
PERGAMON

Journal of Quantitative Spectroscopy & Radiative Transfer 77 (2003) 417–432

Journal of Quantitative Spectroscopy & Radiative Transfer

www.elsevier.com/locate/jqsrt

The linearized Boltzmann equation: a concise and accurate solution of the temperature-jump problem

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Received 25 June 2002; received in revised form 17 July 2002; accepted 24 July 2002

Abstract

Polynomial expansion procedures, along with an analytical discrete-ordinates method, are used to solve the temperature-jump problem based on a rigorous version of the linearized Boltzmann equation for rigid-sphere interactions. In particular, the temperature and density perturbations and the temperature-jump coefficient are obtained (essentially) analytically in terms of a modern version of the discrete-ordinates method. The developed algorithms are implemented for general values of the accommodation coefficient to yield numerical results that can be considered a new standard of reference.

Keywords: Boltzmann equation; Rarefied gas dynamics; Temperature-jump problem

1. Introduction

In the general area of rarefied gas dynamics we typically have to make a choice between: (i) an analytically and computationally elegant solution of a problem based on one of the many models of the linearized Boltzmann equation and (ii) a strictly numerical solution of the true linearized Boltzmann equation for rigid-sphere interactions. In three recent works [1–3] we have reported what we consider to be concise and accurate (essentially analytical) solutions of the temperature-jump problem based on different model equations. The first work [1] used the analytical discrete-ordinates (ADO) method [4] to solve the temperature-jump problem for the classical BGK model [5]. This work was subsequently extended to include the variable collision frequency model (CLF) of Cercignani [6] and Loyalka and Ferziger [7], and most recently [3] the CES model [8] was used to solve this same temperature-jump problem. As a result of these studies we can see clearly that as the models are improved the analysis becomes more difficult, but the obtained numerical results get closer to

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0022-4073/03/$ - see front matter
PII: S0022-4073(02)00172-3

what we have considered reference values. In regard to numerical results for the temperature-jump problem based on the linearized Boltzmann equation, we have found the works by Loyalka [9,10], Sone et al. [11] and Ohwada and Sone [12] to be especially valuable. The two first papers [9,11] were limited to the case of purely diffuse reflection at the wall. However, in subsequent papers [10,12] the earlier work was extended to the general case of a mixture of specular and diffuse reflection at the wall, and improved numerical results were reported. These papers [9–12] are based on what we consider to be strictly numerical methods (finite difference techniques coupled with multi-dimensional numerical quadrature schemes and/or collocation methods) that can be considered computationally intensive; however these works are the best we have available, and so in the past we have used these papers to define reference results against which we have evaluated our solutions to the various model equations. However, we have now extended our work so as to be able to provide what we consider to be a concise and accurate solution to the temperature-jump problem based on the full linearized Boltzmann equation for rigid-sphere collisions. This solution and the associated computational algorithm define what we consider to be a new and improved standard of reference.

To start this work, we consider the homogeneous and linearized Boltzmann equation written for rigid-sphere collisions as

$$c\mu \frac{\partial}{\partial \tau} h(\tau, \boldsymbol{c}) = \varepsilon L\{h\}(\tau, \boldsymbol{c}), \tag{1}$$

where

$$L\{h\}(\tau, \boldsymbol{c}) = -\nu(c) h(\tau, \boldsymbol{c}) + \int_0^\infty \int_{-1}^1 \int_0^{2\pi} \mathrm{e}^{-c'^2} c'^2 h(\tau, \boldsymbol{c}') K(\boldsymbol{c}', \boldsymbol{c}) \, \mathrm{d}\chi' \, \mathrm{d}\mu' \, \mathrm{d}c'. \tag{2}$$

Here the scattering kernel is written in the expanded (Pekeris) form [13], viz.

$$K(\boldsymbol{c}', \boldsymbol{c}) = \frac{1}{4\pi} \sum_{n=0}^{\infty} \sum_{m=0}^{n} (2n+1)(2-\delta_{0,m}) P_n^m(\mu') P_n^m(\mu) k_n(c', c) \cos m(\chi' - \chi), \tag{3}$$

where the *normalized* Legendre functions are given (in terms of the Legendre polynomials) by

$$P_n^m(\mu) = \left[\frac{(n-m)!}{(n+m)!} \right]^{1/2} (1-\mu^2)^{m/2} \frac{\mathrm{d}^m}{\mathrm{d}\mu^m} P_n(\mu), \quad n \geqslant m. \tag{4}$$

In addition,

$$\varepsilon = \sigma_0^2 n_0 \pi^{1/2} l, \tag{5}$$

where l is (at this point) an unspecified mean-free path, n_0 is the density and σ_0 is the scattering diameter of the gas particles. In this work, the spatial variable τ is measured in units of the mean-free path l and $c(2kT_0/m)^{1/2}$ is the magnitude of the particle velocity. Also, k is the Boltzmann constant, m is the mass of a gas particle and T_0 is a reference temperature. The basic unknown $h(\tau, \boldsymbol{c})$ in Eq. (1) is a perturbation from a Maxwellian distribution. Continuing, we note that the functions $k_n(c', c)$ in Eq. (3) are the components in an expansion of the scattering law (for rigid-sphere collisions) reported by Pekeris [13], and

$$\nu(c) = \frac{2c^2+1}{c} \int_0^c \mathrm{e}^{-x^2} \, \mathrm{d}x + \mathrm{e}^{-c^2} \tag{6}$$

is the collision frequency. And finally, we use spherical coordinates $(c', \arccos\mu', \chi')$ and $(c, \arccos\mu, \chi)$ to define the (dimensionless) velocity vectors $\boldsymbol{c}'$ and $\boldsymbol{c}$.

