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Physica A 225 (1996) 235–253

**PHYSICA** A

# Kinetic models for diffusion generated by an external force

C. Marín, J.M. Montanero, V. Garzó

*Departamento de Física, Universidad de Extremadura, E-06071 Badajoz, Spain*

Received 6 November 1995

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## Abstract

Two kinetic models are used to study the homogeneous color diffusion problem in a dilute binary mixture. Both kinetic models incorporate a temperature dependence in the collision frequencies, which allows for the consideration of a general repulsive molecular interaction. The main transport properties as well as the velocity distribution functions are explicitly obtained in terms of the field strength and the parameters characterizing the mixture. The results are illustrated for the two extreme cases of Maxwell molecules and hard spheres. A comparison between both models and with previous results derived from the Boltzmann equation for Maxwell molecules is carried out.

PACS: 51.10.+y; 05.20.Dd; 47.50.+d; 05.60.+w

Keywords: Dilute binary mixture; Kinetic models; Mutual diffusion; Nonlinear transport

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## 1. Introduction

One of the major shortcomings in dealing with the Boltzmann equation is the intricacy of its collision term. This problem has made the search for explicit solutions in general nonequilibrium situations a formidable hard task. As a consequence, simpler kinetic models have been proposed for the Boltzmann collision kernel that preserve the main physical properties, such as the conservation laws. For a single gas, the so-called Bhatnagar–Gross–Krook (BGK) [1] kinetic equation has been shown to be very useful in the past for evaluating transport properties in far from equilibrium states. Specifically, in the case of the uniform shear flow, the elements of the pressure tensor (which characterize the rheological properties of the gas) given by the BGK equation [2] coincide with those obtained from the Boltzmann equation for Maxwell molecules [3] when one chooses the BGK-collision frequency to be a given eigenvalue of the linearized Boltzmann collision operator. This fact shows the relevance of the BGK model for analyzing transport phenomena. Very recently, the exact fourth-degree moments [4] have

also been compared with the ones derived from the BGK model [5], showing a good agreement for not too large shear rates.

For multicomponent systems, several models constructed within the same spirit as the BGK equation have been proposed. Nevertheless, the scarcity of *exact* solutions of the Boltzmann equation for dilute gas mixtures has not allowed to test the range of validity of the above kinetic models. Perhaps, one of the simplest problems where nonlinear transport takes place in a mixture is the so-called “color” conductivity problem [6]. In this problem, mutual diffusion is induced in the system in a spatially homogeneous state by the action of a constant external force. Recently, an exact solution of the two Boltzmann coupled equations for a binary mixture of mechanically different particles subjected to a color field has been found [7]. Explicit expressions for the mass and momentum fluxes were obtained as functions of the color field and the parameters of the mixture, namely the mass ratio, the molar fractions, and the interaction constant ratio. This solution has two limitations: first, it is restricted to the particular case of Maxwell molecules, and second, since the solution is constructed by means of the moment method, explicit expressions for the velocity distribution functions are not known. These limitations can be overcome analytically by using tractable model kinetic equations.

The aim of this paper is to extend our previous solution [7] to general repulsive intermolecular forces by solving two different kinetic models. The reason for considering these two models is that one of them [8] seems to be more suitable for systems of like particles, while the other one [9] is presumably more adequate for disparate masses. Our motivation is twofold. On the one hand, we will examine the virtues of both models by carrying out a comparison with the exact results derived from the Boltzmann equations for Maxwell molecules. On the other hand, we want to assess to what extent the previous exact description for Maxwell molecules is indicative of what happens for general repulsive interactions. In particular, we are interested in evaluating the effect of the interaction potential on the main transport properties of the system.

The plan of the paper is as follows. In Section 2 we describe the color conductivity problem in a binary mixture and give a brief summary of the results derived from the Boltzmann equation for Maxwell molecules. Section 3 is concerned with the results obtained from kinetic models. We derive explicit expressions for the velocity moments and for the velocity distribution functions in terms of the color field, the parameters of the mixture and the interaction model considered. In the case of Maxwell molecules, both models give the same expressions for the color conductivity coefficient and the partial temperature as those obtained from the Boltzmann equation. Apart from these properties, both models lead to different results. In Section 4 we compare the results obtained from both models with the ones derived from the Boltzmann equation. In this comparison we also include recent simulation results [10] obtained for the velocity distribution function in the cases of Maxwell molecules and hard spheres. Finally, we close the paper in Section 5 with some concluding remarks.

## 2. Homogeneous color conductivity problem

Let us consider a binary mixture constituted by particles which are mechanically distinguishable. Particles of different species have a different “color charge”, so that both species can be distinguished even if they are mechanically equivalent. In the color conductivity problem, a constant external field is applied accelerating particles of each species along opposite directions [6]. The action of the color force  $F_r$  ( $r = 1, 2$ ) produces color diffusion in spite of the absence of concentration gradients. This force is given by

$$F_r = -k_B T \epsilon_r, \quad (1)$$

where  $k_B$  is the Boltzmann constant,  $T$  is the temperature of the mixture, and  $\epsilon_r = \epsilon_r \hat{x}$  is a constant vector that mimics the role played by  $\nabla \ln n_r$  in a typical diffusion problem. Since the color force does work on the system, an additional external force must be introduced to compensate for the increase of the temperature and so achieve a stationary state. The simplest choice, which may be derived from Gauss’ Principle of Least Constraint [11], is a drag force of the form  $-\alpha m_r v$ , where  $m_r$  is the mass of a particle of species  $r$  and  $\alpha$  is a thermostat parameter identical for both species. This quantity is determined as a function of the parameters of the problem by consistency. This kind of thermostat force is usually employed in nonequilibrium molecular dynamics simulation.

A complete description for the color conductivity problem can be given if one restricts oneself to a low-density binary mixture. In that case, the one-particle velocity distribution functions  $f_r$  provide all the information on the properties of the system. They obey the set of two coupled Boltzmann equations [12]. When a steady homogeneous state has been reached, the Boltzmann equations corresponding to the color problem read

$$-\frac{k_B T}{m_1} \epsilon_1 \cdot \frac{\partial}{\partial v} f_1 - \alpha \frac{\partial}{\partial v} \cdot (v f_1) = J_{11}[f_1, f_1] + J_{12}[f_1, f_2], \quad (2)$$

$$-\frac{k_B T}{m_2} \epsilon_2 \cdot \frac{\partial}{\partial v} f_2 - \alpha \frac{\partial}{\partial v} \cdot (v f_2) = J_{22}[f_2, f_2] + J_{21}[f_2, f_1], \quad (3)$$

where  $J_{rs}[f_r, f_s]$  is the Boltzmann collision operator. Conservation of total momentum (taken to be zero) and energy yields, respectively,

$$n_1 \epsilon_1 + n_2 \epsilon_2 = \mathbf{0}, \quad (4)$$

$$\alpha = -\frac{\rho}{3nm_1\rho_2} \epsilon_1 \cdot \mathbf{j}_1 = -\frac{\rho}{3nm_2\rho_1} \epsilon_2 \cdot \mathbf{j}_2, \quad (5)$$

where

$$n_r = \int dv f_r \quad (6)$$

is the number density of species  $r$ ,  $n = n_1 + n_2$  is the total number density,  $\rho = \rho_1 + \rho_2 = n_1 m_1 + n_2 m_2$  is the total mass density, and

$$\mathbf{j}_r \equiv \rho_r \mathbf{u}_r = \int d\mathbf{v} m_r \mathbf{v} f_r \quad (7)$$

is the mass flux of species  $r$ . Eq. (4) implies that the color forces acting on the two species are not independent, while Eq. (5) couples  $\alpha$  with the relevant fluxes of the problem. The mass flux  $\mathbf{j}_r$  defines the nonlinear color conductivity coefficient  $\sigma$  through the law

$$\mathbf{j}_r = -\frac{m_1 m_2 n}{\rho} \sigma n_r \boldsymbol{\epsilon}_r. \quad (8)$$

