Two kinetic temperature description for shock waves

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A two kinetic temperature displaced Maxwellian is used as the weight function for a Hermite expansion of the distribution function. The expansion is cut up to fourteen moments following Grad's theory. The moment equations are used to derive under a Knudsen type expansion what one may call two-temperature Navier-Stokes equations (2T-NS). The 2T-NS equations are then solved numerically, for a plane shock wave, and a comparison between Navier-Stokes, Holian theory, and results from molecular dynamics and Monte Carlo is performed. [S1063-651X(98)10009-0]

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I. INTRODUCTION

Shock wave phenomena provide a natural arena for highly nonequilibrium situations in which several theories can be tested. Although most comparisons have been done for small or intermediate Mach numbers [1–6], with the advent of the computer, simulations for Mach numbers of about 100 have been reported [7–9]. Thus it seems interesting to study the different theoretical approaches that have been advanced to explain the structure of shock waves at high Mach numbers. In this paper we concentrate on the simulations that were done for the rigid sphere model at low density using molecular dynamics [9] and the direct simulation Monte Carlo method [7,9]. In this case the questions of what is the true interaction potential and what is the equation of state do not represent additional difficulties that need to be addressed since both are accurately known for the rigid sphere model in the dilute regime. There are various recent references [9–16] in the literature related to the shock wave problem that use different theories, thus reflecting the current interest in the problem. In this work we have focused on some aspects of the problem without trying to be exhaustive.

The Navier-Stokes equations have been used with relative success to obtain velocity profiles for shock waves at high Mach numbers [10]. Another theory that is even more successful is the one advanced by Holian *et al.* [10], which we refer to as the Holian theory. It is based on a conjecture that as yet does not have a microscopic justification; the main idea is to use a different temperature in the expression for the transport coefficients. In fact, the present investigation was undertaken with the hope of providing its kinetic foundation. To get a quantitative idea about the level of prediction of the Navier-Stokes equations, the reader may take a look at Fig. 1 where a comparison of the theories mentioned previously and the results of simulations (for the velocity profiles) can be found. The reduced variables used are defined in Sec. IV. As can be seen from the figure, while the Navier-Stokes theory gives a reasonable profile, the Holian theory gives an important improvement.

The idea of different temperature profiles in nonequilibrium situations is not new and has been used with success in problems where there is an external field and an anisotropy is to be expected. Also, there are many fields where the idea of different temperatures has been applied [17–22].

In this work we use the 14-moment approximation in Grad's solution to the Boltzmann equation focused on obtaining constitutive relations that result in a corresponding Navier-Stokes regime with two temperatures that we refer to as the two-temperature Navier-Stokes theory (2T-NS). The equations have been solved numerically for a plane shock wave as is also done for the Navier-Stokes and Holian equations. A comparison with results from simulations is given and several remarks concerning the comparison are done.

In 1964 Holway [23] claimed that there is no solution for the moment equations in the case of shock waves, no matter how many terms are included in the Hermite polynomial expansion for the distribution function, for Mach numbers greater than 1.851. Such a proof has been recently challenged by Weiss [11] concluding that there is no such restriction. In this work we focus on obtaining constitutive equations for a two-temperature theory and, therefore, the previous remarks are not crucial. The question of why the Navier-Stokes equations, which can be derived from linearized 13-moment Grad's equations, give a solution for high Mach numbers while the linearized Grad equations do not, remains a mystery that we will not attempt to solve here.

In Sec. II we give the kinetic model and the variables that

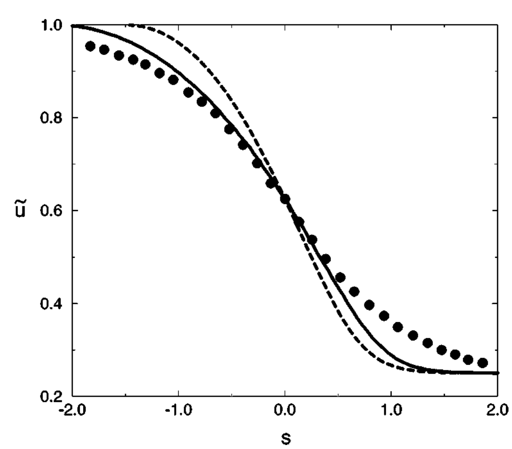

FIG. 1. Velocity profile $\tilde{u}(s)$ vs s. Solid circles correspond to the molecular dynamics calculations ($M_a=134$), dashed line corresponds to the Navier-Stokes equations ($\tau_0=0$), and the solid line to the Holian theory ($\tau_0=0$). We recall for the reader that the MD and DSMC yield similar results.

we will use. Section III gives results concerning the constitutive equations for the two-temperature theory at the level of the Navier-Stokes regime. In Sec. IV the equations to be solved for the shock wave problem are given and the Holian conjecture is explained in detail. The numerical solution of the Navier-Stokes, Holian, and 2T-NS equations is done in Sec. V and Sec. VI is left for some concluding remarks.

II. EXPANSION OF THE DISTRIBUTION FUNCTION

We consider here a stationary plane shock wave propagating in a dilute hard sphere gas whose states are described by the Boltzmann equation. If we take the x axis as the direction of propagation of the wave, its mean velocity will be given by $\mathbf{u}(\mathbf{r},t)=u(x)\mathbf{i}$, and we assume that the mean kinetic energy along x $(mkT_{\parallel}^{(0)}/2)$ is different from the mean kinetic energy along the other axis $(mkT_{\perp}^{(0)}/2)$.

The zero order distribution function is given by a displaced Maxwellian with two temperatures:

$$\begin{aligned} f^{(0)}(\mathbf{c},\mathbf{r},t)=n\left(\frac{m}{2\pi kT_{\perp}^{(0)}}\right)\left(\frac{m}{2\pi kT_{\parallel}^{(0)}}\right)^{1/2} \\ \times\exp(-mC_x^2/2kT_{\parallel}^{(0)}), \\ \times\exp[-m(C_y^2+C_z^2)/2kT_{\perp}^{(0)}], \end{aligned} \tag{1}$$

where $\mathbf{c}$ is the molecular velocity, $\mathbf{u}$ the mass velocity, $\mathbf{C}\equiv\mathbf{c}-\mathbf{u}$ the peculiar velocity, n the number density, k Boltzmann's constant, and m the mass. $T_{\parallel}^{(0)}$ and $T_{\perp}^{(0)}$ are the parallel and perpendicular temperatures, respectively. The superscript in the temperatures is to remind us that they are related to the Maxwellian (local equilibrium temperatures).

With $f^{(0)}(\mathbf{c},\mathbf{r},t)$ as the weight function, the Hermite multidimensional orthogonal polynomials $[\mathcal{H}^{(s)}(\mathbf{v})]$ can be generated in a straightforward way, and the distribution function can be expanded in terms of such a complete basis. Hence [24],

$$\begin{aligned} f(\mathbf{c},\mathbf{r},t)=f^{(0)}(\mathbf{c},\mathbf{r},t)\Bigg(a^{(0)}(\mathbf{r},t)\mathcal{H}^{(0)}(\mathbf{v})+a_i^{(1)}(\mathbf{r},t)\mathcal{H}^{(1)}(\mathbf{v}) \\ +\frac{1}{2!}a_{ij}^{(2)}(\mathbf{r},t)\mathcal{H}_{ij}^{(2)}(\mathbf{v}) \\ +\frac{1}{3!}a_{ijk}^{(3)}(\mathbf{r},t)\mathcal{H}_{ijk}^{(3)}(\mathbf{v})+\cdots\Bigg), \end{aligned} \tag{2}$$

where the components of the dimensionless velocity are defined as

$$\mathbf{v}_x=\left(\frac{m}{kT_{\parallel}^{(0)}}\right)^{1/2}\mathbf{C}_x, \quad \mathbf{v}_{y,z}=\left(\frac{m}{kT_{\perp}^{(0)}}\right)^{1/2}\mathbf{c}_{y,z}, \tag{3}$$

the quantities $a_{i_1,\ldots,i_s}^{(s)}(\mathbf{r},t)$ are the corresponding moments, which are given by

$$a_{\cdots}^{(s)}=\frac{1}{n}\int f(\mathbf{c},\mathbf{r},t)\mathcal{H}_{\cdots}^{(s)}\,d\mathbf{c}. \tag{4}$$

The Hermite polynomials that we use in this work are

$$\begin{aligned} \mathcal{H}^{(0)}=1, \\ \mathcal{H}_i^{(1)}=\mathbf{v}_i, \\ \mathcal{H}_{ij}^{(2)}=\mathbf{v}_i\mathbf{v}_j-\delta_{ij}, \\ \mathcal{H}_{ijk}^{(3)}=\mathbf{v}_i\mathbf{v}_j\mathbf{v}_k-(\mathbf{v}_i\delta_{jk}+\mathbf{v}_j\delta_{ik}+\mathbf{v}_k\delta_{ij}+) \\ \vdots \end{aligned} \tag{5}$$

and higher order ones, which are unnecessary to list [24].

According to Grad [25] we use the approximation in which the heat flow and the pressure tensor are the relevant physical moments needed in the description. This amounts to taking $a^{(s)}(\mathbf{r},t)=0,\forall s\geqslant 4$ and in addition to assume, as is usual in the thirteen-moment approximation, that

$$\mathring{a}_{ijk}^{(3)}\mathring{\mathcal{H}}_{ijk}^{(3)}=0. \tag{6}$$

The overcircle indicates that we are speaking of the *corresponding* traceless tensor. It is convenient to introduce further simplifications corresponding to a situation prevailing in one-dimensional shock waves. First, since $\mathbf{u}=u(x)\mathbf{i}$ we assume that we have cylindrical symmetry. Furthermore, assuming that the density and mean velocity are given by the local Maxwellian, we will propose that

$$f=f^{(0)}(1+\tilde{\xi}). \tag{7}$$

The quantity $\tilde{\xi}$ measures the deviation from the Maxwellian distribution function and can be expressed in terms of either the moments or the physical relevant variables, namely,

$$\begin{aligned} \tilde{\xi}=\mu_{xx}\left(\mathbf{C}_x^2-\frac{kT_{\parallel}^{(0)}}{m}\right)+\mu_{xy}(\mathbf{C}_x\mathbf{c}_y+\mathbf{C}_x\mathbf{c}_z) \\ +\mu_{yy}\left(\mathbf{c}_{\perp}^2-\frac{2kT_{\perp}^{(0)}}{m}\right)+\mu_{yz}\mathbf{c}_y\mathbf{c}_z+\theta_x\mathbf{C}_x \\ \times\left(\frac{m\mathbf{C}_x^2}{kT_{\parallel}^{(0)}}+\frac{m\mathbf{c}_{\perp}^2}{kT_{\perp}^{(0)}}-5\right)+\theta_y(\mathbf{c}_y+\mathbf{c}_z)\left(\frac{m\mathbf{C}_x^2}{kT_{\parallel}^{(0)}}+\frac{m\mathbf{c}_{\perp}^2}{kT_{\perp}^{(0)}}-5\right), \end{aligned} \tag{8}$$