Since the component kernels $k_n(c', c)$ used in Eq. (3) are essential to our work here, we restate some basic results developed and reported by Pekeris [13], Pekeris and Alterman [14] and Pekeris et al. [15]. First of all, Pekeris [13] gives (in our notation) the expression

$$k_n(c', c) = 2\int_0^\pi [(2/R)\mathrm{e}^{\omega^2} - R]P_n(\cos\theta)\sin\theta\,\mathrm{d}\theta, \tag{7}$$

where

$$R = |\boldsymbol{c}' - \boldsymbol{c}| \tag{8a}$$

and

$$\omega = (1/R)c'c\sin\theta \tag{8b}$$

and where θ is the angle between $\boldsymbol{c}'$ and $\boldsymbol{c}$. In Ref. [14] Pekeris and Alterman discussed the coefficients of viscosity and heat conduction and used the kernel functions $k_1(c', c)$ and $k_2(c', c)$ to define the Chapman–Enskog integral equations for viscosity and heat conduction. We write these equations here as

$$\nu(c)c^2 b(c) - \int_0^\infty \mathrm{e}^{-c'^2} b(c')k_2(c', c)c'^4\,\mathrm{d}c' = c^2 \tag{9}$$

and

$$\nu(c)ca(c) - \int_0^\infty \mathrm{e}^{-c'^2} a(c')k_1(c', c)c'^3\,\mathrm{d}c' = c(c^2 - 5/2) \tag{10a}$$

with

$$\int_0^\infty \mathrm{e}^{-c^2} a(c)c^4\,\mathrm{d}c = 0. \tag{10b}$$

Now, as discussed (for example) in Refs. [14,16], if we wish to use a mean-free path based on the viscosity, i.e.

$$l = l_p = (\mu_*/p_0)(2kT_0/m)^{1/2} \tag{11}$$

where μ_* is the viscosity and $p_0 = n_0 kT_0$ is the pressure, then we should use in Eq. (1)

$$\varepsilon = \varepsilon_p = \frac{16}{15\pi^{1/2}}\int_0^\infty \mathrm{e}^{-c^2} b(c)c^6\,\mathrm{d}c, \tag{12}$$

where $b(c)$ is defined by Eq. (9). On the other hand, if we wish to use a mean-free path based on heat conduction,

$$l = l_t = [4\lambda_*/(5n_0 k)][m/(2kT_0)]^{1/2}, \tag{13}$$

where λ_* is the heat-conduction coefficient, then in Eq. (1) we should use [7,14]

$$\varepsilon = \varepsilon_t = \frac{16}{15\pi^{1/2}}\int_0^\infty \mathrm{e}^{-c^2} a(c)c^6\,\mathrm{d}c \tag{14}$$

where $a(c)$ is defined by Eqs. (10). While only the component kernel functions $k_n(c',c)$, $n=1$–3, are required for the Chapman–Enskog equations for viscosity and heat conduction and the so-called Burnett integral equations [16], we intend to use more of these component kernels in a truncated version of Eq. (3). We note here that in Ref. [15], Pekeris and co-workers have reported an ingenious set of expressions and recursion formulas that they used (along with a computer program) to evaluate analytically the expression listed here as Eq. (7). Pekeris et al. [15] also give explicit results for the cases up to and including $k_8(c',c)$, but we believe there is at least one misprint in those (extensive) results. As will be discussed in more detail later in this work, we have used the MAPLE software package to evaluate Eq. (7) analytically for essentially any value of n, but we have actually used the kernel functions (so far) only up to $n=8$.

Due to the presence of a wall located at $\tau=0$, we must supplement Eq. (1) with an appropriate boundary condition. Noting that

$$h(\tau,\boldsymbol{c}) \Leftrightarrow h(\tau,c,\mu,\chi), \tag{15}$$

we express the required boundary condition as

$$h(0,c,\mu,\chi) - (1-\alpha)h(0,c,-\mu,\chi) - \alpha\mathscr{I}\{h\}(0) = 0 \tag{16}$$

for $\mu\in(0,1]$, $c\in[0,\infty)$ and all χ. Here

$$\mathscr{I}\{h\}(0) = \frac{2}{\pi}\int_0^\infty \int_0^1 \int_0^{2\pi} \mathrm{e}^{-c^2} c^3 h(0,c,-\mu,\chi)\mu \,\mathrm{d}\chi\,\mathrm{d}\mu\,\mathrm{d}c \tag{17}$$

and $\alpha\in(0,1]$ is the accommodation coefficient. In this formulation of the temperature-jump problem there is no driving term in Eq. (1), and so in addition to the boundary condition listed as Eq. (16), we will include in our statement of the problem a condition on $h(\tau,\boldsymbol{c})$ as τ tends to infinity. This condition will be seen clearly once we have expressed the quantities of interest in terms of $h(\tau,\boldsymbol{c})$.

2. Quantities of interest

Following the discussion from Ref. [3], we see that, while our problem is defined in terms of the unknown $h(\tau,\boldsymbol{c})$, we require only two elementary integrals of $h(\tau,\boldsymbol{c})$ in order to establish the density and temperature perturbations [17] defined by

$$N(\tau) = \frac{1}{\pi^{3/2}}\int_0^\infty \int_{-1}^1 \int_0^{2\pi} \mathrm{e}^{-c^2} c^2 h(\tau,c,\mu,\chi)\,\mathrm{d}\chi\,\mathrm{d}\mu\,\mathrm{d}c \tag{18}$$

and

$$T(\tau) = \frac{2}{3\pi^{3/2}}\int_0^\infty \int_{-1}^1 \int_0^{2\pi} \mathrm{e}^{-c^2} c^2(c^2-3/2) h(\tau,c,\mu,\chi)\,\mathrm{d}\chi\,\mathrm{d}\mu\,\mathrm{d}c \tag{19}$$

or

$$N(\tau) = \frac{2}{\pi^{1/2}}\int_0^\infty \int_{-1}^1 \mathrm{e}^{-c^2} c^2 \phi(\tau,c,\mu)\,\mathrm{d}\mu\,\mathrm{d}c \tag{20}$$

and

$$T(\tau) = \frac{4}{3\pi^{1/2}} \int_0^\infty \int_{-1}^1 \mathrm{e}^{-c^2} c^2 (c^2 - 3/2) \phi(\tau, c, \mu) \, \mathrm{d}\mu \, \mathrm{d}c, \tag{21}$$

where

$$\phi(\tau, c, \mu) = \frac{1}{2\pi} \int_0^{2\pi} h(\tau, c, \mu, \chi) \, \mathrm{d}\chi \tag{22}$$

is an azimuthal average. We can integrate Eqs. (1) and (16) over χ to find

$$c\mu \frac{\partial}{\partial \tau} \phi(\tau, c, \mu) + \varepsilon \nu(c) \phi(\tau, c, \mu) = \varepsilon \int_0^\infty \int_{-1}^1 \mathrm{e}^{-c'^2} c'^2 k(c', \mu' : c, \mu) \phi(\tau, c', \mu') \, \mathrm{d}\mu' \, \mathrm{d}c', \tag{23}$$

