s) A(v) \exp\left[-(s+1)x/v\right] dv \right\},$$
(13)

where the continuum matrix is

$$\mathbf{\Phi}(\nu,\mu;s) = \theta \nu P \nu \left(\frac{1}{\nu-\mu}\right) \mathbf{Q}(\mu) (\mathbf{I} + \gamma \nu \mu \mathbf{D}) + \delta(\nu-\mu) e^{\nu^2} \mathbf{Q}^{-T}(\nu) \lambda(\nu;s)$$
(14)

and the discrete vectors are

$$\mathbf{\Phi}(\pm \mathbf{v}_{\alpha}, \mu; s) = \theta \mathbf{v}_{\alpha} \left(\frac{1}{\mathbf{v}_{\alpha} \mp \mu} \right) \mathbf{Q}(\mu) (\mathbf{I} \pm \gamma \mathbf{v}_{\alpha} \mu \mathbf{D}) \mathbf{M}(\mathbf{v}_{\alpha}; s).$$
(15)

Here

$$\theta = (\pi)^{-1/2} \left(\frac{1}{s+1} \right), \qquad \gamma = \frac{2s}{s+1}, \qquad \mathbf{D} = \begin{vmatrix} 0 & 0 \\ 0 & 1 \end{vmatrix}$$
 (16a, b, c)

and the discrete eigenvalues $\pm v_{\alpha}$ are the zeros of $\Lambda(z; s) = \det \Lambda(z; s)$, where

$$\Lambda(z;s) = \mathbf{I} + z \int_{-\infty}^{\infty} \Psi(\mu;s) \frac{d\mu}{\mu - z}$$
(17)

and

$$\Psi(\mu; s) = \theta e^{-\mu^2} \mathbf{Q}^T(\mu) \mathbf{Q}(\mu) (\mathbf{I} + \gamma \mu^2 \mathbf{D}).$$
(18)

In addition, $\mathbf{M}(v_{\alpha}; s)$ is a null vector of $\Lambda(v_{\alpha}; s)$, κ is used to denote the number of \pm pairs of zeros of $\Lambda(z; s)$ in the complex plane cut along the entire real axis, and

$$\lambda(\nu; s) = \mathbf{I} + \nu P \int_{-\infty}^{\infty} \Psi(\mu; s) \frac{d\mu}{\mu - \nu}.$$
 (19)

The scalars $A(\pm v_{\alpha})$ and the two-vector $\mathbf{A}(v)$ appearing in Eqn. (13) are arbitrary expansion coefficients to be used to constrain $\Psi(x, \mu, t)$ to meet appropriate boundary and initial conditions.

3. Orthogonality Relations and Normalization Integrals

In SB proof (for $\kappa = 0$) that the elementary solutions given by Eqns. (14) and (15) are sufficiently general for half-range, $\mu > 0$, boundary conditions was given. Here we wish to show that these eigenvectors are also orthogonal on the half-range to a related adjoint set $\Theta(\xi, \mu; s)$. As will be clearly illustrated in Section IV of this paper, these adjoint functions allow us to develop concisely solutions to typical half-space problems. We consider the adjoint functions

$$\Theta^{T}(\nu,\mu;s) = \pi^{-1}(\nu)\mathbf{H}^{-T}(\nu)\left[\nu P \nu\left(\frac{1}{\nu-\mu}\right) - \frac{2\nu z_{1}}{(z_{1}+\nu)(z_{1}-\mu)}\mathbf{K}\right] + \lambda(\nu;s)\Psi^{-1}(\nu;s)\pi^{-1}(\nu)\mathbf{H}^{-T}(\nu)\,\delta(\nu-\mu), \quad \nu > 0,$$
(20)

and

$$\boldsymbol{\Theta}^{T}(\boldsymbol{v}_{\alpha},\boldsymbol{\mu};\boldsymbol{s}) = \mathbf{M}^{T}(\boldsymbol{v}_{\alpha};\boldsymbol{s})\boldsymbol{\pi}(-\boldsymbol{v}_{\alpha})\mathbf{H}^{-T}(\boldsymbol{v}_{\alpha})\left[\frac{\boldsymbol{v}_{\alpha}}{\boldsymbol{v}_{\alpha}-\boldsymbol{\mu}}-\frac{2\boldsymbol{v}_{\alpha}\boldsymbol{z}_{1}}{(\boldsymbol{z}_{1}+\boldsymbol{v}_{\alpha})(\boldsymbol{z}_{1}-\boldsymbol{\mu})}\mathbf{K}\right], \quad (21)$$

with

$$\mathbf{K} = [\mathbf{I} + \mathbf{H}^{-1}(z_1)\mathbf{D}\mathbf{H}(-z_1)]^{-1}\mathbf{H}^{-1}(z_1)\mathbf{D}\mathbf{H}(-z_1).$$
(22)