where $\mathbf{c}_{\perp}^2\equiv\mathbf{C}_{\perp}^2\equiv c_y^2+c_z^2$ has been introduced in order to simplify the notation. The μ's and θ's are defined in the following way:

$$\mu_{xx}=\frac{m}{2kT_{\parallel}^{(0)}}\left(\frac{\mathbf{P}_{xx}}{nkT_{\parallel}^{(0)}}-1\right),$$

$$\mu_{xy}=\frac{m\mathbf{P}_{xy}}{nk^2T_{\parallel}^{(0)}T_{\perp}^{(0)}},$$

$$\mu_{yy}=\frac{m}{2kT_{\perp}^{(0)}}\left(\frac{\mathbf{P}_{yy}}{nkT_{\perp}^{(0)}}-1\right),$$

$$\mu_{yz}=\frac{m\mathbf{P}_{yz}}{nk^2T_{\perp}^{(0)2}},$$

$$\theta_x = \frac{m}{5kT_\parallel^{(0)}}\left[\frac{\mathbf{q}_x}{nkT_\perp^{(0)}} + \frac{1}{nk}\left(\frac{1}{T_\parallel^{(0)}} - \frac{1}{T_\perp^{(0)}}\right)\mathbf{Q}_x\right],$$

$$\theta_y = \frac{m}{5kT_\perp^{(0)}}\left[\frac{\mathbf{q}_y}{nkT_\perp^{(0)}} + \frac{1}{nk}\left(\frac{1}{T_\parallel^{(0)}} - \frac{1}{T_\perp^{(0)}}\right)\mathbf{Q}_y\right]. \tag{9}$$

The pressure tensor $(\mathbf{P})$, heat flux $(\mathbf{q})$, and $\mathbf{Q}$ are given by

$$\mathbf{P} = \int f(\mathbf{c},\mathbf{r},t) m\mathbf{C}\mathbf{C}\, d\mathbf{C},$$

$$\mathbf{q} = \int f(\mathbf{c},\mathbf{r},t)\frac{m}{2}\mathbf{C}^2\mathbf{C}\, d\mathbf{C},$$

$$\mathbf{Q} = \int f(\mathbf{c},\mathbf{r},t)\frac{m}{2}\mathbf{C}_x^2\mathbf{C}\, d\mathbf{C}. \tag{10}$$

Substitution of Eq. (1) in Eq. (10) yields readily the expression of the pressure in terms of the temperatures, namely,

$$p = \tfrac{1}{3}nkT_\parallel^{(0)} + \tfrac{2}{3}nkT_\perp^{(0)}. \tag{11}$$

Further, the condition $\mathrm{Tr}(\mathbf{P}) = 3p$ also implies that

$$\mu_{xx} = -2\left(\frac{T_\perp}{T_\parallel}\right)^2 \mu_{yy}. \tag{12}$$

The specific internal energy is also given by the usual expression [26] so that using Eq. (1) we also get

$$E(x) = \frac{3}{2}\frac{kT(x)}{m}, \tag{13}$$

where

$$T(x) = \tfrac{1}{3}T_\parallel^{(0)} + \tfrac{2}{3}T_\perp^{(0)} \tag{14}$$

is the total temperature. Finally it is important to mention that, within the present approximation, we have the following relation between $\mathbf{q}_x$ and $\mathbf{Q}_x$:

$$\mathbf{q}_x = \left(1 + \frac{2}{3}\frac{T_\perp^{(0)}}{T_\parallel^{(0)}}\right)\mathbf{Q}_x. \tag{15}$$

Notice that the cylindrical symmetry, which was taken into account in the expression for $\tilde{\xi}$ [Eq. (8)], has reduced the number of variables. At the present level of description we have four variables that appear in the Maxwellian $(n,u,T_\perp^{(0)},T_\parallel^{(0)})$ and 6 fluxes $(\mathring{\mathbf{P}}_{xx},\mathring{\mathbf{P}}_{yy},\mathring{\mathbf{P}}_{xy},\mathring{\mathbf{P}}_{yz},\mathbf{q}_x$, and $\mathbf{q}_y)$. Since Eq. (12) gives a relation between $\mathbf{P}_{xx}$ and $\mathbf{P}_{yy}$, we have nine unknowns. The problem is now to obtain the equations needed to solve for the unknowns, so that besides the conservation equations, *which are granted due to the binary collision hypothesis*, we need constitutive equations for the fluxes. This question will be undertaken in the next section.

III. TRANSPORT EQUATIONS

We derive here the equations for the conserved variables and the fluxes, starting from the Boltzmann equation,

$$\frac{\partial f}{\partial t} + \mathbf{c}\cdot\nabla_r f = J(f,f), \tag{16}$$

where $J(f,f)$ is the collision term whose explicit form is given by

$$J(f,f) \equiv \int d\mathbf{c}_1 d\mathbf{e}\Sigma(\chi,g) g[f(\mathbf{c}',\mathbf{r},t)f(\mathbf{c}_1',\mathbf{r},t) - f(\mathbf{c},\mathbf{r},t)f(\mathbf{c}_1,\mathbf{r},t)], \tag{17}$$

where the primes denote the final velocities of the molecules in the binary collision, $\Sigma(\chi,g)$ is the differential cross section, $g = |\mathbf{c} - \mathbf{c}_1|$ the relative speed, and $d\mathbf{e}$ denotes the integration over the solid angle [26]. The transport equation for an arbitrary function $\Psi(\mathbf{c})$ is obtained from the Boltzmann equation when we multiply it by $\Psi(\mathbf{c})$ and integrate in the velocity space, so

$$\int d\mathbf{c}\mathcal{D}(f)\Psi(\mathbf{c}) = \int d\mathbf{c}J(f,f)\Psi(\mathbf{c}), \tag{18}$$

where $\mathcal{D}$ is a shorthand notation for the drift term in the Boltzmann equation.

If $\psi(\mathbf{c})$ corresponds to a summational invariant, we obtain the corresponding conservation equation [26]. For a stationary plane shock wave along the $\mathbf{i}$ direction, all the relevant quantities depend only on the x coordinate and the conservation equations can be integrated once [10] to give for the conservation of mass:

$$\rho(x)u(x) = C_1, \tag{19}$$

the conservation of momentum

$$\mathbf{P}_{xx} + \rho(x)u^2(x) = C_2, \tag{20}$$

the energy conservation

$$\rho(x)[E(x) + \tfrac{1}{2}u^2(x)]u(x) + u(x)\mathbf{P}_{xx} + \mathbf{q}_x = C_3, \tag{21}$$

where C_1, C_2, C_3 are constants and the specific internal energy is given by Eq. (13). Equations (19), (20), and (21), *must* be supplemented by additional constitutive relations for $\mathbf{P}_{xx}$ and $\mathbf{q}_x$, which we now obtain.

For $\Psi(\mathbf{c}) = (3m/2)\mathbf{C}_x^2$, and assuming that the fluxes depend only on x, we obtain for the drift terms in the stationary case

$$\frac{\partial}{\partial x}\{[\mathbf{P}_{xx}(x) - \mathbf{P}_{yy}(x)]u(x) + 3\mathbf{Q}_x(x) - \mathbf{q}_x(x)\} + 2\mathbf{P}_{xx}(x)\frac{\partial u(x)}{\partial x} = \int d\mathbf{c}\frac{3m}{2}\mathbf{C}_x^2 J(f,f), \tag{22}$$

and using $\Psi(\mathbf{c}) = m\mathbf{C}_x^3/2$ (we prefer to use this function instead of the usual $\Psi(\mathbf{c}) = m\mathbf{C}^2\mathbf{C}_x/2$ since the collision terms can be evaluated more easily) we obtain for the drift term:

$$\frac{\partial}{\partial x}[u(x)\mathbf{Q}_x]+\frac{3\mathbf{P}_{xx}}{2}u(x)\frac{\partial u(x)}{\partial x}+3\mathbf{Q}_x\frac{\partial u(x)}{\partial x} + \frac{\partial}{\partial x}\left[\frac{3kT_{\parallel}^{(0)}}{m}\mathbf{P}_{xx}-\frac{3}{2}\frac{nk^2T_{\parallel}^{(0)2}}{m}\right]=\int d\mathbf{c}\frac{m\mathbf{C}_x^2}{2}\mathbf{C}_x J(f,f). \tag{23}$$

While it is in principle necessary to consider more functions Ψ to obtain equations for the other fluxes, it turns out that they are not required if we consider the linear part (in the fluxes) of the collision term, as will become clear later on.

A. The collision terms

Our main objective is to obtain a generalization of the Navier-Stokes equations when we have two temperatures in the Maxwellian. With this idea in mind we do not study the equations for the moments in their full generality, instead we want to obtain the corresponding constitutive relations. In order to achieve this objective we will consider a Knudsen type expansion of the moment equations. The main idea is to consider that the fluxes represent small corrections to the distribution function, typically of the order of the Knudsen number, and so the nonlinear contributions from the fluxes can be neglected if the Knudsen number is small enough. So, when evaluating the collision term we will only consider linear contributions in the fluxes.