for $\tau > 0$, $\mu \in [-1, 1]$ and $c \in [0, \infty)$, and

$$\phi(0, c, \mu) - (1 - \alpha) \phi(0, c, -\mu) - 4\alpha \int_0^\infty \int_0^1 \mathrm{e}^{-c'^2} c'^3 \phi(0, c', -\mu') \mu' \, \mathrm{d}\mu' \, \mathrm{d}c' = 0 \tag{24}$$

for $\mu \in (0, 1]$ and $c \in [0, \infty)$. In regard to Eq. (23), we note that

$$k(c', \mu' : c, \mu) = \int_0^{2\pi} K(\boldsymbol{c}', \boldsymbol{c}) \, \mathrm{d}\chi \tag{25}$$

or

$$k(c', \mu' : c, \mu) = \frac{1}{2} \sum_{n=0}^\infty (2n + 1) P_n(\mu') P_n(\mu) k_n(c', c). \tag{26}$$

As Eqs. (1) and (16) are homogeneous, we must specify a driving term for the temperature-jump problem. We do this implicitly by requiring that $h(\tau, \boldsymbol{c})$ diverge as τ tends to infinity. More specifically, we impose the condition that the temperature perturbation satisfies the Welander condition [18]

$$\lim_{\tau \to \infty} \frac{\mathrm{d}}{\mathrm{d}\tau} T(\tau) = \mathscr{K} \tag{27}$$

where $\mathscr{K}$ is considered specified.

In Ref. [8] five exact solutions (collisional invariants) of Eq. (1) that are independent of τ and three exact (in terms of solutions of the Chapman–Enskog integral equations for viscosity and heat conduction) solutions linear in τ were listed. However, since Eq. (23) is an azimuthal average of Eq. (1) only four of the mentioned solutions are relevant to Eq. (23). These four solutions allow us to write *a component* of the complete solution of Eq. (23) as

$$\phi_{\mathrm{a}}(\tau, c, \mu) = A + Bc\mu + D(c^2 - 5/2) + (\mathscr{K}/\varepsilon)[(c^2 - 5/2)\varepsilon\tau - \mu A(c)], \tag{28}$$

where the constants A, B, D and $\mathscr{K}$ are arbitrary. To be clear, we consider that the Chapman–Enskog function $A(c) = ca(c)$ is available [16,19]. We therefore write

$$\phi(\tau, c, \mu) = (\mathscr{K}/\varepsilon)[\phi_*(\tau, c, \mu) + (c^2 - 5/2)\varepsilon\tau - \mu A(c)], \tag{29}$$

where $\phi_*(\tau,c,\mu)$ is a solution of Eq. (23) that is bounded as τ tends to infinity and satisfies the boundary condition that is obtained once we use Eq. (29) in Eq. (24), viz.

$$\phi_*(0,c,\mu)-(1-\alpha)\phi_*(0,c,-\mu)-4\alpha\int_0^\infty\int_0^1 \mathrm{e}^{-c'^2}c'^3\phi_*(0,c',-\mu')\mu'\,\mathrm{d}\mu'\,\mathrm{d}c'=\mathscr{R}(c,\mu) \tag{30}$$

for $\mu\in(0,1]$ and $c\in[0,\infty)$. Here

$$\mathscr{R}(c,\mu)=(2-\alpha)\mu A(c). \tag{31}$$

Finally, in regard to the quantities of interest here, we can use Eq. (29) in Eqs. (20) and (21) to obtain

$$N(\tau)=\mathscr{K}\left[-\tau+\frac{2}{\varepsilon\pi^{1/2}}\int_0^\infty\int_{-1}^1 \mathrm{e}^{-c^2}c^2\phi_*(\tau,c,\mu)\,\mathrm{d}\mu\,\mathrm{d}c\right] \tag{32}$$

and

$$T(\tau)=\mathscr{K}\left[\tau+\frac{4}{3\varepsilon\pi^{1/2}}\int_0^\infty\int_{-1}^1 \mathrm{e}^{-c^2}c^2(c^2-3/2)\phi_*(\tau,c,\mu)\,\mathrm{d}\mu\,\mathrm{d}c\right]. \tag{33}$$

In order to complete the computation of the temperature and density perturbations, we now must establish a bounded (as τ tends to infinity) solution of Eq. (23) that satisfies the boundary condition listed as Eq. (30). While we are unable to find this bounded solution exactly, we are able to establish a concise and accurate approximate result that we can use to compute well the desired temperature and density perturbations as given by Eqs. (32) and (33).

3. A polynomial representation

We seek a bounded (as τ tends to infinity) solution of

$$c\mu\frac{\partial}{\partial\tau}\phi_*(\tau,c,\mu)+\varepsilon\nu(c)\phi_*(\tau,c,\mu)=\varepsilon\int_0^\infty\int_{-1}^1 \mathrm{e}^{-c'^2}c'^2k(c',\mu':c,\mu)\phi_*(\tau,c',\mu')\,\mathrm{d}\mu'\,\mathrm{d}c' \tag{34}$$

that satisfies the boundary condition

$$\phi_*(0,c,\mu)-(1-\alpha)\phi_*(0,c,-\mu)-4\alpha\int_0^\infty\int_0^1 \mathrm{e}^{-c'^2}c'^3\phi_*(0,c',-\mu')\mu'\,\mathrm{d}\mu'\,\mathrm{d}c'=\mathscr{R}(c,\mu), \tag{35}$$

where

$$\mathscr{R}(c,\mu)=(2-\alpha)\mu A(c). \tag{36}$$

Here the scattering kernel $k(c',\mu':c,\mu)$ is given by Eq. (26), but we now make our first approximation: we truncate Eq. (26) and write

$$k(c',\mu':c,\mu)=\frac{1}{2}\sum_{l=0}^{L}(2l+1)P_l(\mu')P_l(\mu)k_l(c',c). \tag{37}$$

At this point we approximate the required solution by a representation in terms of Legendre polynomials, viz.