Here we use the superscript T to denote the transpose operation and the superscript -T to denote the transpose-inverse operation. In addition we let v_{α} be the 'positive' eigenvalue of the pair $\pm v_{\alpha}$, and

$$\pi(z) = \mathbf{I} - \left(\frac{z}{z_1}\right) \mathbf{D},\tag{23}$$

where $\sqrt{\gamma} z_1 = i$. The **H** matrix appearing in Eqns. (20) and (21) is that introduced for this problem in SB. To establish the desired orthogonality relations, we consider that the **H** matrix is the solution to the singular integral equation

$$\mathbf{H}^{T}(\mu)\boldsymbol{\pi}(\mu)\boldsymbol{\lambda}(\mu;s)\boldsymbol{\pi}^{-1}(\mu) = \mathbf{I} + \mu P \int_{0}^{\infty} \mathbf{H}^{T}(x)\Psi_{*}(x;s)\frac{dx}{x-\mu}, \quad \mu \in [0,\infty), \quad (24)$$

and the constraints (for $\kappa > 0$)

$$\left[\mathbf{I} + v_{\alpha} \int_{0}^{\infty} \mathbf{H}^{T}(x) \Psi_{*}(x;s) \frac{dx}{x - v_{\alpha}}\right] \pi(v_{\alpha}) \mathbf{M}(v_{\alpha};s) = \mathbf{0}, \quad \alpha = 1, 2, \dots, \kappa,$$
(25)

where

$$\Psi_*(x;s) = \pi(x)\Psi(x;s)\pi^{-1}(x).$$
(26)

Once $\mathbf{H}(\mu)$, $\mu \in [0, \infty)$, is established by solving iteratively

$$\mathbf{H}^{-1}(\mu) = \mathbf{I} - \mu \int_{0}^{\infty} \mathbf{H}^{T}(x) \Psi_{*}(x;s) \frac{dx}{x+\mu}, \quad \mu \in [0,\infty),$$
(27)

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the representation

$$\mathbf{H}^{-1}(z) = \mathbf{I} - z \int_0^\infty \mathbf{H}^T(x) \Psi_*(x;s) \frac{dx}{x+z}, \quad z \notin (-\infty, 0],$$
(28)

yields $H^{-1}(z)$ off of the cut. In addition to Eqns. (24) and (25), we note from SB that H(z) can be used to factor

$$\mathbf{\Omega}(z;s) = \mathbf{\Omega}^{T}(-z;s) = \pi(z)\mathbf{\Lambda}(z;s)\pi^{-1}(z)$$
⁽²⁹⁾

in the manner

$$\mathbf{\Omega}^{T}(z;s) = \mathbf{H}^{-T}(-z)\mathbf{H}^{-1}(z).$$
(30)

Equations (24), (25), (28) and (30), along with the fact that

$$\Omega(v_{\alpha}; s)\pi(v_{\alpha})\mathbf{M}(v_{\alpha}; s) = \mathbf{0}, \tag{31}$$

can now be used to establish the following summary of orthogonality relations and normalization integrals:

$$\int_{0}^{\infty} \Theta^{T}(v,\mu;s) \mathbf{H}^{T}(\mu) \pi(\mu) \mathbf{Q}^{T}(\mu) \Phi(v_{\alpha},\mu;s) e^{-\mu^{2}} \mu d\mu = \mathbf{0}, \quad v \in (0,\infty), \quad (32a)$$

$$\int_{0}^{\infty} \Theta^{T}(v,\mu;s) \mathbf{H}^{T}(\mu) \pi(\mu) \mathbf{Q}^{T}(\mu) \Phi(v',\mu;s) e^{-\mu^{2}} \mu d\mu = v \mathbf{L}(v) \,\delta(v-v'), \quad v, v' \in (0,\infty), \quad (32b)$$

$$\int_0^\infty \mathbf{\Theta}^T(\mathbf{v}_{\alpha},\mu;s)\mathbf{H}^T(\mu)\boldsymbol{\pi}(\mu)\mathbf{Q}^T(\mu)\mathbf{\Phi}(\mathbf{v}',\mu;s) \, e^{-\mu^2}\,\mu\,d\mu = \mathbf{0}, \quad \mathbf{v}' \in (0,\infty), \tag{32c}$$

$$\int_{0}^{\infty} \boldsymbol{\Theta}^{T}(\boldsymbol{v}_{\alpha},\boldsymbol{\mu};s) \mathbf{H}^{T}(\boldsymbol{\mu}) \boldsymbol{\pi}(\boldsymbol{\mu}) \mathbf{Q}^{T}(\boldsymbol{\mu}) \boldsymbol{\Phi}(\boldsymbol{v}_{\beta},\boldsymbol{\mu};s) e^{-\boldsymbol{\mu}^{2}} \boldsymbol{\mu} d\boldsymbol{\mu} = N(\boldsymbol{v}_{\alpha}) \,\delta_{\alpha,\beta}.$$
(32d)