Using Eqs. (7) and (17) we obtain for the linearized collision term

$$\begin{aligned}\int d\mathbf{c}\Psi(\mathbf{c})J(f,f)\big|_L &=\frac{1}{2}[\Psi(\mathbf{c}),1]+\mu_{xx}\left[\Psi(\mathbf{c}),\left(\mathbf{C}_x^2-\frac{kT_{\parallel}^{(0)}}{m}\right)\right]\\ &+\mu_{xy}[\Psi(\mathbf{c}),(\mathbf{C}_x\mathbf{c}_y+\mathbf{C}_x\mathbf{c}_z)]\\ &+\mu_{yy}\left[\Psi(\mathbf{c}),\left(\mathbf{c}_{\perp}^2-\frac{2kT_{\perp}^{(0)}}{m}\right)\right]+\mu_{yz}[\Psi(\mathbf{c}),\mathbf{c}_y\mathbf{c}_z]\\ &+\theta_x\left[\Psi(\mathbf{c}),\mathbf{C}_x\left(\frac{m\mathbf{C}_x^2}{2kT_{\parallel}^{(0)}}+\frac{m\mathbf{C}_{\perp}^2}{2kT_{\perp}^{(0)}}-5\right)\right]\\ &+\theta_y\left[\Psi(\mathbf{c}),(\mathbf{c}_y+\mathbf{c}_z)\left(\frac{m\mathbf{C}_x^2}{2kT_{\parallel}^{(0)}}+\frac{m\mathbf{C}_{\perp}^2}{2kT_{\perp}^{(0)}}-5\right)\right],\end{aligned} \tag{24}$$

where [,] is a shorthand notation for the terms that contain the collision dynamics,

$$[\Psi(\mathbf{c}),\Phi(\mathbf{c})]\equiv\int d\mathbf{c}\int d\mathbf{c}_1 d\mathbf{e}\Sigma(\chi,g)gf^{(0)}(\mathbf{c},\mathbf{r},t)f^{(0)}\times(\mathbf{c_1},\mathbf{r},t)\Psi(\mathbf{c})\Delta^{\star}[\Phi(\mathbf{c})], \tag{25}$$

$$\Delta^{\star}[\Phi(\mathbf{c})]=\exp[-\Delta(\phi)][\Phi(\mathbf{c}')+\Phi(\mathbf{c}_1')]-[\Phi(\mathbf{c})+\Phi(\mathbf{c}_1)], \tag{26}$$

and $\Delta(\phi)$ is given by

$$\Delta(\phi)=\frac{m}{2k}\left(\frac{1}{T_{\parallel}^{(0)}}-\frac{1}{T_{\perp}^{(0)}}\right)[\mathbf{C}_{1x}'^2+\mathbf{C}_x'^2-\mathbf{C}_{1x}^2-\mathbf{C}_x^2]. \tag{27}$$

With $\Psi(\mathbf{c})=(3m/2)\mathbf{C}_x^2$ and $\Psi(\mathbf{c})=(m/2)\mathbf{C}_x^2\mathbf{C}_x$ it turns out that all the collision integrals can be evaluated for the rigid sphere model, the details of which are given in the Appendix. We therefore obtain

$$\int d\mathbf{c}\frac{3m}{2}\mathbf{C}_x^2J(f,f)\big|_L=\frac{3m}{2}\{\xi_{xx}+\mu_{xx}\Xi\}, \tag{28}$$

where

$$\xi_{xx}\equiv\frac{1}{2}[\mathbf{C}_x^2,1], \tag{29}$$

and

$$\Xi\equiv\left[\mathbf{C}_x^2,\left(\mathbf{C}_x^2-\frac{kT_{\parallel}^{(0)}}{m}\right)-\frac{1}{c^2}\left(\mathbf{c}_y^2-\frac{kT_{\perp}^{(0)}}{m}\right)\right]. \tag{30}$$

Equations (29) and (30) give the relevant collision integrals and can be expressed in terms of the temperature ratio:

$$c\equiv\frac{T_{\perp}^{(0)}}{T_{\parallel}^{(0)}}, \tag{31}$$

which measures the temperature asymmetry in the system. For $\Psi(\mathbf{c})=(m/2)\mathbf{C}_x^2\mathbf{C}_x$ we have that

$$\int d\mathbf{c}\frac{m}{2}\mathbf{C}_x^2\mathbf{C}_xJ(f,f)\big|_L=\frac{m}{2}\theta_x\Gamma_q, \tag{32}$$

where

$$\Gamma_q=\left[\mathbf{C}_x^3,\mathbf{C}_x\left(\frac{m\mathbf{C}_x^2}{kT_{\parallel}^{(0)}}+\frac{m\mathbf{C}_{\perp}^2}{kT_{\perp}^{(0)}}-5\right)\right]. \tag{33}$$

Expressions for reduced collision integrals defined as

$$\xi^{\star}(c)\equiv\frac{\xi_{xx}}{(kT_{\parallel}^{(o)}/m)^{3/2}\sigma^2n^2\sqrt{\pi}},$$

$$\Xi^{\star}(c)\equiv\frac{\Xi}{(kT_{\parallel}^{(o)}/m)^{5/2}\sigma^2n^2\sqrt{\pi}}, \tag{34}$$

$$\Gamma_q^{\star}(c)\equiv\frac{\Gamma_q}{(kT_{\parallel}^{(0)}/m)^{5/2}\sigma^2n^2\sqrt{\pi}}, \tag{35}$$

can be found in the Appendix. All of them can be expressed as a function of the ratio of the Maxwellian temperatures. Figure 2 gives their behavior as a function of c. Notice that for $c=1$ (equal temperatures) their values are 0, $-32/5$, and $-64/5$, respectively.

B. The constitutive relations

Direct substitution of the result for the collision terms given by Eq. (28) in Eq. (22) gives a way to obtain the constitutive relation for $\mathbf{P}_{xx}$:

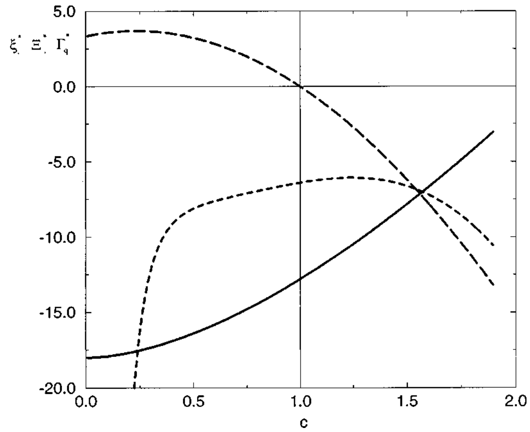

FIG. 2. Collision integrals $\xi^\star$ (long dashed line), $\Xi^\star$ (solid line), and $\Gamma_q^\star$ (small dashed line) as a function of $c=T_\perp^{(0)}/T_\parallel^{(0)}$. For $c=1$ their values are 0, $-32/5$, and $-64/5$, respectively.

$$\frac{\partial}{\partial x}[[\mathbf{P}_{xx}(x)-\mathbf{P}_{yy}(x)]u(x)+3\mathbf{Q}_x(x)-\mathbf{q}_x(x)]$$
$$+2\mathbf{P}_{xx}(x)\frac{\partial u(x)}{\partial x}=\frac{3m}{2}\{\xi_{xx}+\mu_{xx}\Xi\}. \tag{36}$$

Following Grad [25], in the left hand of the equation we make the approximation $\mathbf{P}_{xx}=nkT_\parallel^{(0)}$, $\mathbf{P}_{yy}=nkT_\perp^{(0)}$ and $\mathbf{q}=0$ (zero order expression for the fluxes in a Knudsen expansion). This approximation can be regarded as a way to obtain the first order correction in a Knudsen expansion for the fluxes, thus leading to

$$\frac{\partial}{\partial x}[(nkT_\parallel^{(0)}-nkT_\perp^{(0)})u(x)]+2nkT_\parallel^{(0)}\frac{\partial u(x)}{\partial x}$$
$$=\frac{3m}{2}\{\xi_{xx}+\mu_{xx}\Xi\}. \tag{37}$$

Using the definition of μ_{xx} we obtain that

$$\mathbf{P}_{xx}=nkT_\parallel^{(0)}+\frac{8n^2k^3T_\parallel^{(0)3}}{3m^2}\Xi^{-1}\frac{\partial u(x)}{\partial x}$$
$$+\frac{2}{3m}\Xi^{-1}\frac{\partial}{\partial x}[(nkT_\parallel^{(0)}-nkT_\perp^{(0)})u(x)]-\xi_{xx}\Xi^{-1}. \tag{38}$$

However, if $f=f^{(0)}$ is the two-temperature Maxwellian, which corresponds to zero transport coefficients that is $\Xi^{-1}=0$ or $\sigma=\infty$ (zero mean free path), we do not recover $nkT_\parallel^{(0)}$. The reason is that Ξ and ξ_{xx} have the same σ dependence [see Eq. (34)], so that in the limit $\sigma\to\infty$ the last term of Eq. (38) gives a nonzero limiting value. To get the correct limiting case it is necessary that the sum of the last two members terms in Eq. (38) is zero, which implies that the pressure tensor is given by

$$\mathbf{P}_{xx}=nkT_\parallel^{(0)}+\frac{8n^2k^3T_\parallel^{(0)3}}{3m^2}\Xi^{-1}\frac{\partial u(x)}{\partial x}. \tag{39}$$

Equation (39) is the generalization of the usual constitutive equation for one temperature, the second term is proportional to the mean free path and represents a first order Knudsen correction. The viscosity, which we denote by η_{xx}, is then given by

$$\eta_{xx}=-\frac{2n^2k^3T_\parallel^{(0)3}}{m^2}\Xi^{-1}, \tag{40}$$

using the value of Ξ for equal temperatures given at the end of the preceding section, we conclude that for such a case we have

$$\eta=\frac{5m}{16\sigma^2}\left(\frac{kT}{\pi m}\right)^{1/2}, \tag{41}$$

which is the first approximation in a Sonine expansion for the viscosity. For rigid spheres the exact value of the viscosity is known [26] and is equal to 1.016 034 times Eq. (41). If this more accurate value for the viscosity is used, and also the corresponding one for the thermal conductivity [see Eq. (48)], it turns out that there is a minor modification to the solution of the Navier-Stokes equations (than with the first Sonine expansion expression for the transport coefficients). The numerical calculations for the Navier-Stokes equations, to be given later, were obtained with the first order Sonine expansion expression for the transport coefficients, that is, using Eqs. (41) and (48).

On the other hand, the condition that the last two terms of Eq. (38) is zero implies a relationship between the temperature gradients and the collision integral ξ_{xx}, which is itself a function of $T_\parallel^{(0)}$ and $T_\perp^{(0)}$,

$$\frac{\partial}{\partial x}[(nkT_\parallel^{(0)}-nkT_\perp^{(0)})u(x)]=\frac{3m}{2}\xi_{xx}. \tag{42}$$

Hence, Eq. (42) may be regarded as a constitutive relation for the temperatures. When there are no gradients for $T_\parallel^{(0)}$, $T_\perp^{(0)}$, and u, we infer from Eq. (42) and Fig. 2 that the Maxwellian temperatures should be equal. We will say more about Eq. (42) later on.