In general,  $\sigma$  is a function of the field strength  $\boldsymbol{\epsilon}$  and the parameters of the mixture. In accordance with the original spirit of the color field method, the color conductivity  $\sigma$  must reduce to the mutual diffusion coefficient  $D$  in the zero-field limit. This equivalence was the original motivation to introduce the color method in computer simulations. Furthermore, we define the pressure tensor of species  $r$ ,

$$P_r = \int d\mathbf{v} m_r (\mathbf{v} - \mathbf{u}_r) (\mathbf{v} - \mathbf{u}_r) f_r, \quad (9)$$

which measures the contribution of each species to the total momentum flux. It is also interesting to introduce a partial temperature  $T_r$  for species  $r$  through <sup>1</sup>

$$\frac{3}{2} n_r k_B T_r = \int d\mathbf{v} \frac{1}{2} m_r (\mathbf{v} - \mathbf{u}_r)^2 f_r, \quad (10)$$

which is related to the mean kinetic energy of each species. From these partial temperatures, the temperature of the mixture  $T$  (which is the relevant one at a hydrodynamic level) is

$$n k_B T = \sum_{r=1}^2 \left( n_r k_B T_r + \frac{1}{3} \rho_r u_r^2 \right). \quad (11)$$

A general solution, valid for arbitrary interaction potentials, to the set of Eqs. (2) and (3) can only be obtained from a perturbation expansion in powers of the field strength, although the corresponding expressions for the fluxes are generally not useful far from equilibrium. Nevertheless, the Boltzmann equations (2) and (3) can be *exactly* solved by the moment method if one considers the particular case of Maxwell molecules (particles interacting via the inverse fifth power force). For this interaction, the collision rate is independent of the relative velocity so that a moment of order  $k$  of the collision operator only involves moments of order less than or equal to  $k$ . As a consequence, all the velocity moments can be explicitly obtained *in principle* in a recursive way. In particular, explicit expressions for the mass and momentum fluxes for arbitrary values of the color field were derived in Ref. [7]. Writing the color conductivity coefficient in appropriate reduced units, this coefficient happens to be a nonlinear function independent of the parameters characterizing the mixture of the reduced field strength. This general

<sup>1</sup> Note that the definition of the partial temperature  $T_r$  given here differs from the one used in Ref. [7].

character disappears for higher-order moments, such as the temperature of each species or the pressure tensor. Although the recursive scheme could be followed if one knew the corresponding collisional moments, it would be a very difficult task to get higher-order moments.

The extension to other interaction models requires the use of simple kinetic equations or simulation techniques. Here, we adopt the first approach by considering two appropriate kinetic models. This will be the goal of the next section.

### 3. Kinetic models for the color conductivity problem

The complex structure of the Boltzmann equations has motivated the search of several kinetic models that, while being mathematically simpler, keep the main physical features of the Boltzmann equation. Constructed in the same spirit as the BGK model [1] for a single gas, the general idea is to replace the exact collision integrals  $J_{rs}\{f_r, f_s\}$  by simple relaxation terms of the form

$$J_{rs}\{f_r, f_s\} \longrightarrow -\nu_{rs}(f_r - f_{rs}), \tag{12}$$

where  $\nu_{rs}$  is a velocity-independent effective collision frequency verifying the general property  $n_r \nu_{rs} = n_s \nu_{sr}$ . The reference distribution function  $f_{rs}$  is determined by requiring that Eq. (12) preserves the relevant physical properties of  $J_{rs}$ . Its explicit form depends on the specific model considered.

In the context of the models of type (12), the kinetic equation (2) for  $f_1$  becomes

$$-\frac{k_B T}{m_1} \epsilon_1 \frac{\partial}{\partial v_x} f_1 - \alpha \frac{\partial}{\partial \mathbf{v}} \cdot (\mathbf{v} f_1) + \nu_1 f_1 = \Phi_1, \tag{13}$$

where  $\Phi_1 \equiv \nu_{11} f_{11} + \nu_{12} f_{12}$ , and  $\nu_1 = \nu_{11} + \nu_{12}$  is the total collision frequency for particles of species 1. In the following, we will focus on the transport properties of species 1. The properties of species 2 can be obtained by changing adequately the indices. In order to get information about the transport properties, let us introduce the dimensionless velocity moments  $M_{k_1, k_2, k_3}$  as

$$M_{k_1, k_2, k_3} = \frac{1}{n_1} \left( \frac{m_1}{2k_B T} \right)^{k/2} \int d\mathbf{v} v_x^{k_1} v_y^{k_2} v_z^{k_3} f_1, \tag{14}$$

$k \equiv k_1 + k_2 + k_3$  being the degree of  $M_{k_1, k_2, k_3}$ . Taking velocity moments in Eq. (13), one gets

$$\left( k_B T / 2m_1 \right)^{1/2} \epsilon_1 k_1 M_{k_1-1, k_2, k_3} + (\nu_1 + \alpha k) M_{k_1, k_2, k_3} = N_{k_1, k_2, k_3}, \tag{15}$$

where

$$N_{k_1, k_2, k_3} = \frac{1}{n_1} \left( \frac{m_1}{2k_B T} \right)^{k/2} \int d\mathbf{v} v_x^{k_1} v_y^{k_2} v_z^{k_3} \Phi_1 \tag{16}$$

is a known function of  $\epsilon_1$  and the parameters of the mixture. The solution of Eq. (15) can be cast into the form

$$M_{k_1, k_2, k_3} = \sum_{q=0}^{k_1} \left( \frac{k_B T}{2m_1} \right)^{q/2} \frac{k_1!}{(k_1 - q)!} \frac{(-\epsilon_1)^q}{\prod_{p=0}^q [\nu_1 + \alpha(k - p)]} N_{k_1 - q, k_2, k_3}. \tag{17}$$

Eq. (17) provides all the physical information about the partial contribution to the total transport properties due to species 1. This expression is general since it is not restricted to any specific form of  $\Phi_1$ . In order to get the explicit dependence of  $M_{k_1, k_2, k_3}$  on the field strength and the parameters of the system, particular forms of  $\Phi_1$  must be considered.