$$\phi_*(\tau,c,\mu)=\sum_{k=0}^{K}P_k(2\mathrm{e}^{-c}-1)g_k(\tau,\mu), \tag{38}$$

where the functions $g_k(\tau,\mu)$ are to be determined. We now substitute Eq. (38) into Eq. (34), multiply the resulting equation by

$$W_i(c) = c^2 \mathrm{e}^{-c^2} P_i(2\mathrm{e}^{-c} - 1) \tag{39}$$

and integrate over all c to obtain the coupled system

$$\mu \frac{\partial}{\partial \tau} \boldsymbol{A}\boldsymbol{G}(\tau,\mu) + \varepsilon \boldsymbol{S}\boldsymbol{G}(\tau,\mu) = \varepsilon \sum_{l=0}^{L} \boldsymbol{B}_l P_l(\mu) \int_{-1}^{1} P_l(\mu') \boldsymbol{G}(\tau,\mu')\, \mathrm{d}\mu'. \tag{40}$$

Here the $K+1$ vector-valued function $\boldsymbol{G}(\tau,\mu)$ has components $g_k(\tau,\mu)$ and the $(K+1)\times(K+1)$ constants are given by

$$\boldsymbol{A} = \int_0^\infty \mathrm{e}^{-c^2} \boldsymbol{P}^{\mathrm{T}}(c) \boldsymbol{P}(c) c^3\, \mathrm{d}c, \tag{41}$$

$$\boldsymbol{S} = \int_0^\infty \mathrm{e}^{-c^2} \boldsymbol{P}^{\mathrm{T}}(c) \boldsymbol{P}(c) \nu(c) c^2\, \mathrm{d}c \tag{42}$$

and

$$\boldsymbol{B}_l = \frac{2l+1}{2} \int_0^\infty \int_0^\infty \mathrm{e}^{-c'^2} \mathrm{e}^{-c^2} k_l(c',c) \boldsymbol{P}^{\mathrm{T}}(c') \boldsymbol{P}(c) c'^2 c^2\, \mathrm{d}c'\, \mathrm{d}c, \tag{43}$$

where the superscript T is used to denote the transpose operation, and where

$$\boldsymbol{P}(c) = [P_0(2\mathrm{e}^{-c} - 1), P_1(2\mathrm{e}^{-c} - 1), \ldots, P_K(2\mathrm{e}^{-c} - 1)]. \tag{44}$$

We note, since $k_l(c',c) = k_l(c,c')$, that the matrices $\boldsymbol{B}_l$ are symmetric. We note also that a computation of the matrices listed as Eq. (43) will require some care to do well; however, an evaluation of all the input matrices $\boldsymbol{A}$, $\boldsymbol{S}$ and $\boldsymbol{B}_l$ can be done once only and stored for later use. Some details of these initially required computations will be given in a subsequent section of this work.

Now in regard to the boundary condition subject to which we must solve Eq. (40), we use Eq. (38) in Eq. (35) and then multiply the resulting equation by $W_i(c)$ and integrate over all c to obtain

$$\boldsymbol{F}[\boldsymbol{G}(0,\mu) - (1-\alpha)\boldsymbol{G}(0,-\mu)] - 4\alpha \boldsymbol{J} \int_0^\infty \boldsymbol{G}(0,-\mu')\mu'\, \mathrm{d}\mu' = (2-\alpha)\mu \boldsymbol{T} \tag{45}$$

for $\mu \in (0,1]$. Here the additional input constants are

$$\boldsymbol{F} = \int_0^\infty \mathrm{e}^{-c^2} \boldsymbol{P}^{\mathrm{T}}(c) \boldsymbol{P}(c) c^2\, \mathrm{d}c, \tag{46}$$

$$\boldsymbol{J} = \boldsymbol{P}_0^{\mathrm{T}} \boldsymbol{P}_1 \tag{47}$$

and

$$\boldsymbol{T} = \int_0^\infty \mathrm{e}^{-c^2} \boldsymbol{P}^{\mathrm{T}}(c) A(c) c^2\, \mathrm{d}c, \tag{48}$$

where, in general,

$$\boldsymbol{P}_n = \int_0^\infty \mathrm{e}^{-c^2} \boldsymbol{P}(c) c^{n+2}\, \mathrm{d}c. \tag{49}$$

And so, we now must solve Eq. (40) subject to the boundary condition given as Eq. (45); however, in order to make use of a previously reported [20] ADO solution of a multigroup neutron transport problem, we multiply Eq. (40) by $\boldsymbol{A}^{-1}$ and Eq. (45) by $\boldsymbol{F}^{-1}$ to obtain the final forms we solve, viz.

$$\mu\frac{\partial}{\partial\tau}\boldsymbol{G}(\tau,\mu)+\varepsilon\boldsymbol{\Sigma}\mathbf{G}(\tau,\mu)=\varepsilon\sum_{l=0}^{L}\boldsymbol{C}_l P_l(\mu)\int_{-1}^{1}P_l(\mu')\boldsymbol{G}(\tau,\mu')\,\mathrm{d}\mu' \tag{50}$$

and

$$\boldsymbol{G}(0,\mu)-(1-\alpha)\boldsymbol{G}(0,-\mu)-4\alpha\boldsymbol{D}\int_0^{\infty}\boldsymbol{G}(0,-\mu')\mu'\,\mathrm{d}\mu'=(2-\alpha)\mu\boldsymbol{Q} \tag{51}$$

for $\mu\in(0,1]$. Here

$$\boldsymbol{\Sigma}=\boldsymbol{A}^{-1}\boldsymbol{S}, \tag{52a}$$

$$\boldsymbol{C}_l=\boldsymbol{A}^{-1}\boldsymbol{B}_l, \tag{52b}$$

$$\boldsymbol{D}=\boldsymbol{F}^{-1}\boldsymbol{J} \tag{52c}$$

and

$$\boldsymbol{Q}=\boldsymbol{F}^{-1}\boldsymbol{T}. \tag{52d}$$

And so now we continue by developing our analytical discrete-ordinates solution of the transport problem defined by Eqs. (50) and (51).