To obtain the constitutive relation for the heat flux we first note that the equation for conservation of momentum can be written as

$$u\frac{\partial u}{\partial x}=-\frac{1}{\rho}\frac{\partial \mathbf{P}_{xx}}{\partial x}. \tag{43}$$

Using Eqs. (32) and (43), Eq. (23) can be rewritten as

$$\frac{\partial}{\partial x}[u(x)\mathbf{Q}_x]+\frac{3\mathbf{P}_{xx}}{2}\left[-\frac{1}{\rho}\frac{\partial \mathbf{P}_{xx}}{\partial x}\right]+3\mathbf{Q}_x\frac{\partial u(x)}{\partial x}$$
$$+\frac{\partial}{\partial x}\left[\frac{3kT_\parallel^{(0)}}{m}\mathbf{P}_{xx}-\frac{3}{2}\frac{nk^2T_\parallel^{(0)2}}{m}\right]=\frac{m}{2}\theta_x\Gamma_q. \tag{44}$$

If, as was done to obtain the viscosity, in the left hand of the Eq. (44) we make the approximation $\mathbf{P}_{xx}=nkT_\parallel^{(0)}$ and $\mathbf{Q}$

$=0$ (zero order expression for the fluxes in a Knudsen expansion), then using the expression for θ_x we have from Eq. (44) that

$$\mathbf{q}_x = \frac{3}{2} A n k T_{\parallel}^{(0)} \frac{k}{m} \frac{\partial}{\partial x} T_{\parallel}^{(0)}, \tag{45}$$

where

$$A = \frac{kT_{\parallel}^{(0)}}{m} \frac{10nkT_{\perp}^{(0)}}{m} \frac{1}{\Gamma_q} \frac{1}{1+(c-1)/(1+2c/3)}. \tag{46}$$

Equation (45) is a generalization of Fourier's law, with a thermal conductivity given by

$$\lambda = -\frac{15n^2}{\Gamma_q}\left(\frac{kT_{\parallel}^{(0)}}{m}\right)^2 \frac{kT_{\perp}^{(0)}}{m} \frac{k}{1+(c-1)/(1+2c/3)}, \tag{47}$$

which in the limit of equal temperatures ($\Gamma_q^{\star} = -64/5$) becomes the usual first order Sonine expansion expression for the thermal conductivity:

$$\lambda = \frac{75k}{64\sigma^2}\left[\frac{kT}{\pi m}\right]^{1/2}. \tag{48}$$

The exact value for the rigid spheres model, in the Chapman-Enskog expansion [26], is 1.025 13 times Eq. (48).

Equations (39), (42), and (45) are the main results of this work. Together with the expressions for the collision integrals given in the Appendix, they provide the constitutive relations needed to close the conservation equations for a two-temperature theory.

At the present level of approximation we have a closed set of equations for the variables n, u, $T_{\parallel}^{(0)}$, $T_{\perp}^{(0)}$, $\mathbf{P}_{xx}$, and $\mathbf{q}_x$. That is, we have three equations for the conserved variables [Eqs. (19), (20), and (21)] and three constitutive equations [Eqs. (39), (42), and (45)]. We are now in a position to solve numerically the equations for a plane shock wave using the proper dimensionless variables.

IV. THE REDUCED EQUATIONS

In order to compare with previous work it is convenient to use the same dimensionless variables as Holian *et al.* [10]:

$$s \equiv x/l, \quad l = \frac{5m}{12\rho_0\sigma^2\sqrt{\pi}}, \quad \tau_{\parallel}(s) \equiv \frac{kT_{\parallel}^{(0)}(x)}{mu_0^2},$$

$$\tau_{\perp}(s) \equiv \frac{kT_{\perp}^{(0)}(x)}{mu_0^2}, \quad \tilde{u} \equiv u/u_0, \quad \tau_0 \equiv \frac{P_0}{\rho_0 u_0^2}, \tag{49}$$

where l is the ''mean free path'' and the origin is chosen in such a way that the velocity at this point is equal to $(u_1 + u_0)/2$. The subscript ''0'' refers to the asymptotic values in the low density region of the shock wave whereas the subscript ''1'' refers to the denser asymptotic values of the shock wave. In particular P_0 is the pressure in the low density part of the shock. The pressures, temperatures, and velocities at the asymptotic regions of the shock (P_0, P_1, T_0, T_1, u_0, u_1), are of course related by the Rankine-Hugoniot equations, which can be obtained from the conservation equations, in terms of the previous reduced variables, they read

$$\tilde{u}_1 = \tfrac{5}{4}\tau_0 + \tfrac{1}{4}, \quad \tau_1 = \tfrac{7}{8}\tau_0 + \tfrac{3}{16} - \tfrac{5}{16}\tau_0^2, \quad \tilde{u}_0 = 1. \tag{50}$$

Thus, given τ_0 the reduced values of the velocity and temperature at the high density part of the shock can be determined. We define the Mach number (M_a) [9] as the velocity of the shock wave divided by the sound velocity, both quantities being evaluated at the low density part of the shock, the ratio of the specific heat at constant pressure divided by the one at constant volume is taken to be 5/3, so that we obtain for the Mach number

$$M_a = \sqrt{\frac{3}{5\tau_0}}. \tag{51}$$

In terms of these variables, using the constitutive equations for the pressure tensor and the heat flux [Eqs. (39) and (45)], and using the conservation equations [Eqs. (19), (20), and (21)] we obtain the following set of three equations:

$$\frac{\tau_{\parallel}}{\tilde{u}(s)} + \frac{32}{5}\frac{\sqrt{\tau_{\parallel}(s)}}{\Xi^{\star}(c)}\frac{\partial}{\partial s}u(s) = \tau_0 + 1 - \tilde{u}(s),$$

$$\frac{\partial}{\partial s}\tau_{\parallel}(s) - \frac{\partial}{\partial s}\tau_{\perp}(s) = \frac{5}{8}\frac{\tau_{\parallel}(s)^{3/2}\xi^{\star}(c)}{\tilde{u}(s)^2}, \tag{52}$$

$$\frac{1}{2}\tau_{\parallel}(s) + \tau_{\perp}(s) + \frac{36c\,\tau_{\parallel}(s)}{\Gamma_q^{\star}(c)[1+(c-1)/(1+2c/3)]}\frac{\partial}{\partial s}\tau_{\parallel}(s)$$
$$= \frac{3}{2}\tau_o + \frac{1}{2}[1-\tilde{u}(s)]^2 + \tau_0[1-\tilde{u}(s)].$$

The first of Eqs. (52) is the reduced form of conservation of momentum, the second one is the constitutive relation for the temperature difference, and the last one is the equation for energy conservation. We have then a closed system of three equations with three unknowns.

For the single temperature case ($\tau_{\parallel} = \tau_{\perp} = \tau$) Eqs. (52) reduce as it should be to the dimensionless Navier-Stokes equations:

$$\frac{\tau(s)}{\tilde{u}(s)} - \tau^{1/2}(s)\tilde{u}'(s) = \tau_0 + 1 - \tilde{u}(s),$$

$$\tfrac{3}{2}\tau(s) - \tfrac{45}{16}\tau^{1/2}(s)\tilde{\tau}'(s) = \tfrac{3}{2}\tau_0 + \tfrac{1}{2}[1-\tilde{u}(s)]^2 + \tau_0[1-\tilde{u}(s)]. \tag{53}$$

The Holian [10] conjecture can now be explained in terms of the previous reduced Navier-Stokes equations. Holian *et al.* noticed that the temperature defined as $nkT_{\parallel} \equiv \mathbf{P}_{xx}$ is in general different from the temperature that appears in the Maxwellian (T) and also in the expression for the transport coefficients. Hence, they proposed that the temperature in the expression of the transport coefficients should be replaced by $T_{\parallel}$, which, in the notation used here, amounts to replacing

$\sqrt{\tau}$ with $\sqrt{\tilde{u}(\tau_0+1-\tilde{u})}$ in the Navier-Stokes equations. In this way they obtained that Eqs. (53) now become

$$\frac{\tau(s)}{\tilde{u}(s)}-\sqrt{\tilde{u}(\tau_0+1-\tilde{u})}\tilde{u}'(s)=\tau_0+1-\tilde{u}(s)$$

$$\tfrac{3}{2}\tau(s)-\tfrac{45}{16}\sqrt{\tilde{u}(\tau_0+1-\tilde{u})}\tilde{\tau}'(s)=\tfrac{3}{2}\tau_0+\tfrac{1}{2}[1-\tilde{u}(s)]^2 + \tau_0[1-\tilde{u}(s)]. \tag{54}$$

They were then able to obtain a closed system of equations, which they solved using finite difference methods. For each of the three versions of equations that we have described—2T-NS [Eq. (52)], NS [Eq. (53)], and HO [Eq. (54)]—we must give initial or boundary conditions. In order to compare, we have taken the same initial conditions as Holian *et al.* [10] and solved the equations using three different methods, as will be explained below. It should be emphasized that Eqs. (52) are a result obtained solely from the constitutive relations for two temperatures and thus represent an important result of this work.

V. NUMERICAL CALCULATIONS

The molecular dynamics data with which we compare were taken from the work by Holian *et al.* [10] who did not report the Mach (M_a) number to which the data correspond, although since they refer to the molecular dynamics data reported by Salomons and Mareschal [9] for a Mach number value of 134 we infer that the Mach number, as defined by Salomons and Mareschal [9], is equal to 134. In order to compare with results of molecular dynamics, which incidentally gives identical results to the direct simulation Monte Carlo method [9], we follow Holian *et al.* [10] and make the simplifying assumption that $\tau_0=0$, for $M_a=134$ we obtain from Eq. (51) that $\tau_0\approx 3.34\times 10^{-5}$, we would like to stress that the condition $\tau_0=0$ is only a reasonable and simplifying assumption [10]. Hence, the Rankine-Hugoniot equations imply the following asymptotic values:

$$\tilde{u}_0=1,\quad \tilde{u}_1=1/4,\quad \tau_1=3/16. \tag{55}$$

Thus the preceding equations (52), (53), and (54) are simplified. Holian *et al.* [10] proposed to give initial conditions with values $\tilde{u}_i=1/4+10^{-6},\tau_i=3/16$ and then found the initial ''time'' s_i that gave the correct value (0.625) of $\tilde{u}$ at the origin. The same procedure will be followed here. Holian *et al.* also mentioned that the finite difference method used by them was unstable when the integration was done in a direction opposite to that of the heat flow, a point that will be analyzed later on, so we also started at the high density region of the shock wave. It is interesting to notice that if the exact asymptotic values of the variables are given, all three theories give the same constant result that corresponds to the Euler solution. The reason for this is that all three theories give derivatives for u and the temperatures that are zero when the exact asymptotic values are used and since the numerical methods use the information of the derivatives to estimate the next point, it is clear that they will give the same value for the next point and so on.