The general description of the color conductivity problem requires the knowledge of the velocity distribution functions. While in the case of the Boltzmann equation information about the distribution functions is obtained only indirectly through the knowledge of a finite number of moments, the use of the simplified collision term (12) allows one to explicitly get  $f_1$ . In the steady state, a formal solution to Eq. (13) compatible with the moments (17) can be written as

$$f_1(\nu) = \left[ \nu_1 - 3\alpha - \frac{k_B T}{m_1} \epsilon_1 \frac{\partial}{\partial \nu_x} - \alpha \nu \cdot \frac{\partial}{\partial \nu} \right]^{-1} \Phi_1(\nu) \\ = \int_0^\infty ds e^{-(\nu_1 - 3\alpha)s} \exp \left( \frac{k_B T}{m_1} \epsilon_1 s \frac{\partial}{\partial \nu_x} + \alpha s \nu \cdot \frac{\partial}{\partial \nu} \right) \Phi_1(\nu). \tag{18}$$

The explicit expression for  $f_1$  can be obtained when one takes into account the action of the exponential operator (see the appendix) in Eq. (18),

$$\exp \left( \frac{k_B T}{m_1} \epsilon_1 s \frac{\partial}{\partial \nu_x} + \alpha s \nu \cdot \frac{\partial}{\partial \nu} \right) \Phi_1(\nu_x, \nu_y, \nu_z) \\ = \Phi_1 \left( e^{\alpha s} (\nu_x - \lambda \frac{k_B T}{m_1} \epsilon_1 s) + \frac{k_B T}{m_1} \epsilon_1 s, e^{\alpha s} \nu_y, e^{\alpha s} \nu_z \right), \tag{19}$$

where

$$\lambda = e^{-\alpha s} \left( 1 + \frac{1}{\alpha s} \right) - \frac{1}{\alpha s}. \tag{20}$$

By substituting Eq. (19) into Eq. (18), one derives the corresponding expression for  $f_1$  in terms of the parameters of the problem.

As stated above, so far the results are general. In order to get the explicit dependence on  $\epsilon_1$ , particular forms for  $\nu_{rs}$  and  $f_{rs}$  must be considered. Here, we will take two well-known choices.

### 3.1. Results from the Gross-Krook (GK) model

In the GK model, the reference function  $f_{rs}$  is defined as [9]

$$f_{rs} = n_r \left( \frac{m_r}{2\pi k_B T_{rs}} \right)^{3/2} \exp \left( -\frac{m_r}{2k_B T_{rs}} (\mathbf{v} - \mathbf{u}_{rs})^2 \right). \quad (21)$$

The quantities  $\mathbf{u}_{rs}$  and  $T_{rs}$  are defined by imposing that the total momentum and energy are conserved and that the first five collisional moments as computed with Eqs. (12) and (21) be the same as those computed with the exact  $J_{rs}[f_r, f_s]$ . Since the last requirement can only be exactly evaluated for Maxwell molecules, one may introduce approximate forms for the above collisional moments in the case of non-Maxwell molecules and hence derive the corresponding expressions for  $\mathbf{u}_{rs}$  and  $T_{rs}$ . Therefore, for molecules interacting via a repulsive force law  $\mathcal{F}_{rs} = \kappa_{rs} r^{-\gamma} \hat{\mathbf{r}}$  ( $\gamma = 5, \dots, \infty$ ), it can be proved that  $\mathbf{u}_{rs}$  and  $T_{rs}$  have the same expressions as those obtained in the conventional GK model for Maxwell molecules ( $\gamma = 5$ ), i.e. [9],

$$\mathbf{u}_{rs} = \frac{m_r \mathbf{u}_r + m_s \mathbf{u}_s}{m_r + m_s}, \quad (22)$$

$$T_{rs} = T_r + 2 \frac{m_r m_s}{(m_r + m_s)^2} \left[ (T_s - T_r) + \frac{m_s}{6k_B} (\mathbf{u}_r - \mathbf{u}_s)^2 \right], \quad (23)$$

but  $\nu_{rs}$  is identified as

$$\nu_{rs} = A(\beta) n_s \left( \kappa_{rs} \frac{m_r + m_s}{m_r m_s} \right)^{(1-\beta)/2} \left( \frac{2k_B T_r}{m_r} + \frac{2k_B T_s}{m_s} \right)^{\beta/2}. \quad (24)$$

Here,  $\beta \equiv (\gamma - 5)/(\gamma - 1)$  and  $A(\beta)$  is a constant for a given interparticle potential that is tabulated in Ref. [12]. The kinetic model defined by Eqs. (21)–(24) can be seen as an extension of the conventional GK model to inverse power laws. Recently, this model has been used to study tracer diffusion under shear flow [13].

Once  $\Phi_1$  has been defined, one may evaluate the integral (16) and obtain the velocity moments (17) of the GK model. The only nonvanishing moments correspond to even values of  $k_2$  and  $k_3$ , in which case one gets

$$\begin{aligned} M_{k_1, k_2, k_3} &= \pi^{-3/2} \sum_{\substack{q=0 \\ k_1+q+\ell=\text{even}}}^{k_1} \sum_{\ell=0}^{k_1-q} \left( \frac{k_B T}{2m_1} \right)^{q/2} \\ &\times \frac{k_1!}{(k_1 - q - \ell)!} \Gamma \left( \frac{k_1 - q - \ell + 1}{2} \right) \Gamma \left( \frac{k_2 + 1}{2} \right) \Gamma \left( \frac{k_3 + 1}{2} \right) \\ &\times \frac{(-\epsilon_1)^q}{\prod_{p=0}^q [\nu_1 + \alpha(k - p)]} \left[ \nu_{11} \chi_1^{(k-q)/2} \left( \frac{m_1 u_1^2}{2k_B T_1} \right)^{\ell/2} \right. \\ &\left. + \nu_{12} \chi_{12}^{(k-q)/2} \left( \frac{m_1 u_{12}^2}{2k_B T_{12}} \right)^{\ell/2} \right], \quad (25) \end{aligned}$$

where  $\chi_1 \equiv T_1/T$  and  $\chi_{12} \equiv T_{12}/T$ . Note that the expression (25) is not closed since  $M_{k_1, k_2, k_3}$  is given in terms of the first nontrivial moments of  $f_1$ , namely  $j_1$  and  $T_1$ . These moments can be consistently determined from the requirements

$$M_{100} = n_1 u_1 \quad (26)$$

and

$$M_{200} + M_{020} + M_{002} = 3 \frac{n_1 k_B T_1}{m_1} + n_1 u_1^2. \quad (27)$$

Nevertheless, as the collision frequencies are nonlinear functions of the partial temperatures, the corresponding equations for  $j_r$  and  $T_r$  must be solved in general numerically.