4. An analytical discrete-ordinates solution

Since our discrete-ordinates solution of Eqs. (50) and (51) follows closely work previously reported [20] in the context of fully-coupled multigroup neutron transport theory, our presentation here can be brief. We begin by using a "half-range" quadrature scheme to approximate the integral term in Eq. (50), and so we write

$$\mu\frac{\partial}{\partial\tau}\boldsymbol{G}(\tau,\mu)+\varepsilon\boldsymbol{\Sigma}\mathbf{G}(\tau,\mu)=\varepsilon\sum_{l=0}^{L}P_l(\mu)\boldsymbol{C}_l\sum_{n=1}^{N}w_n\boldsymbol{G}_{l,n}(\tau), \tag{53}$$

where to compact our notation we have introduced

$$\boldsymbol{G}_{l,n}(\tau)=P_l(\mu_n)[\boldsymbol{G}(\tau,\mu_n)+(-1)^l\boldsymbol{G}(\tau,-\mu_n)]. \tag{54}$$

Here the N quadrature points $\{\mu_n\}$ and the N weights $\{w_n\}$ are defined for use on the integration interval $[0,1]$. Eq. (53) clearly has separable exponential solutions, so we use ν as a separation constant and substitute

$$\boldsymbol{G}(\tau,\mu)=\boldsymbol{\Phi}(\nu,\mu)\mathrm{e}^{-\varepsilon\tau/\nu} \tag{55}$$

into that equation to find

$$[\boldsymbol{\Sigma}-(\mu/\nu)\boldsymbol{I}]\boldsymbol{\Phi}(\nu,\mu)=\sum_{l=0}^{L}P_l(\mu)\boldsymbol{C}_l\sum_{n=1}^{N}w_n\boldsymbol{\Phi}_{l,n}(\nu), \tag{56}$$

where $\boldsymbol{I}$ is the identity matrix and

$$\boldsymbol{\Phi}_{l,n}(\nu) = P_l(\mu_n)[\boldsymbol{\Phi}(\nu,\mu_n) + (-1)^l \boldsymbol{\Phi}(\nu,-\mu_n)]. \tag{57}$$

If we now evaluate Eq. (56) at $\mu = \pm\mu_i$, for $i = 1,2,\ldots,N$, then we can obtain

$$[\boldsymbol{D} - (1/\nu)\boldsymbol{M}]\boldsymbol{\Phi}_+(\nu) = \sum_{l=0}^{L} \boldsymbol{\Pi}_l \boldsymbol{C}_l \boldsymbol{G}_l(\nu) \tag{58a}$$

and

$$[\boldsymbol{D} + (1/\nu)\boldsymbol{M}]\boldsymbol{\Phi}_-(\nu) = \sum_{l=0}^{L} (-1)^l \boldsymbol{\Pi}_l \boldsymbol{C}_l \boldsymbol{G}_l(\nu), \tag{58b}$$

where

$$\boldsymbol{\Phi}_+(\nu) = [\boldsymbol{\Phi}^{\mathrm{T}}(\nu,\mu_1), \boldsymbol{\Phi}^{\mathrm{T}}(\nu,\mu_2), \ldots, \boldsymbol{\Phi}^{\mathrm{T}}(\nu,\mu_N)]^{\mathrm{T}} \tag{59a}$$

and

$$\boldsymbol{\Phi}_-(\nu) = [\boldsymbol{\Phi}^{\mathrm{T}}(\nu,-\mu_1), \boldsymbol{\Phi}^{\mathrm{T}}(\nu,-\mu_2), \ldots, \boldsymbol{\Phi}^{\mathrm{T}}(\nu,-\mu_N)]^{\mathrm{T}}. \tag{59b}$$

In addition, we have used the $J \times J$ matrices

$$\boldsymbol{M} = \mathrm{diag}\{\mu_1\boldsymbol{I}, \mu_2\boldsymbol{I}, \ldots, \mu_N\boldsymbol{I}\} \tag{60a}$$

and

$$\boldsymbol{D} = \mathrm{diag}\{\boldsymbol{\Sigma}, \boldsymbol{\Sigma}, \ldots, \boldsymbol{\Sigma}\} \tag{60b}$$

along with

$$\boldsymbol{G}_l(\nu) = \boldsymbol{\Pi}_l^{\mathrm{T}} \boldsymbol{W}[\boldsymbol{\Phi}_+(\nu) + (-1)^l \boldsymbol{\Phi}_-(\nu)]. \tag{61}$$

Note that we have introduced the composite dimension $J = N(K+1)$ and that here the matrix

$$\boldsymbol{W} = \mathrm{diag}\{w_1\boldsymbol{I}, w_2\boldsymbol{I}, \ldots, w_N\boldsymbol{I}\} \tag{62a}$$

is also $J \times J$, while the matrices

$$\boldsymbol{\Pi}_l = [P_l(\mu_1)\boldsymbol{I}, P_l(\mu_2)\boldsymbol{I}, \ldots, P_l(\mu_N)\boldsymbol{I}]^{\mathrm{T}} \tag{62b}$$

are $J \times (K+1)$. We now let

$$\boldsymbol{U} = \boldsymbol{\Phi}_+(\nu) + \boldsymbol{\Phi}_-(\nu) \tag{63a}$$

and

$$\boldsymbol{V} = \boldsymbol{\Phi}_+(\nu) - \boldsymbol{\Phi}_-(\nu), \tag{63b}$$

so that we can take the sum and the difference of Eqs. (58) to obtain

$$\boldsymbol{E}\boldsymbol{X} = \frac{1}{\nu}\boldsymbol{Y} \tag{64a}$$

and

$$\boldsymbol{H}\boldsymbol{Y} = \frac{1}{\nu}\boldsymbol{X}, \tag{64b}$$

where

$$\boldsymbol{E} = \left\{ \boldsymbol{D} - \sum_{l=0}^{L} \boldsymbol{\Pi}_l \boldsymbol{C}_l [1 + (-1)^l] \boldsymbol{\Pi}_l^{\mathrm{T}} \boldsymbol{W} \right\} \boldsymbol{M}^{-1}, \tag{65a}$$

$$\boldsymbol{H} = \left\{ \boldsymbol{D} - \sum_{l=0}^{L} \boldsymbol{\Pi}_l \boldsymbol{C}_l [1 - (-1)^l] \boldsymbol{\Pi}_l^{\mathrm{T}} \boldsymbol{W} \right\} \boldsymbol{M}^{-1}, \tag{65b}$$

$$\boldsymbol{X} = \boldsymbol{M}\boldsymbol{U} \tag{66a}$$

and

$$\boldsymbol{Y} = \boldsymbol{M}\boldsymbol{V}. \tag{66b}$$

We can eliminate between Eqs. (64) to obtain the eigenvalue problems

$$(\boldsymbol{H}\boldsymbol{E})\boldsymbol{X} = \lambda \boldsymbol{X} \tag{67a}$$

and

$$(\boldsymbol{E}\boldsymbol{H})\boldsymbol{Y} = \lambda \boldsymbol{Y}, \tag{67b}$$