To solve the three different set of equations we first made some calculations for the Navier-Stokes equations using three different methods in order to see if the solution was dependent on the method. The three methods are Adams (AD), backward differentiation formula (BDF), and Runge-Kutta (RK) [27]. The tolerance was varied to infer the expected accuracy in each of the numerical methods. It turns out that only for the BDF method the tolerance can be varied to about the smallest positive model number, which for the machine used is about 2.2×10^{-308}. For the other two methods (AD and RK) the minimum tolerance that can be used is about 10^{-15}; for smaller tolerances both methods are not able to provide the solution to the requested tolerance.

For the RK method three different variants of order of accuracy 3, 5, and 8 were used. Only results for the method RK(7-8) of accuracy 8 are reported. The results of our calculations are given in Table I.

The AD method was used to determine the initial ''time'' for the previous mentioned initial conditions, so that the numerical solution gave the correct value of $\tilde{u}$ at the origin (0.625) to a certain tolerance. The initial ''time'' found in this way is $s_i=2.488\,513$ for the Navier-Stokes equations. This value of s_i together with $\tilde{u}_i=0.250\,006$ and $\tau_i=0.1875$ were used to solve the Navier-Stokes equations with the other two methods (RK and BDF), and the results are given in Table I.

From the results of Table I we see that the results from the RK(7-8) method are rather similar to the AD method. The AD method gives $\tilde{u}(0)=0.625\,000\,30$ with an estimated accuracy of few parts in 10^9, whereas for the RK(7-8) we have $\tilde{u}(0)=0.625\,000\,30$ with again about the same estimated accuracy as for the AD method. Thus, we are tempted to conclude that with any of the two methods [RK(7-8),AD] the numerical solution is the same with an estimated accuracy of few parts in 10^9. The results from the BDF method show that the numerical solution has an estimated accuracy of 16 digits, which is the maximum accuracy that can be obtained with double precision, and that the method has a better behavior as the tolerance is varied. An accuracy of 16 digits seems too good to be true and later on we will come to this point. However, the difference between the BDF method and the other two is about 4 parts in 10^4, which seems to imply that the methods are converging to different values. It should be pointed out that in the graphs for the velocity profiles given by Holian *et al.* [10] this difference cannot be noticed, but in problems in which sensitivity to initial conditions is to be expected, it can be important.

We have made an analysis to investigate the ''stability'' of the methods when the integration is done in a direction opposite to the heat flow. Let us examine the Adams' integration scheme when we integrate from the hot side of the shock wave to the cold part. In Table II the Navier-Stokes equations are integrated from different initial ''times'' to different final values with the AD method. In row ''a'' of Table II we see the initial values (s_i, $\tilde{u}_i$, and τ_i), discussed previously, and the corresponding final values (s_f, $\tilde{u}_f$, and τ_f). In row ''c'' of the same table we see that the initial value of s is taken to be s_{fa}, that is, the final value of s that appears in row ''a'' ($s_{fa}=0$). The initial velocity and temperature are taken as their final values in row ''a'' of Table II. In

TABLE I. Solution of the reduced Navier-Stokes equations at $s=0$ with three different methods and different tolerances. The initial values are given in row (a) of Table II and are the same for the three methods used.

Tolerance	$\tilde{u}(0)$	$\tau(0)$
	Adams method	
10^{-9}	0.624 963 315 174 621 1	0.125 637 756 970 500 7
10^{-10}	0.624 997 997 208 800 0	0.125 629 385 120 289 6
10^{-12}	0.625 000 281 414 129 2	0.125 628 833 711 147 2
10^{-13}	0.625 000 300 794 112 1	0.125 628 829 032 846 6
10^{-14}	0.625 000 301 988 302 6	0.125 628 828 744 566 4
10^{-15}	0.625 000 302 068 455 9	0.125 628 828 725 217 3
	RK(7−8) method	
10^{-9}	0.625 000 014 402 597 9	0.125 628 898 167 095 5
10^{-11}	0.625 000 156 383 882 5	0.125 628 863 893 462 5
10^{-13}	0.625 000 302 077 649 8	0.125 628 828 722 997 6
10^{-14}	0.625 000 302 079 943 1	0.125 628 828 722 444 2
10^{-15}	0.625 000 302 080 741 2	0.125 628 828 722 251 5
	BDF method	
10^{-22}	0.625 322 569 829 112 1	0.125 550 997 767 003 2
10^{-23}	0.625 322 569 829 187 0	0.125 550 997 766 985 1
10^{-24}	0.625 322 569 829 182 8	0.125 550 997 766 986 2
10^{-28}	0.625 322 569 829 182 8	0.125 550 997 766 986 2
10^{-307}	0.625 322 569 829 182 8	0.125 550 997 766 986 2

other words, given the initial values $s_i=2.488\,513$, $\tilde{u}_i=0.250\,006$, and $\tau_i=0.1875$ we integrate the NS equation to $s=0$ and then use the values found as initial values and integrate to $s=2.488\,513$. The results of Table II show that there is a difference from the expected values ($\tilde{u}_i=0.250\,006$ and $\tau_i=0.1875$), but the difference is really marginal and can be understood in terms of the roundoff error. Our conclusion is that there is a range in which the AD method is not unstable when the integration is carried out in a direction contrary to the heat flow. So, irreversibility and local ‘‘instability’’ of the numerical methods are not in general related.

We can now analyze the behavior of the solution for larger values of s and integrate the NS equations to $s=4.5$. In row ‘‘b’’ of Table II we start with the initial values; $s=2.488\,513$, $\tilde{u}_i=0.250\,006$, $\tau_i=0.1875$ and integrate to $s=4.5$. We see that the final value of $\tilde{u}$ is greater than its value at $s=2.488\,513$, which means that the profile is nonmonotonic. The results of row ‘‘d’’ in Table II show that the accuracy of the method starts to deteriorate; nevertheless, the conclusion of a nonmonotonic profile is true, as can be shown by integrating to a lower value of s. We interpret this fact as being a result of the approximation of using initial values instead of boundary ones as explained previously.

We have investigated the ‘‘stability’’ of the BDF method in the same way as described previously for the AD method, but the results are not shown in the tables. We found the initial time ($s_i=2.487\,856$) so that we obtained approximately the correct value of the velocity profile at zero [$\tilde{u}(0)\approx 0.625\,000\,049$]. Using the values obtained at $s=0$ we integrate to $s^{\star}=2.487\,856$ to predict a value for the velocity profile of $\tilde{u}(s^{\star})\approx 0.250\,003\,4$, which should be compared with the initial value given ($\tilde{u}=0.250\,006$). We conclude that an accuracy of the method of a few parts in 10^7 is probably a more reasonable expectation. Nevertheless, it is not enough to explain the different values obtained with the other two methods.

TABLE II. Numerical solution of the reduced Navier-Stokes equations with the Adams method, a tolerance of 10^{-14}, and different initial values.

	s_i	$\tilde{u}_i$	τ_i	s_f	$\tilde{u}_f$	τ_f
a	2.488 513	0.250 006	0.1875	0.0	0.625 000 301 988 303	0.125 628 828 744 566
b	s_{ia}	$\tilde{u}_{ia}$	τ_{ia}	4.5	0.250 044 358 523 472	0.187 532 170 949 702
c	s_{fa}	$\tilde{u}_{fa}$	τ_{fa}	2.488 513	0.250 006 000 000 343	0.187 500 000 000 253
d	s_{fb}	$\tilde{u}_{fb}$	τ_{fb}	0.0	0.624 999 884 960 198	0.125 628 929 415 134

TABLE III. Numerical solution of the reduced Holian equations with the Adams method, a tolerance of 10^{-15}, and different initial values.

	s_i	$\tilde{u}_i$	τ_i	s_f	$\tilde{u}_f$	τ_f
a	2.674 459	0.250 006	0.1875	0.0	0.625 000 097 246 471 7	0.125 628 878 169 247 6
b	s_{ia}	$\tilde{u}_{ia}$	τ_{ia}	4.5	0.250 030 127 377 060 2	0.187 521 849 729 052 4
c	s_{fa}	$\tilde{u}_{fa}$	τ_{fa}	2.674 459	0.250 006 000 000 020 9	0.187 500 000 000 015 5
d	s_{fb}	$\tilde{u}_{fb}$	τ_{fb}	0.0	0.625 000 179 401 722 6	0.125 628 858 336 972 1

For the Holian equations, the initial ''time'' was determined so that with the initial conditions mentioned before the solution at $s=0$ was approximately $\tilde{u}=0.625$; in row ''a'' of Table III the initial conditions and final results can be found. We have done similar calculations as mentioned before and similar conclusions can be obtained from the table; there is a region in which the equations can be integrated in a direction opposite to the heat flow without having ''instability'' of the method and the velocity and temperature profiles are nonmonotonic.

For the 2T-NS theory similar calculations can be done but it is not necessary to do them in order to obtain the conclusion that the theory does not give the correct asymptotic behavior for different temperatures. In fact from the constitutive relation for the temperatures given by Eq. (42) and Fig. 2 the conclusion can be obtained. Suppose that at $s=0.0$ we have $T_{\parallel}^{(0)}>T_{\perp}^{(0)}$, that is, $c<1$, from Fig. 2 we see that $\xi^{\star}<0$ and from Eq. (42) we see that the variation of the temperature difference is negative so when integrating to higher values of s the difference will decrease. However, if we integrate to values lower than $s=0.0$ the situation is just the opposite and we will have that the difference will increase, but the asymptotic behavior for a normal shock wave is that the asymptotic states correspond to equilibrium, so the 2T-NS equations cannot give this behavior. It should be pointed out that if equal temperatures are taken then the results of the 2T-NS equations are the same as the Navier-Stokes equations, so the 2T-NS equations do not give anything new for normal shock waves. The idea that a two-temperature displaced Maxwellian can offer an improvement to the Navier-Stokes equations is not true if only the first correction in the Knudsen expansion is considered. The conclusion is valid only for normal shock waves although the 2T-NS theory developed here could find applications in other situations.

We have calculated the shock wave thickness (λ_{ST}), which is defined as [10]

$$\lambda_{\mathrm{ST}}\equiv\frac{u_1-u_0}{u'(0)}=\frac{(\tilde{u}_1-1)\ l}{\tilde{u}'(0)}, \tag{56}$$

obtaining that, using $M_a=134$, for the Navier-Stokes equations and the Holian *et al.* theory it has values of 1.53 l and 2.09 l, respectively, and for the molecular dynamics simulations its value is equal to 2.35 l [10]. While the shock thickness has been used in the past to compare the results of simulations or experiment with the results of continuum theories, it must be pointed out that a more stringent test would be to compare the distribution function itself as pointed out by Bird [7]. However, there is an intermediate option of comparing the profiles, which is the one used here. In this respect, it should be pointed out that while the theory advanced by Holian *et al.* represents an important improvement over the Navier-Stokes equations, there is room to improve the temperature profiles that are shown in Fig. 3.