In order to study the nonlinear transport properties of the system, it is convenient to introduce dimensionless quantities. To parallel the results derived from the Boltzmann equation [7], we introduce the reduced field strength

$$\epsilon^* \equiv \left( \frac{2}{3} \frac{k_B T m_1 m_2}{\tau^2 \rho n} \frac{n_1}{n_2} \right)^{1/2} \epsilon_1, \quad (28)$$

where

$$\tau \equiv A(\beta) \kappa_{12}^{(1-\beta)/2} \left( \frac{m_1 m_2}{m_1 + m_2} \right)^{1/2} (2k_B T)^{\beta/2}. \quad (29)$$

In terms of these units, it is a matter of algebra to write the right-hand side of (25) in dimensionless form. In particular, in the zero-field limit,  $\sigma \equiv D = (k_B T / \tau n)$ ,  $D$  being the mutual diffusion coefficient of a binary mixture with general repulsive intermolecular forces [12].

Despite the general mathematical complexity of Eq. (25), there is a particular interaction model for which the conditions (26) and (27) for  $j_1$  and  $T_1$  reduce to simple linear algebraic equations. This corresponds to Maxwell molecules ( $\beta = 0$ ), for which  $\nu_{rs}$  is a constant independent of  $T_r$  and  $T_s$ . In this case, the reduced color conductivity coefficient  $\sigma^* = \sigma / D$  can be written as

$$\sigma^*(\epsilon^*) = \epsilon^{*-2} [(1 + 2\epsilon^{*2})^{1/2} - 1]. \quad (30)$$

This expression is the same as the one derived from the exact Boltzmann equation [7]. In terms of  $\epsilon^*$ ,  $\sigma^*$  adopts a general form, independent of the parameters of the mixture. From the knowledge of  $\sigma^*$ , the reduced partial temperature  $\chi_1$  can be obtained. In the same way as  $\sigma^*$ , its expression is identical to that of the Boltzmann equation [7], i.e.,

$$\chi_1 = (1 + \delta) \frac{4\mu\delta + 2(1 + \mu)\sigma^*\epsilon^{*2} - 2\mu\sigma^{*2}\epsilon^{*2} - (1 + \mu)\sigma^{*3}\epsilon^{*4}}{4\mu\delta(1 + \delta) + 2(1 + \mu)\delta(1 + \mu\delta)\sigma^*\epsilon^{*2}}, \quad (31)$$

where  $\mu \equiv m_1/m_2$  is the mass ratio and  $\delta \equiv n_1/n_2$  is the concentration ratio. Eq. (31) clearly shows that  $\chi_1$  is a function of  $\epsilon^*$  that depends on  $\mu$  and  $\delta$  although it is independent of the force constant ratio. In terms of  $\sigma^*$  and  $\chi_1$ , higher-order moments can be easily obtained from Eq. (25), their expressions being different from those obtained with the Boltzmann equation.

When  $\beta \neq 0$ ,  $\sigma^*$  and  $\chi_1$  cannot be ascertained analytically except in some limiting cases. Thus, for small field strengths one gets

$$\sigma^* \approx 1 - \left[ \beta \frac{\delta^3 \mu^3 - \delta^2 \mu(2\mu + 1) - \delta \mu(\mu + 2) + 1}{4\delta \mu(\delta + 1)(\mu + 1)} + \frac{1}{2} \right] \epsilon^{*2}, \quad (32)$$

$$\chi_1 \approx 1 - \left[ \frac{1}{2\delta\mu} - \frac{(1 + \mu)(1 + \mu\delta)}{2\mu(1 + \delta)} \right] \epsilon^{*2}, \tag{33}$$

whereas for large field strengths,

$$\sigma^* \approx \sqrt{2} |\epsilon^*|^{-1}, \tag{34}$$

$$\chi_1 \approx \frac{2}{\sqrt{2}} (1 + \delta) \frac{1 + \mu(1 + \delta)}{\delta(1 + \mu)(1 + \mu\delta)} |\epsilon^*|^{-1}. \tag{35}$$

This means that in the limit of  $\epsilon^*$  going to infinity,  $\langle v \rangle^2 = \langle v^2 \rangle$  for each species, so that the velocity distribution functions become  $\delta$ -distributions. This conclusion was already obtained in the case of the Maxwell interaction [7]. The fact that  $j_1$  and  $T_1$  reach the same saturation values for all the interaction models is not surprising, since in the limit of very large fields the system behaves as a collisionless gas. With respect to the behavior for small values of  $\epsilon^*$ , Eq. (32) indicates that  $\sigma^*$  is not a universal function of  $\epsilon^*$ , while Eq. (33) shows that the dependence of  $\chi_1$  on  $\beta$  appears beyond the “Burnett” approximation (second order in  $\epsilon^*$ ). Furthermore, Eqs. (32) and (33) also show that  $\sigma^*$  and  $\chi_1$  do not present a monotonic behavior. Only in the case of Maxwell molecules,  $\sigma^*$  always decreases as  $\epsilon^*$  increases. For  $\beta \neq 0$ , there exist combinations of  $\mu$  and  $\delta$  for which  $\sigma^*$  increases with the field strength, reaches a maximum, and then decreases. This behavior agrees qualitatively with recent molecular dynamics simulations [6,14].

Let us now determine the velocity distribution function  $f_1(v)$ . Its explicit form can be directly obtained from the general expressions (18)–(20). In order to write  $f_1$  in a compact form, we introduce the effective collision frequency  $\zeta \equiv [(m_1 + m_2)/m_1 m_2] n \tau$  and we define the dimensionless quantities  $\nu_1^* \equiv \nu_1/\zeta$ ,  $\nu_{11}^* \equiv \nu_{11}/\zeta$ ,  $\nu_{12}^* \equiv \nu_{12}/\zeta$ , and  $\alpha^* \equiv \alpha/\zeta$ . Henceforth, we will omit the asterisks of these quantities. In addition, we also introduce the reduced velocity  $\xi \equiv (2k_B T/m_1)^{1/2} v$ . Thus, in terms of these quantities, the velocity distribution function  $f_1(v)$  can be written as

$$f_1(v) = n_1 \left( \frac{m_1}{2k_B T} \right)^{3/2} \Psi_1(\xi), \tag{36}$$

where the reduced distribution  $\Psi_1(\xi)$  is a function of the field strength  $\epsilon^*$  and the parameters of the mixture, namely, the mass ratio  $\mu$ , the concentration ratio  $\delta$ , the force constant ratio  $\kappa_{11}/\kappa_{12}$  and the interaction parameter  $\beta$ . Its expression is

$$\begin{aligned} \Psi_1(\xi) = \pi^{-3/2} \int_0^\infty ds e^{-(\nu_1 - 3\alpha)s} \left\{ \nu_{11} \chi_1^{-3/2} \exp \left[ -\chi_1^{-1} (\tilde{\xi} - \tilde{u}_1)^2 \right] \right. \\ \left. + \nu_{12} \chi_{12}^{-3/2} \exp \left[ -\chi_{12}^{-1} (\tilde{\xi} - \tilde{u}_{12})^2 \right] \right\}, \end{aligned} \tag{37}$$