where $\lambda = 1/\nu^2$. We note that the required separation constants $\{\nu_j\}$ are readily available once we find the eigenvalues $\{\lambda_j\}$ defined by either of Eqs. 67. We choose to express our results in terms of the eigenvalues and eigenvectors defined by Eq. (67a). Continuing, we let λ_j and $\boldsymbol{X}(\lambda_j)$, for $j = 1, 2, \ldots, J$, denote the collection of eigenvalues and eigenvectors of Eq. (67a). The separation constants we require clearly occur in plus–minus pairs, and so letting ν_j, for $j = 1, 2, \ldots, J$, denote the reciprocal of the positive square root of λ_j, we can use Eqs. (63), (64) and (66) to obtain

$$\boldsymbol{\Phi}_+(\nu_j) = \tfrac{1}{2}\boldsymbol{M}^{-1}(\boldsymbol{I} + \nu_j \boldsymbol{E})\boldsymbol{X}(\lambda_j) \tag{68a}$$

and

$$\boldsymbol{\Phi}_-(\nu_j) = \tfrac{1}{2}\boldsymbol{M}^{-1}(\boldsymbol{I} - \nu_j \boldsymbol{E})\boldsymbol{X}(\lambda_j) \tag{68b}$$

for $j = 1, 2, \ldots, J$. We note that $\boldsymbol{I}$ in Eqs. (68) is the $J \times J$ identity matrix and that

$$\boldsymbol{\Phi}_+(-\nu_j) = \boldsymbol{\Phi}_-(\nu_j) \tag{69}$$

and so at this point we have available all we require for defining our discrete-ordinates solution to Eq. (53). We therefore write

$$\boldsymbol{G}(\tau, \pm\mu_i) = \sum_{j=1}^{J} [A_j \boldsymbol{\Phi}(\nu_j, \pm\mu_i) \mathrm{e}^{-\varepsilon\tau/\nu_j} + B_j \boldsymbol{\Phi}(\nu_j, \mp\mu_i) \mathrm{e}^{\varepsilon\tau/\nu_j}] \tag{70}$$

for $i = 1, 2, \ldots, N$. Here the arbitrary constants $\{A_j\}$ and $\{B_j\}$ are to be determined by the boundary conditions of any given problem, and to be clear we note that the quantities $\boldsymbol{\Phi}(\nu_j, \mu_i)$ and $\boldsymbol{\Phi}(\nu_j, -\mu_i)$ are to be taken from the components of $\boldsymbol{\Phi}_\pm(\nu_j)$ that are available from Eqs. 68.

For the considered temperature-jump problem, we seek a bounded (as τ tends to infinity) solution, $\phi_*(\tau, c, \mu)$, and so we neglect the terms with positive exponentials in Eq. (70) and write

$$\boldsymbol{G}(\tau, \pm\mu_i) = \sum_{j=1}^{J} A_j \boldsymbol{\Phi}(\nu_j, \pm\mu_i) \mathrm{e}^{-\varepsilon\tau/\nu_j} \tag{71}$$

for $i = 1, 2, \ldots, N$. Now, as was anticipated, we have observed in our numerical work that two of the separation constants, say ν_1 and ν_2 tend to infinity as the order J of the eigenvalue system is increased. And so our procedure is to ignore these two constants in Eq. (71) and to use instead two of the bounded exact solutions from Eq. (28). This means that we now write a discrete-ordinates version of Eq. (38) as

$$\phi_*(\tau, c, \pm\mu_i) = \pm A_1 c\mu_i + A_2(c^2 - 5/2) + \boldsymbol{P}(c) \sum_{j=3}^{J} A_j \boldsymbol{\Phi}(\nu_j, \pm\mu_i) \mathrm{e}^{-\varepsilon\tau/\nu_j}, \tag{72}$$

where $\boldsymbol{P}(c)$ is given by Eq. (44). While Eq. (30) and (subsequently) Eq. (51) are the boundary conditions relative to $\phi_*(\tau, c, \mu)$ and $\boldsymbol{G}(\tau, \mu)$, we use a discrete-ordinates version of the boundary condition to determine the constants $\{A_j\}$ we require to complete our solution. And so we rewrite Eq. (30) as

$$\phi_*(0, c, \mu_i) - (1 - \alpha)\phi_*(0, c, -\mu_i) - 4\alpha \sum_{n=1}^{N} w_n \mu_n \int_0^\infty \mathrm{e}^{-c'^2} c'^3 \phi_*(0, c', -\mu_n)\, \mathrm{d}c' = \mathscr{R}(c, \mu_i) \tag{73}$$

for $i = 1, 2, \ldots, N$. To find a linear system to define the required constants, we substitute Eq. (72) into Eq. (73), multiply by $\boldsymbol{P}^{\mathrm{T}}(c)\mathrm{e}^{-c^2}c^2$ and integrate over all c to find

$$A_1 \boldsymbol{V}_1 + A_2 \boldsymbol{V}_2 + \sum_{j=3}^{J} A_j \boldsymbol{V}(\nu_j) = (2 - \alpha)\boldsymbol{R} \tag{74}$$

where

$$\boldsymbol{V}_1 = (2 - \alpha)[\mu_1 \boldsymbol{E}_1^{\mathrm{T}}, \mu_2 \boldsymbol{E}_1^{\mathrm{T}}, \ldots, \mu_N \boldsymbol{E}_1^{\mathrm{T}}]^{\mathrm{T}} + (\alpha/2)\pi^{1/2}[\boldsymbol{E}_0^{\mathrm{T}}, \boldsymbol{E}_0^{\mathrm{T}}, \ldots, \boldsymbol{E}_0^{\mathrm{T}}]^{\mathrm{T}}, \tag{75a}$$

$$\boldsymbol{V}_2 = \alpha[\boldsymbol{E}_2^{\mathrm{T}}, \boldsymbol{E}_2^{\mathrm{T}}, \ldots, \boldsymbol{E}_2^{\mathrm{T}}]^{\mathrm{T}} + (\alpha/2)[\boldsymbol{E}_0^{\mathrm{T}}, \boldsymbol{E}_0^{\mathrm{T}}, \ldots, \boldsymbol{E}_0^{\mathrm{T}}]^{\mathrm{T}} \tag{75b}$$

and, for $j = 3, 4, \ldots, J$,

$$\boldsymbol{V}(\nu_j) = [\boldsymbol{\Gamma}_1^{\mathrm{T}}(\nu_j), \boldsymbol{\Gamma}_2^{\mathrm{T}}(\nu_j), \ldots, \boldsymbol{\Gamma}_N^{\mathrm{T}}(\nu_j)]^{\mathrm{T}}. \tag{76}$$