As a test of our numerical calculations for low Mach numbers we have compared the maximum slope shock thickness (Δ) as defined by Gilbarg and Paolucci [28]. Recently Ruggeri [29] has recalculated Gilbarg and Paolucci values for a soft sphere model (power law potential), apparently not for the rigid sphere case, for which the temperature dependence of the transport coefficients goes like T^s, with $s=0.816$, obtaining good agreement. Our calculations for l_0/Δ, where l_0 is the mean free path [28], for the rigid sphere model are the same as the values reported by Gilbarg and Paolucci at $M_a=1.2$, but are 0.7% and 1.8% higher than their values for $M_a=2.0$ and $M_a=3.0$, respectively. Apparently they had problems in calculating the maximum slope shock thickness for Mach numbers greater than 3 for the rigid sphere model and for a soft sphere model with $s=0.816$, however, Ruggeri reported numerical calculations up to $M_a=11$ in the last case.

With respect to the condition $\tau_0=0$ we would like to

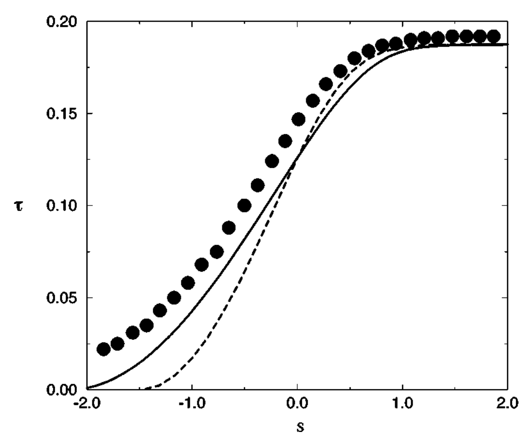

FIG. 3. Temperature profile $\tau(s)$ vs s. Solid circles correspond to the molecular dynamics calculations ($M_a=134$), dashed line corresponds to the Navier-Stokes equations ($\tau_0=0$), and the solid line to the Holian theory ($\tau_0=0$). We recall for the reader that the MD and DSMC yield similar results.

TABLE IV. Shock thickness for the rigid sphere model as a function of the Mach number for the Navier-Stokes (NS) equations and the Holian *et al.* theory (HO).

M_a	λ_{ST}/l (NS)	λ_{ST}/l (HO)	M_a	λ_{ST}/l (NS)	λ_{ST}/l (HO)
1.2	13.749	13.897	8.0	1.616	2.160
2.0	3.323	3.706	10.0	1.584	2.134
3.0	2.208	2.680	134	1.528	2.087
5.0	1.757	2.282	∞	1.528	2.087

mention that, as far as the numerical methods are concerned, the numerical solution cannot be continued beyond the point at which the solution is very near its asymptotic values at the low density region of the shock wave. In fact for lower values of s than about 1.5 for the Navier-Stokes equations and 2.1 for the Holian theory, we get a floating point exception, which in our opinion is a result of the condition $\tau_0=0$. Such behavior is the result of taking $M_a=\infty$ and for finite Mach numbers this problem does not show up. In fact the general methodology of perturbing the initial velocity at the high density region of the shock can be used to numerically generate the profiles for finite Mach numbers. In Table IV we have included the calculations of the shock thickness for different Mach numbers. Finally, it is worth pointing out that the local topology of the Holian *et al.* theory at the critical points is the same as the Navier-Stokes equations, that is, the upflow critical point (low density region) is an unstable node and the other one is a saddle.

VI. DISCUSSION

As mentioned in the Introduction, the present research was initiated with the hope of providing a theoretical basis for the Holian conjecture, which is known to give an important improvement over the Navier-Stokes equations. Our point of departure was Grad's moment method with a two-temperature displaced Maxwellian as a weight function and our goal is to obtain constitutive equations from the moment equations. We showed that, if the first order Knudsen expansion of the moment equations is taken, it is possible to obtain constitutive relations for the heat flow, the viscous pressure tensor, and the temperature difference. This allows us to close the conservation equations, providing us with a well posed problem for shock waves. The idea is motivated by the observation that the Navier-Stokes equations give a reasonable velocity profile for high Mach numbers and so perturbations around it could result in an improvement. To first order in the Knudsen number we find that the equations derived are not capable of providing the correct asymptotic behavior for normal shock waves. In this respect, it should be pointed out that from the molecular dynamics results [9,10] it is not clear that the asymptotic behavior for the shock corresponds to that of a normal one since their results are not given for a wide interval of distances. On the other hand, our calculations for the collision integrals are valid in the range $0<T_{\perp}^{(0)}<2T_{\parallel}^{(0)}$, the upper limit may possibly be extended if the analytic continuation to the hypergeometric series is used. Nevertheless, we do not think that such an extension can change our conclusion about the asymptotic behavior.

The Holian conjecture gives higher values for the transport coefficients, viscosity, and thermal conductivity, than the ones corresponding to the usual Navier-Stokes regime. For $c<1$, where $c=T_{\perp}^{(0)}/T_{\parallel}^{(0)}$, the 2T-NS theory predicts a higher value for the viscosity while the thermal conductivity is lower than the corresponding Navier-Stokes results, whereas in the case $c>1$ the situation is just the opposite. For $c=1$ the 2T-NS theory gives identical results as the Navier-Stokes equations. In this case the solution to the 2T-NS equations is stable in the sense that once the temperatures are equal they remain equal regardless of whether the integration is performed in the direction of the heat flow or in the opposite direction. In this respect it is interesting to mention that if different temperatures are given and the integration is carried out in the direction in which the temperatures tend to be equal, then, once they are equal (up to the machine's precision) and the integration is carried out in the opposite direction, as initially done, we do not obtain different temperatures.

We have provided evidence that shows how different classes of numerical methods may converge to different points. While for the present problem this is not important, as far as velocity profiles are concerned, it is important in situations where sensitivity to initial conditions is to be expected. We also find that there are some numerical methods that are not locally ''unstable'' when the integration is carried out in a direction opposite to that of the heat flux, meaning that irreversibility of nature and local ''instability'' of the numerical methods are in general not related.

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APPENDIX

Here we show how to evaluate the collision integrals. Consider, for example, the expression for Ξ given by Eq. (30). Using Eq. (25) and the linear properties of the integral we obtain

$$\begin{aligned}\Xi&=[\mathbf{C}_x^2,\mathbf{C}_x^2]-\frac{kT_{\parallel}^{(0)}}{m}[\mathbf{C}_x^2,1]-\frac{1}{c^2}[\mathbf{C}_x^2,\mathbf{c}_y^2]+\frac{kT_{\perp}^{(0)}}{c^2m}[\mathbf{C}_x^2,1]\\&=[\mathbf{C}_x^2,\mathbf{C}_x^2]-\frac{1}{c^2}[\mathbf{C}_x^2,\mathbf{c}_y^2]+\frac{1-c}{c}\frac{kT_{\parallel}^{(0)}}{m}[\mathbf{C}_x^2,1].\end{aligned}\tag{A1}$$

We now show how to evaluate $[\mathbf{C}_x^2,\mathbf{C}_x^2]$. For rigid spheres we have that $\Sigma(\chi,g)=\sigma^2/4$ [26], where σ is the rigid sphere diameter, then from Eqs. (1), (25), (26), and (27) we have

$$[\mathbf{C}_x^2,\mathbf{C}_x^2]=\frac{n^2\sigma^2}{32\pi^3}\left(\frac{kT_\perp^{(0)}}{m}\right)^{-2}\left(\frac{kT_\parallel^{(0)}}{m}\right)^{-1}\int d\mathbf{c}\,d\mathbf{c}_1 d\mathbf{e}\exp(-m\mathbf{C}_{1x}^2/2kT_\parallel^{(0)})\exp[-m(\mathbf{C}_{1\perp}^2)/2kT_\perp^{(0)}]\exp(-m\mathbf{C}_x^2/2kT_\parallel^{(0)})$$
$$\times\exp[-m(\mathbf{C}_\perp^2)/2kT_\perp^{(0)}]g\mathbf{C}_x^2\left\{\exp\left[-\frac{m}{2k}\left(\frac{1}{T_\parallel^{(0)}}-\frac{1}{T_\perp^{(0)}}\right)\right](\mathbf{C}_{1x}'^2+\mathbf{C}_x'^2)-(\mathbf{C}_{1x}^2+\mathbf{C}_x^2)\right\}. \quad (A2)$$

In terms of the center of mass and relative coordinates given by

$$\mathbf{C}=\mathbf{G}-\mathbf{g}/2,\quad \mathbf{C}'=\mathbf{G}-\mathbf{g}'/2,\ \ \mathbf{C}_1=\mathbf{G}+\mathbf{g}/2,\quad \mathbf{C}_1'=\mathbf{G}+\mathbf{g}'/2, \quad (A3)$$

Eq. (A2) can be written as

$$[\mathbf{C}_x^2,\mathbf{C}_x^2]=\Omega\int d\tau(\mathbf{G}_x-\mathbf{g}_x/2)^2 g\left\{\exp\left[-\frac{m}{4k}\left(\frac{1}{T_\parallel^{(0)}}-\frac{1}{T_\perp^{(0)}}\right)[\mathbf{g}_x'^2-\mathbf{g}_x^2]\right][(\mathbf{G}_x+\mathbf{g}_x'/2)^2+(\mathbf{G}_x-\mathbf{g}_x'/2)^2]-(\mathbf{G}_x+\mathbf{g}_x/2)^2$$
$$-(\mathbf{G}_x-\mathbf{g}_x/2)^2\right\}, \quad (A4)$$

where $d\tau$ and Ω have been introduced for simplicity; they are given by

$$d\tau\equiv\exp(-m\mathbf{G}_x^2/kT_\parallel^{(0)})\exp[-m(\mathbf{G}_y^2+\mathbf{G}_y^2)/kT_\perp^{(0)}]$$
$$\times\exp(-m\mathbf{g}_x^2/4kT_\parallel^{(0)})$$
$$\times\exp[-m(\mathbf{g}_y^2+\mathbf{g}_y^2)/4kT_\perp^{(0)}]d\mathbf{G}d\mathbf{g}d\mathbf{e},$$
$$\Omega\equiv\frac{n^2\sigma^2}{32\pi^3}\left(\frac{kT_\perp^{(0)}}{m}\right)^2\left(\frac{kT_\parallel^{(0)}}{m}\right). \quad (A5)$$

It is convenient to evaluate separately the two integrals I_1 and I_2 defined as

$$I_1\equiv\Omega\int d\tau\,(\mathbf{G}_x-\mathbf{g}_x/2)^2\ g\ \exp\left[-\frac{m}{4k}\left(\frac{1}{T_\parallel^{(0)}}-\frac{1}{T_\perp^{(0)}}\right)\right.$$
$$\left.\times[\mathbf{g}_x'^2-\mathbf{g}_x^2]\right]\ [(\mathbf{G}_x+\mathbf{g}_x'/2)^2+(\mathbf{G}_x-\mathbf{g}_x'/2)^2], \quad (A6)$$

$$I_2\equiv\Omega\int d\tau\,(\mathbf{G}_x-\mathbf{g}_x/2)^2 g[(\mathbf{G}_x+\mathbf{g}_x/2)^2+(\mathbf{G}_x-\mathbf{g}_x/2)^2]. \quad (A7)$$

Note that $[\mathbf{C}_x^2,\mathbf{C}_x^2]=I_1-I_2$.