where we have introduced the quantities

$$\tilde{\xi}_i \equiv e^{\alpha s} \xi_i - \frac{\theta \epsilon^*}{\alpha} (1 - e^{\alpha s}) \delta_{ix}, \tag{38}$$

$$\theta \equiv \frac{1}{2} (1 + \mu)^{-1} \left[ 3 \frac{1 + \mu\delta}{\delta(1 + \delta)} \right]^{1/2}, \tag{39}$$

$$\tilde{u}_1 \equiv -\frac{1}{2} \left[ 3 \frac{1 + \delta}{\delta(1 + \mu\delta)} \right]^{1/2} \sigma^* \epsilon^*, \tag{40}$$

$$\tilde{u}_{12} \equiv \frac{\mu}{1 + \mu} (1 - \delta) \tilde{u}_1. \tag{41}$$

Eq. (37) gives the explicit expression for the velocity distribution function of species 1 representing the solution to the GK model for molecules interacting through general repulsive forces and subjected to an external color field. This function presents a highly nonlinear dependence on the field strength as well as the parameters of the mixture. For non-Maxwell molecules, the dependence on  $\epsilon^*$  appears even through the collision frequencies  $\nu_{11}$  and  $\nu_{12}$ .

### 3.2. Results from the Garzó–Santos–Brey (GSB) model

Although the GK model has been widely used in the past, especially in the case of disparate-mass mixtures, it has the following shortcoming: when one considers the case of mechanically equivalent particles ( $m_1 = m_2, \kappa_{11} = \kappa_{22} = \kappa_{12}$ ),  $f = f_1 + f_2$  does not obey a closed equation (BGK model), in contrast to what happens with the exact Boltzmann equation. This is due to the highly nonlinear character of  $f_{rs}$  in Eq. (21). The above drawback is not relevant as long as disparate masses are considered. In order to avoid this problem, Garzó, Santos and Brey (GSB) [8] proposed a model of type (12) but now  $f_{rs}$  is given by

$$f_{rs} = n_r \left( \frac{m_r}{2\pi k_B T} \right)^{3/2} \exp \left( -\frac{mv^2}{2k_B T} \right) [1 + A_{rs} + \mathbf{B}_{rs} \cdot \mathbf{v} + C_{rs} v^2], \tag{42}$$

with

$$A_{rs} = -3(k_B T/m_r) C_{rs}, \tag{43}$$

$$\mathbf{B}_{rs} = (m_r/k_B T) \mathbf{u}_{rs}, \tag{44}$$

$$C_{rs} = \frac{m_r}{2k_B T} \left( \frac{T_{rs} - T}{T} + \frac{m_r}{3k_B T} u_{rs}^2 \right), \tag{45}$$

where  $\mathbf{u}_{rs}$  and  $T_{rs}$  are defined by Eqs. (22) and (23) and we have assumed that the flow velocity of the mixture is zero. Furthermore, and according to the spirit of the GSB model, the collision frequencies  $\nu_{rs}$  depend on the temperature of the mixture  $T$  instead of the partial temperature  $T_r$ , i.e.,

$$\nu_{rs} = A(\beta) n_s \kappa_{rs}^{(1-\beta)/2} [(m_r + m_s)/m_r m_s]^{1/2} (2k_B T)^{\beta/2}. \tag{46}$$

Although the GSB model is not restricted to any range of mass ratio, the collision term defined through Eq. (42) suggests that it is more suitable for systems of like particles. In this sense, the GK and GSB models can complement each other in the analysis of transport phenomena in mixtures where no restriction on the mass ratio is considered. The GSB model has been recently used to analyze from a kinetic theory point of view the problem of gas flows condensing on a plane condensed phase [15].

According to Eq. (46),  $\nu_{rs}$  is a constant in the color conductivity problem. Consequently, the results derived from the GSB model are the same for all the interaction models when one takes the appropriate reduced units defined in Eqs. (28) and (29). Thus, from Eqs. (42)–(45) it is straightforward to show that the velocity moments are now given by

$$M_{k_1, k_2, k_3} = \pi^{-3/2} \sum_{q=0}^{k_1} \left( \frac{k_B T}{2m_1} \right)^{q/2} \frac{k_1!}{(k_1 - q)!} \frac{(-\epsilon_1)^q}{\Pi_{p=0}^q [\nu_1 + \alpha(k - p)]} \times (\nu_{11} N_{k_1 - q, k_2, k_3}^{(11)} + \nu_{12} N_{k_1 - q, k_2, k_3}^{(12)}), \tag{47}$$

where

$$N_{k_1, k_2, k_3}^{(rs)} = K_{k_2} K_{k_3} \left[ K_{k_1} + 2K_{k_1+1} \left( \frac{m_r}{2k_B T} \right)^{1/2} u_{rs} + \frac{k}{2} K_{k_1} \left( \frac{T_{rs} - T}{T} + \frac{m_r}{3k_B T} u_{rs}^2 \right) \right], \tag{48}$$

and  $K_n = \Gamma(n)$  if  $n = \text{odd}$ , being zero otherwise. In contrast to what happens in the GK model, now all the moments can be obtained analytically. In particular, it is easy to see that the expressions of  $\sigma^*$  and  $\chi_1$  are identical to those given by the GK model and the Boltzmann equation in the case of Maxwell molecules. Beyond these moments, both kinetic models predict different results. These discrepancies will be analyzed in the next section along with a comparison with Boltzmann results.

Finally, the velocity distribution can be obtained in a similar way as in the GK model. After some algebra, the reduced distribution  $\Psi_1(\xi)$  is given by

$$\Psi_1(\xi) = \pi^{-3/2} \int_0^\infty ds e^{-(\nu_1 - 3\alpha)s} \left\{ \nu_{11} \left[ 1 + 2\tilde{\xi}_x \tilde{u}_1 + \left( \tilde{\xi}^2 - \frac{3}{2} \right) \left( \chi_1 - 1 + \frac{2}{3} \tilde{u}_1^2 \right) \right] + \nu_{12} \left[ 1 + 2\tilde{\xi}_x \tilde{u}_{12} + \left( \tilde{\xi}^2 - \frac{3}{2} \right) \left( \chi_{12} - 1 + \frac{2}{3} \tilde{u}_{12}^2 \right) \right] \right\} e^{-\xi^2}, \tag{49}$$

where all the quantities and notation are as previously defined.

#### 4. Comparison between the Boltzmann and kinetic model equations for the color conductivity problem

The explicit results derived in the above section allows one to carry out a detailed comparison with the corresponding transport properties given by the Boltzmann equation. We focus our attention on the reduced color conductivity coefficient  $\sigma^*$  (which is the most relevant transport coefficient of the problem), the partial temperature ratio  $\chi_1 = T_1/T$ , the reduced normal element of the pressure tensor  $P_{1,yy}^* \equiv P_{1,yy}/n_1 k_B T$ , and the distribution function. In order to illustrate the main features we have concentrated on the two extreme cases of Maxwell molecules ( $\beta = 0$ ) and hard spheres ( $\beta = 1$ ).