Here

$$\boldsymbol{\Gamma}_i(\nu_j) = \boldsymbol{\Phi}(\nu_j, \mu_i) - (1 - \alpha)\boldsymbol{\Phi}(\nu_j, -\mu_i) - 4\alpha \sum_{n=1}^{N} w_n \mu_n \boldsymbol{\Phi}(\nu_j, -\mu_n) \tag{77}$$

and

$$\boldsymbol{R} = [\mu_1 \boldsymbol{Q}^{\mathrm{T}}, \mu_2 \boldsymbol{Q}^{\mathrm{T}}, \ldots, \mu_N \boldsymbol{Q}^{\mathrm{T}}]^{\mathrm{T}}, \tag{78}$$

where $\boldsymbol{Q}$ is given by Eqs. (52d) and (48). In addition,

$$\boldsymbol{E}_0 = \boldsymbol{F}^{-1}\boldsymbol{P}_0^{\mathrm{T}}, \tag{79a}$$

$$\boldsymbol{E}_1 = \boldsymbol{F}^{-1}\boldsymbol{P}_1^{\mathrm{T}} \tag{79b}$$

and

$$\boldsymbol{E}_2 = \boldsymbol{F}^{-1}[\boldsymbol{P}_2^{\mathrm{T}} - (5/2)\boldsymbol{P}_0^{\mathrm{T}}], \tag{79c}$$

where we have used the definitions given in Eq. (49). Finally, we note that while we have used the defined quadrature scheme to compute the component in $\boldsymbol{V}(\nu_j)$ that results from diffuse reflection, we have used exact integration to compute this component in $\boldsymbol{V}_1$ and $\boldsymbol{V}_2$.

Once we have solved the $J \times J$ system of linear equations listed as Eq. (74), we can compute our final results by using Eq. (72) in Eqs. (32) and (33) to find

$$N(\tau) = \mathscr{K}\left[-\tau - \zeta + \sum_{j=3}^{J} A_j N_j \mathrm{e}^{-\varepsilon\tau/\nu_j}\right] \tag{80}$$

and

$$T(\tau) = \mathscr{K}\left[\tau + \zeta + \sum_{j=3}^{J} A_j T_j \mathrm{e}^{-\varepsilon\tau/\nu_j}\right], \tag{81}$$

where

$$N_j = (2/\varepsilon)\pi^{-1/2}\boldsymbol{P}_0\boldsymbol{N}(\nu_j) \tag{82}$$

and

$$T_j = [4/(3\varepsilon)]\pi^{-1/2}[\boldsymbol{P}_2 - (3/2)\boldsymbol{P}_0]\boldsymbol{N}(\nu_j). \tag{83}$$

Again we have used Eq. (49), and we have introduced

$$\boldsymbol{N}(\nu_j) = \sum_{n=1}^{N} w_n[\boldsymbol{\Phi}(\nu_j, \mu_n) + \boldsymbol{\Phi}(\nu_j, -\mu_n)]. \tag{84}$$

To conclude this section we note that the temperature-jump coefficient is given by

$$\zeta = A_2/\varepsilon. \tag{85}$$

5. Numerical results

Our solution to the temperature-jump problem as based on the linearized Boltzmann equation for rigid-sphere interactions involves various analytical and numerical approximations which must be mentioned. First of all, the infinite series in Eq. (26) has been truncated after $L + 1$ terms so as to yield the representation given by Eq. (37). To date, we have used at most nine terms ($L = 8$) in the expansion. The Maple software package was used to obtain analytical expressions

for the component kernels; however, because we observed some loss of accuracy when using these analytical expressions, we have included in our computation some asymptotic expansions for small values of c', when $c' < c$. Our next approximation is illustrated by Eq. (38) where $K+1$ terms in a polynomial expansion were used to model the speed dependence (the c variable) of our solution. Then after a projection against the functions listed in Eq. (39), we obtained the coupled system of transport equations and boundary conditions listed as Eqs. (50) and (51). At this point we have introduced our analytical discrete-ordinates method by approximating the integral term in Eq. (50) by an N-point half-range quadrature scheme, viz. a standard Gauss-Legendre scheme mapped onto the interval [0,1]. Finally we have evaluated all the input parameters, for example Eqs. (41)–(43), by mapping an M-point Gauss–Legendre quadrature scheme onto the positive real axis. And so in this work we have four approximation parameters: $\{L, M, K, N\}$. In regard to linear algebra, we have used the driver program RG from the EISPACK collection [21] to solve our eigenvalue/eigenvector problem and packages from the LINPACK collection [22] to solve our linear system. We note, in regard to Eq. (67a) and the fact that $\nu = 1/\lambda^{1/2}$, that we have not encountered any complex separation constants (ν_j, for $j = 3, 4, \ldots, J$) for the solution parameters used to date.

We list in Tables 1–3 our results for some typical cases using [8,14]

$$\varepsilon = \varepsilon_t = 0.679630049\ldots \tag{86}$$

to define a mean-free path based on thermal conductivity. While we believe our results to be correct to within one unit in last digit given, we have no proof of the accuracy of our results. However, we have found our solution to be stable with regard to changes in the approximation parameters $\{L, M, K, N\}$. Although we have made no special effort to find the minimum values of $\{L, M, K, N\}$ to achieve a given accuracy, we have typically used the values $\{8, 200, 40, 30\}$. In addition to the fact that our solution appears to be stable with respect to the approximation parameters, we have looked at the special cases of (i) the BGK model and (ii) the CES model. Results for these two models were obtained simply by replacing the true component kernels (and the collision frequency for the case of the BGK model) by relevant model kernel functions ($L = 1$ for BGK and $L = 2$ for CES). In this way, we were able to confirm, to seven figures of accuracy for the temperature-jump coefficient and to six figures of accuracy for the temperature and density perturbations, the results reported in Ref. [3].