To evaluate I_2, note that integration over $d\mathbf{e}$ gives 4π since the integrand does not depend on the dispersion angles, furthermore in the integration over $\mathbf{G}_x$ only the even parts in $\mathbf{G}_x$ need to be considered and the resulting integrals can readily be done since they are Gaussian, so we have

$$I_2=4\pi\Omega\pi\left(\frac{kT_\perp^{(0)}}{m}\right)\int d\mathbf{g}\ \exp(-m\mathbf{g}_x^2/4kT_\parallel^{(0)})$$
$$\times\exp[-m(\mathbf{g}_y^2+\mathbf{g}_y^2)/4kT_\perp^{(0)}]\ g\left[\frac{3\sqrt{\pi}}{2}\left(\frac{kT_\parallel^{(0)}}{m}\right)^{5/2}\right.$$
$$\left.+\frac{\sqrt{\pi}}{2}\left(\frac{kT_\parallel^{(0)}}{m}\right)^{3/2}\mathbf{g}_x^2+\frac{\sqrt{\pi}}{8}\left(\frac{kT_\parallel^{(0)}}{m}\right)^{1/2}\mathbf{g}_x^4\right]. \quad (A8)$$

In terms of cylindrical coordinates given by $\mathbf{g}_y=\mathbf{g}_\perp\cos(\theta)$, $\mathbf{g}_z=\mathbf{g}_\perp\ \sin(\theta)$, and $\mathbf{g}_x$, the integration over θ can readily be done to obtain

$$I_2=8\pi^{7/2}\Omega\left(\frac{kT_\perp^{(0)}}{m}\right)\left(\frac{kT_\parallel^{(0)}}{m}\right)^{1/2}\int_{-\infty}^{\infty}d\mathbf{g}_x\int_0^\infty d\mathbf{g}_\perp\,\mathbf{g}_\perp$$
$$\times\exp(-m\mathbf{g}_x^2/4kT_\parallel^{(0)})\exp(-m\mathbf{g}_\perp^2/4kT_\perp^{(0)})$$
$$\times g\left[\frac{3}{2}\left(\frac{kT_\parallel^{(0)}}{m}\right)^2+\frac{1}{2}\left(\frac{kT_\parallel^{(0)}}{m}\right)\mathbf{g}_x^2+\frac{1}{8}\mathbf{g}_x^4\right]. \quad (A9)$$

Using the change of variables given by $u_x=m\mathbf{g}_x^2/4kT_\parallel^{(0)}$ and $u_y=m\mathbf{g}_\perp^2/4kT_\perp^{(0)}$, we obtain for I_2

$$I_2=128\pi^{7/2}\Omega\left(\frac{kT_\perp^{(0)}}{m}\right)^2\left(\frac{kT_\parallel^{(0)}}{m}\right)^{3/2}\int_{-\infty}^{\infty}du_x\int_0^\infty du_y\ u_y$$
$$\times\exp(-u_x^2-u_y^2)\ (u_x^2+cu_y^2)^{1/2}$$
$$\times\left[\frac{3}{2}\left(\frac{kT_\parallel^{(0)}}{m}\right)^2+2\left(\frac{kT_\parallel^{(0)}}{m}\right)^2u_x^2+2\left(\frac{kT_\parallel^{(0)}}{m}\right)^2u_x^2\right]. \quad (A10)$$

Using polar coordinates, $u_x=r\ \cos(\theta)$ and $u_y=r\ \sin(\theta)$, we obtain

$$I_2=128\pi^{7/2}\Omega\left(\frac{kT_\perp^{(0)}}{m}\right)^2\left(\frac{kT_\parallel^{(0)}}{m}\right)^{7/2}\int_0^\infty dr\ r\int_0^\pi d\theta r^2\sin(\theta)$$
$$\times[\cos^2(\theta)+c\ \sin^2(\theta)]^{1/2}\exp(-r^2)$$
$$\times[3/2+2r^2\cos^2(\theta)+2r^4\cos^4(\theta)]. \quad (A11)$$

The integration over the radial coordinate can readily be done to obtain

$$I_2=128\pi^{7/2}\Omega\left(\frac{kT_\perp^{(0)}}{m}\right)^2\left(\frac{kT_\parallel^{(0)}}{m}\right)^{7/2}\times\left[\frac{35}{4}F(1,c)-14F(3,c)+6F(5,c)\right], \quad (A12)$$

where $F(n,c)$ is defined as

$$F(n,c)=\int_0^\pi d\theta\,\sin^n(\theta)\,[\cos^2(\theta)+c\,\sin^2(\theta)]^{1/2}. \quad (A13)$$

$F(n,c)$ can be obtained from tables of integrals [30] or computer algebra, their explicit form is

$$F(1,c)=1+\frac{c}{2\sqrt{1-c}}\ln\left[\frac{1+\sqrt{1-c}}{1-\sqrt{1-c}}\right],$$

$$F(3,c)=\frac{3-4c}{4(1-c)}+\frac{c}{2\sqrt{1-c}}\ln\left[\frac{1+\sqrt{1-c}}{1-\sqrt{1-c}}\right]+\frac{c^2}{8(1-c)^{3/2}}\ln\left[\frac{1+\sqrt{1-c}}{1-\sqrt{1-c}}\right],$$

$$F(5,c)=\frac{15c^2-26c+8}{24(1-c)^2}+\frac{c}{2\sqrt{1-c}}\ln\left[\frac{1+\sqrt{1-c}}{1-\sqrt{1-c}}\right]+\frac{c^2}{4(1-c)^{3/2}}\ln\left[\frac{1+\sqrt{1-c}}{1-\sqrt{1-c}}\right]+\frac{c^3}{16(1-c)^{5/2}}\ln\left[\frac{1+\sqrt{1-c}}{1-\sqrt{1-c}}\right]. \quad (A14)$$

The limiting case of equal temperatures $(c=1)$ [see Eq. (A13)] gives $F(1,1)=2$, $F(3,1)=4/3$, and $F(5,1)=16/15$. Using Eqs. (A12) and (A5) we obtain that I_2 for $c=1$ is given by

$$I_2\big|_{c=1}=\frac{314}{15}n^2\sigma^2\sqrt{\pi}\left(\frac{kT}{m}\right)^{5/2}. \quad (A15)$$

Let us now evaluate I_1, which from Eqs. (A7) and (A5) is given by

$$I_1=\Omega\int d\mathbf{G}\,d\mathbf{g}\,d\mathbf{e}\exp(-m\mathbf{G}_x^2/kT_\parallel^{(0)})\exp[-m(\mathbf{G}_y^2+\mathbf{G}_z^2)/kT_\perp^{(0)}]\exp(-m\mathbf{g}^2/4kT_\perp^{(0)})(\mathbf{G}_x-\mathbf{g}_x/2)^2g\times\exp\left[-\frac{m}{4k}\left(\frac{1}{T_\parallel^{(0)}}-\frac{1}{T_\perp^{(0)}}\right)\mathbf{g}_x'^2\right][(\mathbf{G}_x+\mathbf{g}_x'/2)^2+(\mathbf{G}_x-\mathbf{g}_x'/2)^2]. \quad (A16)$$

The integration over the center of mass coordinates can be done to obtain

$$I_1=\Omega\left(\frac{kT_\perp^{(0)}}{m}\right)\pi\int d\mathbf{g}\,d\mathbf{e}\,\exp(-m\mathbf{g}^2/4kT_\perp^{(0)})\exp\left[\frac{m}{4k}\left(\frac{1}{T_\parallel^{(0)}}-\frac{1}{T_\perp^{(0)}}\right)\mathbf{g}_x'^2\right]g\left[\frac{3\sqrt{\pi}}{2}\left(\frac{kT_\parallel^{(0)}}{m}\right)^{5/2}+\frac{\sqrt{\pi}}{4}\left(\frac{kT_\parallel^{(0)}}{m}\right)^{3/2}\mathbf{g}_x'^2+\frac{\sqrt{\pi}}{4}\left(\frac{kT_\parallel^{(0)}}{m}\right)^{3/2}\mathbf{g}_x^2+\frac{\sqrt{\pi}}{8}\left(\frac{kT_\parallel^{(0)}}{m}\right)^{1/2}\mathbf{g}_x'^2\mathbf{g}_x^2\right]. \quad (A17)$$

To evaluate the integration over the solid angle $d\mathbf{e}$, we first give some useful results. If $\mathbf{g}$ and $\mathbf{g}'$ are the relative velocities before and after the collision, then with the dispersion angles ξ and ϵ we have, using spherical coordinates for $\mathbf{g}$ $(\theta,\phi$ and $g)$, that:

$$\mathbf{g}_x'=g\,\cos(\theta)\cos(\phi)\sin(\xi)\cos(\epsilon)-g\,\sin(\phi)\sin(\xi)\sin(\epsilon)+g\cos(\phi)\cos(\xi)\sin(\theta),$$

$$\mathbf{g}_y'=g\,\cos(\theta)\sin(\phi)\sin(\xi)\cos(\epsilon)+g\cos(\phi)\sin(\xi)\sin(\epsilon)+g\sin(\theta)\sin(\phi)\cos(\xi), \quad (A18)$$

$$\mathbf{g}_z'=g\,\cos(\theta)\cos(\xi)-g\sin(\theta)\sin(\xi)\cos(\epsilon).$$

Note that $\mathbf{g}\cdot\mathbf{g}'=g^2\cos(\xi)$ and $\|\mathbf{g}\|=\|\mathbf{g}'\|$, as expected. Using computer algebra we inferred by induction that for any natural number n we have

$$\int d\mathbf{e}\,\mathbf{g}_x'^{2n}=\int_0^\pi\sin(\xi)\,d\xi\int_0^{2\pi}d\epsilon\,\mathbf{g}_x'^{2n}=\frac{4\pi}{(2n+1)}g^{2n}. \quad (A19)$$

This relation can be checked out more easily by taking $\mathbf{g}$ along the z axis, for the purpose of integrating over the solid angle, so that $\mathbf{g}_x'=g\,\sin(\xi)\cos(\epsilon)$, the resulting integrals can then be expressed in terms of β functions, which are well known [31].