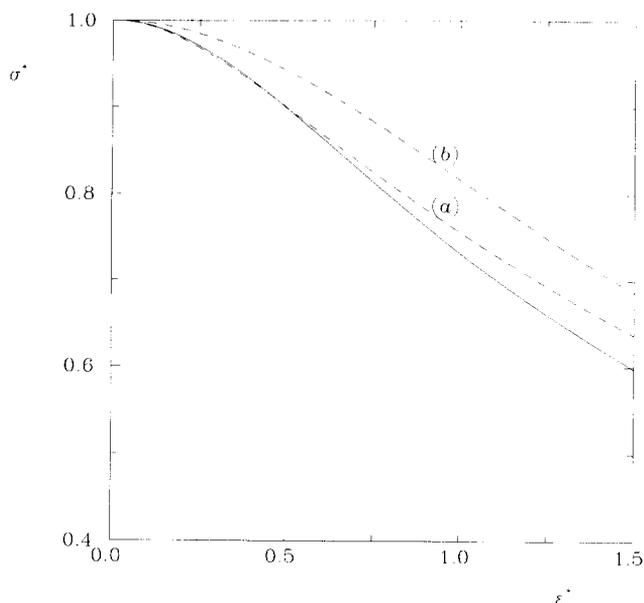


Fig. 1. Plot of the reduced color conductivity coefficient  $\sigma^*(\epsilon^*)$  for the concentration ratio  $\delta = 2$  and for two values of the mass ratio: (a)  $\mu = 2$ , (b)  $\mu = 0.5$ . The solid line corresponds to Maxwell molecules and the dashed lines refer to hard spheres.

Fig. 1 shows  $\sigma^*$  as a function of  $\epsilon^*$  for  $\delta = 2$  and several values of  $\mu$ . In the case of Maxwell molecules, the exact expression of  $\sigma^*$  coincides with the one given by both kinetic models. This coefficient is a function of the reduced field strength that is independent of the parameters of the mixture. This independence disappears when one considers other interaction potentials in the case of the GK model, while in the GSB model  $\sigma^*(\epsilon^*)$  is universal, i.e., independent of the potential law. As clearly seen in this figure, the general dependence of  $\sigma^*$  on the color field predicted by the GK model is not greatly affected by the power of the repulsive law. The effect of the potential model becomes more noticeable as  $\epsilon^*$  increases, specially when the particles of the excess species are lighter than the particles of the defect species. In addition, for a given value of  $\epsilon^*$ ,  $\sigma^*$  increases as  $\beta$  increases.

The partial temperature ratio  $\chi_1$  is plotted in Fig. 2 for the same values as in the previous figure. As happened with  $\sigma^*$ , both kinetic models give the same expression of  $\chi_1$  as the one derived from the Boltzmann equation for Maxwell molecules. In general,  $\chi_1$  is not a monotonic function of the field strength although for the cases considered here it decreases as  $\epsilon^*$  increases. With respect to the influence of the interaction potential, we observe again that it is more significant, for a concentration ratio larger (smaller) than 1, when the mass ratio is smaller (larger) than 1. In the region of small field strengths,  $\chi_1$  is practically the same for both potentials, while it decreases with increasing  $\beta$  as the field strength increases. Anyway, and according to the behavior given by (32) and (33), the effect of the potential on the temperature ratio is less significant than for the color conductivity coefficient.

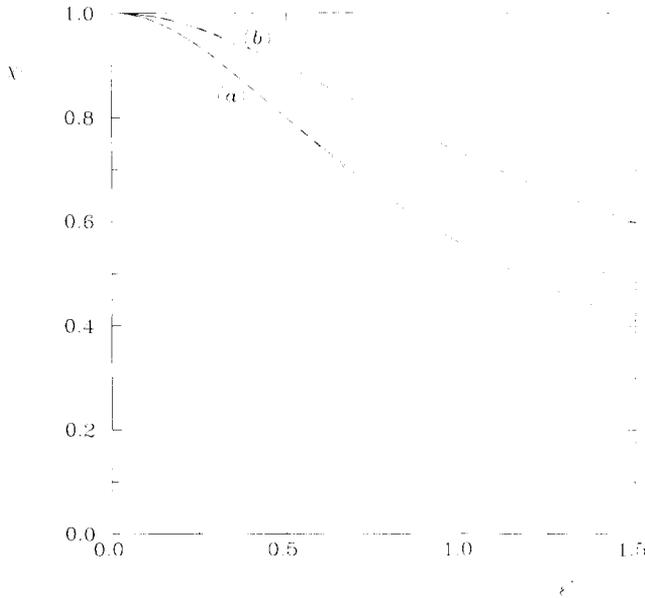


Fig. 2. Plot of the reduced partial temperature  $\chi_1 = T_1/T$  as a function of  $\epsilon^*$  for  $\delta = 2$  and for two values of the mass ratio: (a)  $\mu = 2$ , (b)  $\mu = 0.5$ . The solid lines refer to Maxwell molecules and the dashed lines refer to hard spheres.

The first velocity moment that is different in both models, even in the particular case of Maxwell molecules, is the pressure tensor. Its expression also differs from the exact one. In Fig. 3 we plot  $P_{1,yy}^*$  for  $\delta = 2$  and  $\mu = 2$ . Since  $P_{1,yy}^*$  depends on the force constant ratio, for simplicity we have chosen here  $\kappa_{11} = \kappa_{22} = \kappa_{12}$ . In the case of Maxwell molecules, the deviation from equilibrium is slightly overestimated by the GK model and slightly underestimated by the GSB model. For not too large field strengths, the predictions of both models are reasonably good although the discrepancies increase as  $\epsilon^*$  increases. For instance, for  $\epsilon^* \approx 1.5$  (where the color conductivity coefficient is about twice smaller than its zero-field value) and for the case considered in the figure, the relative difference between the GK model and the Boltzmann value is around 7% while it is around 6.7% in the GSB model. These conclusions can be qualitatively extended to other choices of  $\delta$  and  $\mu$ . We also observe that, in general,  $P_{1,yy}^*$  monotonically decreases as the field strength increases whatever the interaction model considered is. However, at a given value of the concentration ratio, there may be mass ratios for which  $P_{1,yy}^*$  has a maximum in the region of small field strengths. Concerning the potential model considered, we note that the inhibition of the momentum transport along an orthogonal direction to the external field decreases as the intermolecular repulsion becomes softer. According to the comparison made for  $\sigma^*$ ,  $\chi_1$ , and  $P_{1,yy}^*$ , one can conclude in summary that both kinetic models can be seen as good approximations to the first moments of the Boltzmann equation in the color conductivity problem.