Here the results for the normalization integrals are

$$\mathbf{L}(v) = \boldsymbol{\lambda}(v; s) \boldsymbol{\Psi}^{-1}(v; s) \boldsymbol{\lambda}(v; s) + \pi^2 v^2 \boldsymbol{\Psi}(v; s)$$
(33)

and

$$N(v_{\alpha}) = v_{\alpha}^{2} \mathbf{M}^{T}(v_{\alpha}; s) \frac{d}{dz} [\pi(z)\pi(-z)\Lambda(z; s)]_{z = v_{\alpha}} \mathbf{M}(v_{\alpha}; s).$$
(34)

In addition to Eqns. (32), we note that the following integrals can be useful for parallel plates (i.e., finite slab) problems:

$$\int_{0}^{\infty} \boldsymbol{\Theta}^{T}(\boldsymbol{v},\boldsymbol{\mu};\boldsymbol{s}) \mathbf{H}^{T}(\boldsymbol{\mu}) \boldsymbol{\pi}(\boldsymbol{\mu}) \mathbf{Q}^{T}(\boldsymbol{\mu}) \boldsymbol{\Phi}(-\boldsymbol{v}_{\alpha},\boldsymbol{\mu};\boldsymbol{s}) e^{-\boldsymbol{\mu}^{2}} \boldsymbol{\mu} d\boldsymbol{\mu}$$

$$= v v_{\alpha} \boldsymbol{\pi}^{-1}(\boldsymbol{v}) \mathbf{H}^{-T}(\boldsymbol{v}) \left[\frac{1}{\boldsymbol{v} + \boldsymbol{v}_{\alpha}} \mathbf{I} - \frac{2z_{1}}{(z_{1} + \boldsymbol{v})(z_{1} + \boldsymbol{v}_{\alpha})} \mathbf{K} \right] \mathbf{H}^{-1}(\boldsymbol{v}_{\alpha}) \boldsymbol{\pi}(-\boldsymbol{v}_{\alpha}) \mathbf{M}(\boldsymbol{v}_{\alpha};\boldsymbol{s}), \quad \boldsymbol{v} \in (0, \infty), \quad (35a)$$

$$\int_{0}^{\infty} \Theta^{T}(v, \mu; s) \mathbf{H}^{T}(\mu) \pi(\mu) \mathbf{Q}^{T}(\mu) \Phi(-v', \mu; s) e^{-\mu^{2}} \mu d\mu$$

$$= vv' \pi^{-1}(v) \mathbf{H}^{-T}(v) \left[\frac{1}{v + v'} \mathbf{I} - \frac{2z_{1}}{(z_{1} + v)(z_{1} + v')} \mathbf{K} \right] \mathbf{H}^{-1}(v') \pi(-v'), \quad v, v' \in (0, \infty), \quad (35b)$$

$$\int_{0}^{\infty} \Theta^{T}(v_{\alpha}, \mu; s) \mathbf{H}^{T}(\mu) \pi(\mu) \mathbf{Q}^{T}(\mu) \Phi(-v_{\beta}, \mu; s) e^{-\mu^{2}} \mu d\mu$$

$$= v_{\alpha} v_{\beta} \mathbf{M}^{T}(v_{\alpha}; s) \pi(-v_{\alpha}) \mathbf{H}^{-T}(v_{\alpha}) \left[\frac{1}{v_{\alpha} + v_{\beta}} \mathbf{I} - \frac{2z_{1}}{(z_{1} + v_{\alpha})(z_{1} + v_{\beta})} \mathbf{K} \right] \mathbf{H}^{-1}(v_{\beta}) \pi(-v_{\beta}) \mathbf{M}(v_{\beta}; s), \quad (35c)$$

$$\int_{0}^{\infty} \Theta^{T}(v_{\alpha}, \mu; s) \mathbf{H}^{T}(\mu) \pi(\mu) \mathbf{Q}^{T}(\mu) \Phi(-v', \mu; s) e^{-\mu^{2}} \mu d\mu$$

$$= v_{\alpha} v' \mathbf{M}^{T}(v_{\alpha}; s) \pi(-v_{\alpha}) \mathbf{H}^{-T}(v_{\alpha}) \left[\frac{1}{v_{\alpha} + v'} \mathbf{I} - \frac{2z_{1}}{(z_{1} + v_{\alpha})(z_{1} + v')} \mathbf{K} \right] \mathbf{H}^{-1}(v') \pi(-v'), \quad v' > 0. \quad (35d)$$