If we go back to Eq. (A17) and make a series expansion of the second exponential that appears in it, interchanging the summation and the integral we are led to

$$I_1=\Omega\left(\frac{kT_\perp^{(0)}}{m}\right)\left(\frac{kT_\parallel^{(0)}}{m}\right)^{1/2}\pi^{3/2}\sum_{n=0}^{\infty}\frac{1}{n!}\left(\frac{m}{4kT_\parallel^{(0)}}\right)^n\left(\frac{1}{c}-1\right)^n\int d\mathbf{g}\; g\; \exp(-m\mathbf{g}^2/4kT_\perp^{(0)})$$
$$\times\int d\mathbf{e}\;\mathbf{g}_x'^{2n}\left[\frac{3}{2}\left(\frac{kT_\parallel^{(0)}}{m}\right)^2+\frac{1}{4}\left(\frac{kT_\parallel^{(0)}}{m}\right)^2\mathbf{g}_x'^2+\frac{1}{4}\left(\frac{kT_\parallel^{(0)}}{m}\right)\mathbf{g}_x^2+\frac{1}{8}\mathbf{g}_x'^2\mathbf{g}_x^2\right]. \tag{A20}$$

While 0^0 is not defined, we have used the convention $0^0=1$ in order to simplify the previous equation, so that we do not write explicitly the term corresponding to $n=0$. Using Eq. (A19) to carry out the integration over the solid angle in Eq. (A20) we obtain

$$I_1=4\Omega\left(\frac{kT_\perp^{(0)}}{m}\right)\left(\frac{kT_\parallel^{(0)}}{m}\right)^{1/2}\pi^{5/2}\sum_{n=0}^{\infty}\frac{1}{n!}\left(\frac{m}{4kT_\parallel^{(0)}}\right)^n\left(\frac{1}{c}-1\right)^n$$
$$\times\int d\mathbf{g}\; g\; \exp(-m\mathbf{g}^2/4kT_\perp^{(0)})\left[\frac{3}{2}\left(\frac{kT_\parallel^{(0)}}{m}\right)^2\frac{g^{2n}}{2n+1}+\frac{1}{4}\left(\frac{kT_\parallel^{(0)}}{m}\right)\frac{g^{2n+2}}{2n+3}+\frac{1}{4}\left(\frac{kT_\parallel^{(0)}}{m}\right)\frac{\mathbf{g}_x^2g^{2n}}{2n+1}+\frac{1}{8}\frac{\mathbf{g}_x^2g^{2n+2}}{2n+3}\right]. \tag{A21}$$

Using polar coordinates (g,θ,ϕ), the integration over the angles gives

$$I_1=16\Omega\left(\frac{kT_\perp^{(0)}}{m}\right)\left(\frac{kT_\parallel^{(0)}}{m}\right)^{1/2}\pi^{7/2}\sum_{n=0}^{\infty}\frac{1}{n!}\left(\frac{m}{4kT_\parallel^{(0)}}\right)^n\left(\frac{1}{c}-1\right)^n$$
$$\times\int_0^\infty dg\; g^3\exp(-m\mathbf{g}^2/4kT_\perp^{(0)})\left[\frac{3}{2}\left(\frac{kT_\parallel^{(0)}}{m}\right)^2\frac{g^{2n}}{2n+1}+\frac{1}{4}\left(\frac{kT_\parallel^{(0)}}{m}\right)\frac{g^{2n+2}}{2n+3}+\frac{1}{12}\left(\frac{kT_\parallel^{(0)}}{m}\right)\frac{g^{2n}}{2n+1}+\frac{1}{24}\frac{g^{2n+2}}{2n+3}\right]. \tag{A22}$$

Finally, the integration over g can be expressed in terms of Γ functions so that

$$I_1=16\Omega\left(\frac{kT_\perp^{(0)}}{m}\right)\left(\frac{kT_\parallel^{(0)}}{m}\right)^{1/2}\pi^{7/2}\sum_{n=0}^{\infty}\frac{1}{n!}\left(\frac{m}{4kT_\parallel^{(0)}}\right)^n\left(\frac{1}{c}-1\right)^n\left[\frac{3}{4}\left(\frac{kT_\parallel^{(0)}}{m}\right)^2\left(\frac{4kT_\perp^{(0)}}{m}\right)^{n+2}\frac{\Gamma(n+2)}{2n+1}+\frac{1}{8}\left(\frac{kT_\parallel^{(0)}}{m}\right)\right.$$
$$\left.\times\left(\frac{4kT_\perp^{(0)}}{m}\right)^{n+3}\frac{\Gamma(n+3)}{2n+3}+\frac{1}{24}\left(\frac{kT_\parallel^{(0)}}{m}\right)\left(\frac{4kT_\perp^{(0)}}{m}\right)^{n+3}\frac{\Gamma(n+3)}{2n+1}+\frac{1}{48}\left(\frac{4kT_\perp^{(0)}}{m}\right)^{n+4}\frac{\Gamma(n+4)}{2n+3}\right]. \tag{A23}$$

Equation (A23) can be written as

$$I_1=16\Omega\left(\frac{kT_\perp^{(0)}}{m}\right)^3\left(\frac{kT_\parallel^{(0)}}{m}\right)^{5/2}\pi^{7/2}\sum_{n=0}^{\infty}\frac{1}{n!}(1-c)^n\left[12\frac{\Gamma(n+2)}{2n+1}+8c\frac{\Gamma(n+3)}{2n+3}+\frac{8}{3}c\frac{\Gamma(n+3)}{2n+1}+\frac{16}{3}c^2\frac{\Gamma(n+4)}{2n+3}\right]. \tag{A24}$$

The limiting case of equal temperatures gives

$$I_1|_{c=1}=\frac{50}{3}n^2\sigma^2\sqrt{\pi}\left(\frac{kT^{(0)}}{m}\right)^{5/2}. \tag{A25}$$

All the other integrals were evaluated in the same way; to give the expression for them it is convenient to introduce the following definitions:

$$S_1=\sum_{n=1}^{\infty}\frac{(1-c)^n}{n!}\frac{\Gamma(n+2)}{(2n+1)},$$

$$S_2=\sum_{n=1}^{\infty}\frac{(1-c)^n}{n!}\frac{\Gamma(n+3)}{(2n+3)},$$

$$S_3=\sum_{n=1}^{\infty}\frac{(1-c)^n}{n!}\frac{\Gamma(n+3)}{(2n+1)},$$

$$S_4=\sum_{n=1}^{\infty}\frac{(1-c)^n}{n!}\frac{\Gamma(n+4)}{(2n+3)},$$

$$S_5=\sum_{n=1}^{\infty}\frac{(1-c)^n}{n!}\frac{\Gamma(n+3)}{(2n+1)(2n+3)},$$

$$S_6=\sum_{n=1}^{\infty}\frac{(1-c)^n}{n!}\frac{\Gamma(n+4)}{(2n+1)(2n+3)},$$

$$\eta_1=6S_1+4cS_2+\frac{4c}{3}S_3+\frac{8}{3}c^2S_4,$$

$$\eta_2=35F(1,c)-56F(3,c)+24F(5,c)-6c-\frac{16c^2}{3}-\frac{16c^3}{3},$$

$$\eta_3 = 2S_1 + 4S_5 + \frac{4c}{3}S_3 + \frac{8c}{3}S_6,$$

$$\eta_4 = 5cF(1,c) + 10cF(3,c) - 12cF(5,c) - (14/3 + 8c)c^2,$$

$$\eta_5 = 2cS_1 + \frac{4c^2}{3}S_3,$$

$$\eta_6 = 5F(1,c) - 4F(3,c) - 2c - 8c^2/3,$$

$$\lambda_1 = c(15S_1 + 18cS_2 + 6cS_3 + 12c^2S_4),$$

$$\lambda_2 = \frac{303}{2}F(1,c) - 252F(3,1) + 108F(5,c)$$

$$-c(15 + 24c + 24c^2),$$

$$\lambda_3 = 2c(3S_1 + 6S_5 + 2cS_3 + 4cS_6),$$

$$\lambda_4 = 15F(1,c) + 30F(3,c) - 36F(5,c) - 2c(7 + 12c),$$

$$\lambda_5 = c(6S_1 + 4cS_3),$$

$$\lambda_6 = 15F(1,c) - 12F(3,c) - c(6 + 8c). \qquad \text{(A26)}$$

Then the expressions for the reduced collision integrals given by Eqs. (34) and (35) are given by

$$\xi^\star = \eta_5 - \eta_6,$$

$$\Xi^\star = c\,\eta_1 - \eta_2 - \frac{1}{c^2}(c^2\eta_3 - \eta_4) + 2(\eta_5 - \eta_6)\frac{(1-c)}{c},$$

$$\Gamma_q^\star = \lambda_1 - \lambda_2 + \lambda_3 - \lambda_4 - 5\lambda_5 + 5\lambda_6. \qquad \text{(A27)}$$

The series S_i can be expressed in terms of hypergeometric series whose range of convergence is well known; this is why the the reduced collision integrals shown in Fig. 2 have been given for a restricted range of the temperature ratio c.

Using $F(1,1)=2$, $F(3,1)=4/3$, and $F(5,1)=16/15$, and noting that for $c=1$ all the series $S_i, i=1,\ldots,6$, are zero, we have from Eqs. (A26)

$$\eta_1 = 0, \quad \eta_2 = 64/15, \quad \eta_3 = 0, \quad \eta_4 = -32/15,$$

$$\eta_5 = 0, \quad \eta_6 = 0,$$

$$\lambda_1 = 0, \quad \lambda_2 = 96/5, \quad \lambda_3 = 0, \quad \lambda_4 = -32/5, \quad \lambda_5 = 0,$$

$$\lambda_6 = 0. \qquad \text{(A28)}$$

We finally conclude from Eqs. (A27) and (A26) that

$$\xi^\star\big|_{c=1} = 0, \quad \Xi^\star\big|_{c=1} = -32/5, \quad \Gamma_q^\star\big|_{c=1} = -64/5, \qquad \text{(A29)}$$

which are the values that reproduce the Chapman-Enskog expressions for the transport coefficients for equal temperatures.

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