Let us now investigate whether the above conclusion can be extended to the velocity distribution function. Since no explicit expression for this quantity is known in the

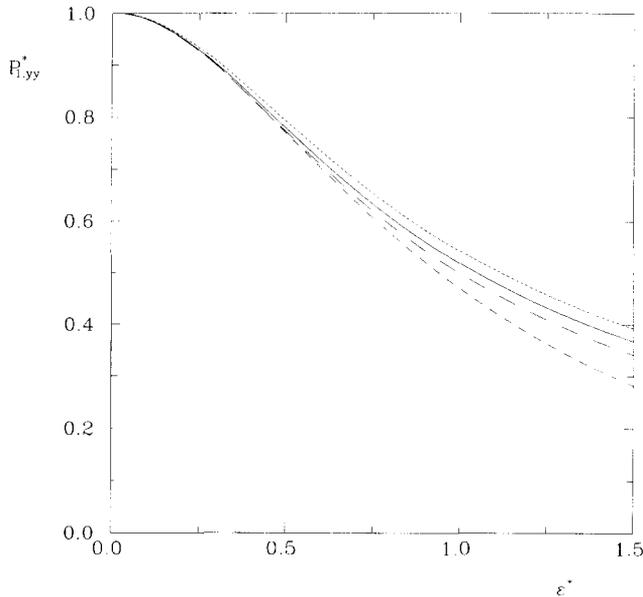


Fig. 3. Plot of  $P_{l,yy}^*$  for  $\delta = 2$  and  $\mu = 2$ . The curves are: Boltzmann equation for Maxwell molecules (—); GK equation for Maxwell molecules (— —); GK equation for hard spheres (- - -); and GSB equation (· · · ·).

context of the Boltzmann equation, we have considered convenient to numerically solve that equation [10] by using the direct simulation Monte Carlo method [16]. This method has been shown to be an important tool to study transport phenomena in rarefied gas dynamics. For the sake of illustration, we have introduced the reduced distribution

$$\varphi(\xi_x) = \pi^{1/2} e^{\xi_x^2} \int_{-\infty}^{+\infty} d\xi_y \int_{-\infty}^{+\infty} d\xi_z \Psi_1(\xi). \tag{50}$$

The behavior of  $\varphi(\xi_x)$  with  $\xi_x$  is plotted in Figs. 4 and 5 for  $\epsilon^* = 1$ ,  $\delta = 4$ ,  $\mu = 1/3$  and for Maxwell molecules and hard spheres, respectively. To compare the results obtained from Maxwell and hard spheres, the force constant ratios for the Maxwell interaction and the diameter ratios for hard spheres have been chosen to give the same equilibrium collision frequencies. In general, a distortion from local equilibrium ( $\varphi(\xi_x) = 1$ ) is clearly observed in both interaction models. In the case of Maxwell molecules, we see that the GK and GSB distributions reproduce satisfactorily the general behavior of the Boltzmann distribution (obtained from the simulation). However, it is evident that there exist important discrepancies in the region of high velocities and near the maximum, specially in the GK model. In particular, we note that the distributions of both models predict well the location of the maximum although not its value. In the case of hard spheres, we observe that the GK distribution describes now much better the behavior of the Boltzmann distribution. In fact, the discrepancies with the simulation data are smaller than the ones given in the case of Maxwell molecules. The comparison between

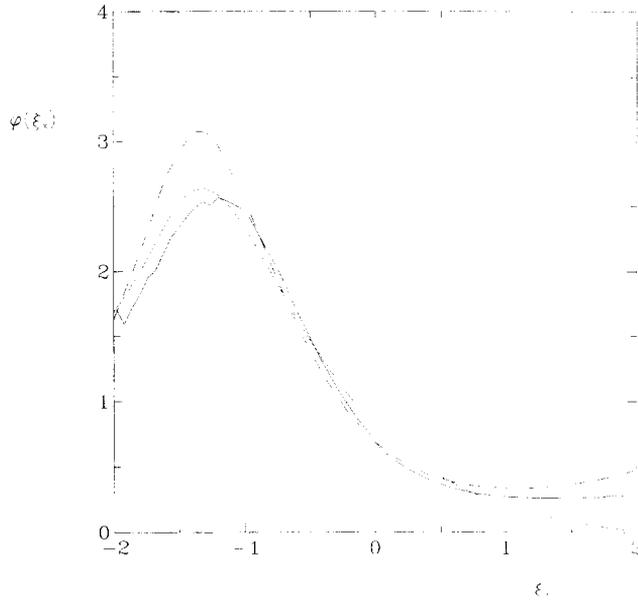


Fig. 4. Reduced distribution function  $\varphi(\xi_x)$  for  $\delta = 4$ ,  $\mu = 1/3$ ,  $\kappa_{12}/\kappa_{11} = 16$ ,  $\kappa_{22}/\kappa_{11} = 81/16$  and  $\epsilon^* = 1$  in the case of Maxwell molecules, as obtained from simulation results (—), the GK model (---) and the GSB model (.....).

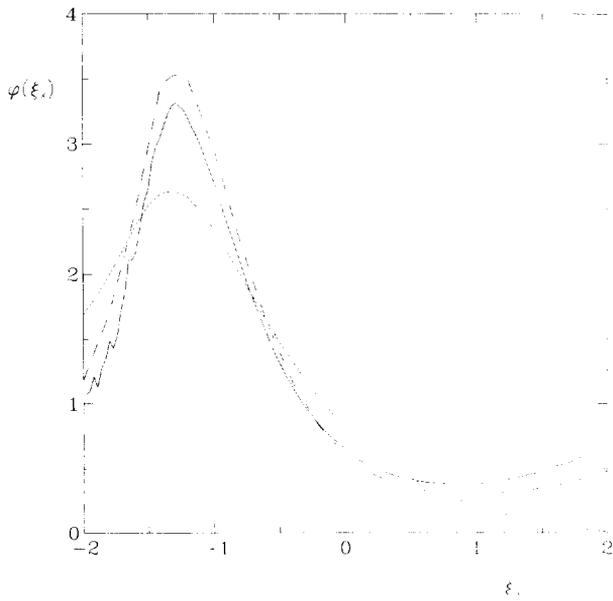


Fig. 5. The same as in Fig. 4, but for hard spheres.

the Boltzmann results for Maxwell molecules and hard spheres clearly shows that the velocity distribution function seems to be rather sensitive to the interaction potential in a far from equilibrium situation. This influence is approximately well predicted by the complicated collision term of the GK model but not by the (universal) GSB model.

## 5. Concluding remarks

In this paper, we have addressed the color conductivity problem in a binary mixture of mechanically different particles in the low-density regime. The physical situation is such that the system is driven to a nonequilibrium homogeneous steady state by the action of an external “color” field. This field produces mutual diffusion in the absence of concentration gradients. The color conductivity coefficient is the main transport coefficient of the problem. It is defined as the ratio between the mass flux and the color field strength. Recently this problem has been studied in the particular case of Maxwell molecules, and explicit expressions for the mass and momentum fluxes have been derived [7]. These fluxes are nonlinear functions of the field strength and the parameters of the mixture. Here, we have extended our previous efforts by addressing the same problem for general repulsive intermolecular forces. Although the problem can be considered as a rather academic one, our results can be taken as a first step toward the understanding of nonlinear electrical conductivity in a coulombic system at low density.