Table 1
The temperature-jump coefficient ζ

α	BGK	CES	[10]	LBE
0.1	21.45012	21.32099	21.349	21.349
0.2	10.34747	10.22670	10.252	10.251
0.3	6.630514	6.517910	6.5398	6.5396
0.4	4.760333	4.655697	4.6747	4.6745
0.5	3.629125	3.532264	3.5708	3.5485
0.6	2.867615	2.778342	2.7924	2.7922
0.7	2.317534	2.235669	2.2476	2.2474
0.8	1.899741	1.825107	1.8350	1.8349
0.9	1.570264	1.502689	1.5109	1.5108
1.0	1.302716	1.242033	1.2486	1.2486

Table 2
The temperature and density perturbations for $\alpha = 0.8$

	$T(\tau)$				$-N(\tau)$			
τ	BGK	CES	[10]	LBE	BGK	CES	[10]	LBE
0.00	1.349	1.382	1.360	1.3597	1.472	1.531	1.502	1.5033
0.25	1.811	1.909	1.860	1.8594	1.900	1.980	1.930	1.9292
0.50	2.147	2.235	2.190	2.1896	2.216	2.278	2.233	2.2327
0.75	2.451	2.523	2.485	2.4846	2.506	2.549	2.513	2.5127
1.00	2.739	2.793	2.763	2.7631	2.784	2.810	2.782	2.7819
1.50	3.290	3.312	3.296	3.2958	3.320	3.320	3.305	3.3045
2.00	3.821	3.820	3.813	3.8125	3.843	3.823	3.817	3.8167

Table 3
The temperature and density perturbations

	$\alpha = 0.3$		$\alpha = 0.5$		$\alpha = 0.9$	
τ	$T(\tau)$	$-N(\tau)$	$T(\tau)$	$-N(\tau)$	$T(\tau)$	$-N(\tau)$
0.0	5.8088	6.0336	2.9250	3.1153	1.0819	1.2111
0.1	6.1567	6.3099	3.2342	3.3647	1.3228	1.4123
0.2	6.3617	6.4811	3.4238	3.5257	1.4843	1.5545
0.3	6.5312	6.6274	3.5831	3.6654	1.6253	1.6821
0.4	6.6820	6.7611	3.7268	3.7944	1.7556	1.8024
0.5	6.8213	6.8870	3.8605	3.9167	1.8790	1.9180
0.6	6.9527	7.0077	3.9874	4.0345	1.9978	2.0305
0.7	7.0782	7.1246	4.1093	4.1491	2.1131	2.1407
0.8	7.1994	7.2387	4.2275	4.2612	2.2258	2.2493
0.9	7.3171	7.3505	4.3428	4.3715	2.3365	2.3565
1.0	7.4322	7.4607	4.4558	4.4802	2.4456	2.4626
2.0	8.5062	8.5125	5.5196	5.5251	3.4904	3.4942

To compare with other works, we have included in Tables 1 and 2, the values obtained by Loyalka [10] from a numerical solution of the linearized Boltzmann equation. With the exception of the temperature-jump coefficient for the case $\alpha = 0.5$ where we suspect Loyalka [10] has a printing error, the agreement between the two sets of results is very good, though not perfect. We have also recomputed the temperature-jump coefficient and other data from Refs. [11,12] using

$$\varepsilon = 2^{1/2}/4. \tag{87}$$

Since our solution is continuous in the spatial variable we were able to compute the temperature and density defects listed by Sone, Ohwada and Aoki [11] and Ohwada and Sone [12] exactly at the grid points listed in those works. First of all, in regard to Ref. [11] that has only the case $\alpha = 1$, we found reasonable agreement for the temperature-jump coefficient (Ref. [11] has $\zeta = 2.3993$ in the notation used there, whereas we found $\zeta = 2.4001$), however, we are of the opinion that the results listed in Table II of Ref. [11] are correct, in general, to no more than three significant figures. In a

more recent work, Ohwada and Sone [12] reported better results and also include a combination of specular and diffuse reflection at the wall. For example, Ref. [12] reports 6.8210, 3.8981 and 2.4001 for the temperature-jump coefficient for the cases of $\alpha = 0.5$, 0.75 and 1, while we have for the same cases 6.8212, 3.8982 and 2.4001. We have also found that we agree significantly better (three to five figures of agreement) with Table III of Ref. [12] than with Table II of Ref [11].

While we have some confidence in our numerical results, there can be some doubt: the use of a maximum value of $L = 8$ could be a source of error. We can emphasize (again) that computing the component kernels $k_n(c', c)$ accurately is no simple task especially as n increases. This too could be a source of error in our final results. On the other hand the approximations used in Eq. (38), the projections defined by Eq. (39) and the analytical discrete-ordinates are all considered exceptionally good procedures for the considered problem.

To conclude this section we give some idea about the computation time required for our FORTRAN implementation of this solution. It should be noted that no special effort was made to "tune" the code for speed and that no optimization options were used. We found that the use of the approximating parameters $\{8, 200, 20, 10\}$ required 20 s of CPU time on a 1.2 GHz mobile Pentium III, without using any stored data, to find the temperature-jump coefficient and the temperature and density perturbations for 10 values of the accommodation coefficient. Using stored input data, we found the code required less than 2 s on the same machine. We found from this timing example what we believe to be five figures of accuracy for the jump coefficient and the temperature and density perturbations for the cases listed in our tables.

6. Concluding comments

We have used a new polynomial expansion technique and the Pekeris [13] expanded form of the scattering kernel basic to the linearized Boltzmann equation for rigid-sphere collisions to define a system of coupled transport problems that has been solved efficiently and accurately with a modern version [4] of the discrete-ordinates method usually associated with Chandrasekhar [23] and the field of radiative transfer. While there exist four basic works [9–12] that report numerical results for the temperature-jump problem solved in this work, we are of the opinion that our (nearly) analytical solution is more efficient in regard to accuracy and computer-time requirements than the older, strictly numerical solutions. The approach developed in this work can be used to solve all the classical flow problems based on the linearized Boltzmann equation, and to include more realistic boundary conditions such as the Cercignani–Lampis boundary condition very recently implemented [24–26] for some model equations should require only minor modifications to the techniques reported in this work. Finally, we are of the opinion that to solve the temperature-jump problem well and to develop a FORTRAN implementation that yields five significant figures of accuracy in less than 2 s seems a good contribution to the general field of rarefied gas dynamics.

Acknowledgements

The author takes this opportunity to thank L.B. Barichello, D. Valougeorgis and A.M. Yacout for helpful discussions regarding this work. The author is also grateful to the Federal University of Rio

Grande do Sul and the University of Thessaly for the kind hospitality extended during recent visits to Brazil and Greece.

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