4. An Example Application and the R Matrix

A typical problem for sound-wave propagation in a half space can be solved concisely in terms of the established formalism. For example, let us seek a solution of Eqn. (8) that is bounded as $x \to \infty$ and satisfies a boundary condition of the form

$$\Psi(0,\mu,t) = e^{i\omega t} \mathbf{F}(\mu), \quad \mu > 0, \tag{36}$$

where $F(\mu)$ is considered given. By taking $s = i\omega$, we can write

$$\Psi(x,\mu;t) = e^{i\omega t} \left\{ \sum_{\alpha=1}^{\kappa} A(v_{\alpha}) \Phi(v_{\alpha},\mu;i\omega) \exp\left[-(i\omega+1)x/v_{\alpha}\right] + \int_{0}^{\infty} \Phi(v,\mu;i\omega) A(v) \exp\left[-(i\omega+1)x/v\right] dv \right\},$$
(37)

where the expansion coefficients are determined by

$$\mathbf{F}(\mu) = \sum_{\alpha=1}^{\kappa} A(v_{\alpha}) \mathbf{\Phi}(v_{\alpha}, \mu; i\omega) + \int_{0}^{\infty} \mathbf{\Phi}(v, \mu; i\omega) \mathbf{A}(v) \, dv, \quad \mu > 0.$$
(38)

Assuming that Eqn. (38) has a solution (this was shown to be true in SB only for

 $\kappa = 0$), we can now multiply Eqn. (38) by $\Theta^T(\nu_{\alpha}, \mu; i\omega)\mathbf{H}^T(\mu)\pi(\mu)\mathbf{Q}^T(\mu)\exp(-\mu^2)\mu$, integrate over μ from 0 to ∞ and use Eqns. (32c) and (32d) to find

$$A(v_{\alpha}) = \frac{1}{N(v_{\alpha})} \int_{0}^{\infty} \Theta^{T}(v_{\alpha}, \mu; i\omega) \mathbf{H}^{T}(\mu) \pi(\mu) \mathbf{Q}^{T}(\mu) \mathbf{F}(\mu) e^{-\mu^{2}} \mu \, d\mu.$$
(39)

In a similar fashion, we can use Eqns. (32a) and (32b) to find

$$\mathbf{A}(\mathbf{v}) = \frac{1}{\mathbf{v}} \mathbf{L}^{-1}(\mathbf{v}) \int_0^\infty \mathbf{\Theta}^T(\mathbf{v}, \mu; i\omega) \mathbf{H}^T(\mu) \pi(\mu) \mathbf{Q}^T(\mu) \mathbf{F}(\mu) \, e^{-\mu^2} \, \mu \, d\mu. \tag{40}$$

If now we set x = 0 in Eqn. (37), enter Eqn. (39) and Eqn. (40) in that equation and consider only $\mu < 0$, then we can evaluate the encountered integrals to obtain the useful result

$$\Psi(0, -\mu, t) = e^{i\omega t} \int_0^\infty \mathbf{R}(\mu' \to \mu) \mathbf{F}(\mu') \, d\mu', \quad \mu \ge 0,$$
(41)

where the **R** matrix is given by

$$\mathbf{R}(\mu' \to \mu) = \frac{\theta \mu'}{\mu' + \mu} e^{-\mu'^2} \mathbf{Q}(\mu) \pi(\mu) \mathbf{H}(\mu)$$
$$\times \left[\mathbf{I} + \frac{2z_1(\mu + \mu')}{(z_1 - \mu')(z_1 - \mu)} \mathbf{K} \right] \mathbf{H}^T(\mu') \pi(\mu') \mathbf{Q}^T(\mu').$$
(42)

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Abstract

A half-range orthogonality relation concerning the elementary solutions of the time-dependent, linearized BGK model of the Boltzmann equation is established, and the required normalization integrals are evaluated. In addition, the half-space reflection matrix $\mathbf{R}(\mu' \rightarrow \mu)$ is developed in order to simplify the evaluation of various surface quantities.

Résumé

On établit une relation d'orthogonalité sur le demi-domaine angulaire pour les solutions élémentaires du modèle BGK linéarisé de l'équation de Boltzmann dépendant du temps et l'on évalue les intégrales de normalisation associées. De plus, on développe la matrice de réflexion du demi-espace $\mathbf{R}(\mu' \to \mu)$ dans le but de simplifier l'évaluation des différentes fonctions de surface.

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