Two different kinetic models (GK and GSB) have been used to get the main transport properties as well as the velocity distribution functions. In these models, the details of the interaction potential are incorporated through effective collision frequencies  $\nu_{rs}$ . In the GK model [9]  $\nu_{rs}$  depends on the temperatures of each species  $T_r$  and  $T_s$ , while  $\nu_{rs}$  is a function of the temperature of the mixture  $T$  in the GSB model [8]. Since in the color problem a drag force maintains the temperature  $T$  constant, the results derived from the GSB model are the same for all the interaction potentials. In addition, the GSB model gives analytical expressions, while the predictions of the GK model are obtained numerically. Starting from both models, we have computed the velocity moments as well as the velocity distribution functions of each species. In the particular case of Maxwell molecules, we find that, in terms of a convenient reduced field strength, the expressions of the reduced color conductivity coefficient  $\sigma^*$  and the reduced partial temperature  $\chi_r$  are the same as those obtained from the exact Boltzmann equation. This equivalence shows the degree of reliability of both models for computing transport properties in the color conductivity problem. For other properties, the results derived from both approximate models as well as from the Boltzmann equation are different, even in the particular case of Maxwell molecules. Nevertheless, the comparison carried out for the normal element of the pressure tensor shows that the approximate results agree quantitatively well (specially the GK model) with the exact ones when one considers not too large field strengths (say  $\epsilon^* < 0.5$ ). Concerning the influence of the potential model the results indicate that, in general, the effect of the power law on the transport properties is not very strong when one uses adequately scaled quantities. In addition,

the GK equation predicts that  $\sigma^*$  is neither a universal function of  $\epsilon^*$  nor a monotonic function of  $\epsilon^*$  when one considers non-Maxwell molecules. These conclusions contrast with the ones previously obtained from the Boltzmann equation for Maxwell molecules. Recent computer simulations [10] confirm the above predictions.

A much more difficult problem is to get the velocity distribution functions in far from equilibrium situations. In particular, no exact solution to the Boltzmann equation at this level is known in the color conductivity problem, even for Maxwell molecules. For this reason, and as a complementary information, we have solved numerically the Boltzmann equation by means of the direct simulation Monte Carlo method in the cases of Maxwell molecules and hard spheres [10]. The comparison between the simulation and kinetic models results shows that, for Maxwell molecules, the models (particularly the GSB) reproduce well the behavior of the actual distribution in the regime of thermal velocities (the latter being slightly better), but significant discrepancies appear in the regime of high velocities. This disagreement is not surprising since the behavior of the velocity distribution function in the kinetic models is governed by the first few moments, namely the mass flux and the partial temperature. In this sense, both models can be considered as good approximations for low-degree moments of the exact distribution function but fail for high-degree moments. This is consistent with the results derived from the BGK model for a single gas [5,17]. In the case of hard spheres, the comparison with the GK solution indicates a good general agreement. Furthermore, the simulation data for both interaction models also show that the velocity distribution function is clearly affected by the interaction considered.

The knowledge of exact solutions to the Boltzmann equation, such as the one derived in Ref. [7], are important not only as means to understand the physical mechanisms involved in nonequilibrium situations but as tests of approximation methods. In this context, the GSB model as well as the GK model can be seen as good approximations of the Boltzmann equation at the level of transport properties. This agreement confirms the usefulness of the kinetic models since the complicated structure of the Boltzmann collision operator (which takes into account the large amount of detail of the two-body interactions) can be replaced by simple relaxation terms which retain the qualitative and average properties of the true collision operator. This replacement is expected to be reliable for the low-degree velocity moments (related to the transport properties), although it becomes less reliable as the degree of the moments increases (as the comparison for the velocity distribution function suggests). Therefore, we expect that the results presented in this paper will stimulate the use of kinetic models as an alternative tool to analyze transport properties in binary mixtures. Finally, and as happens in other nonequilibrium states [17,18], it is interesting to remark that the nonlinear transport coefficients are hardly sensitive to the interaction potential so that the general conclusions obtained from the exact Boltzmann equation for Maxwell molecules can be extended to other interaction potentials.

## Acknowledgements

We are grateful to Andrés Santos and Mariano López the Haro for suggestions for the improvement of the manuscript. This research has been partially supported by the Dirección General de Investigación Científica y Técnica (Spain) through grant no. PB94-1021 and by the Junta de Extremadura (Fondo Social Europeo) through Grant no. EIA94-39. The research of C. M. and J. M. M. has been supported by the Ministerio de Educación y Ciencia (Spain) through predoctoral fellowships.

## Appendix A

Let us consider the operators  $A \equiv av_x \partial / \partial v_x$  and  $B \equiv b \partial / \partial v_x$ , where  $a$  and  $b$  are constants. The commutator  $[A, B] \equiv AB - BA$  is given by

$$[A, B] = ab \left( v_x \frac{\partial^2}{\partial v_x^2} - \frac{\partial}{\partial v_x} v_x \frac{\partial}{\partial v_x} \right) = -ab \frac{\partial}{\partial v_x} \equiv -aB. \quad (\text{A.1})$$

Our goal is to evaluate the action of the operator  $e^{A+B}$  on a given function  $g(v_x)$ . To this end, we define the function

$$F(\gamma) = e^{\gamma A} e^{\gamma B} e^{-\gamma(A+B)}. \quad (\text{A.2})$$

By derivating with respect to  $\gamma$ , one gets

$$\frac{dF(\gamma)}{d\gamma} = e^{\gamma A} [A, e^{\gamma B}] e^{-\gamma(A+B)}. \quad (\text{A.3})$$

In order to integrate Eq. (A.3), we will use the following two well-known properties [19]:

(i) If  $B$  commutes with  $[A, B]$ , then

$$[A, B^n] = nB^{n-1}[A, B]. \quad (\text{A.4})$$

(ii) If the operators  $A$  and  $B$  satisfy the condition  $[A, B] = \alpha B$ ,  $\alpha$  being a constant, then

$$e^A B e^{-A} = e^\alpha B. \quad (\text{A.5})$$

Therefore, by taking into account (A.4), one has

$$[A, e^{\gamma B}] = \sum_{n=0}^{\infty} \frac{\gamma^n}{n!} [A, B^n] = \gamma \sum_{n=0}^{\infty} \frac{\gamma^n}{n!} B^n [A, B] = -\gamma a B e^{\gamma B}, \quad (\text{A.6})$$

so that

$$\begin{aligned} \frac{dF(\gamma)}{d\gamma} &= -\gamma a e^{\gamma A} B e^{-\gamma A} F(\gamma) \\ &= -\gamma a e^{-\gamma a} B F(\gamma), \end{aligned} \quad (\text{A.7})$$

where in the last step use has been made of the identity (A.5). Integration of Eq. (A.7) yields

$$F(\gamma) = \exp \left[ e^{-\gamma a} \left( \gamma + \frac{1}{a} \right) B - \frac{B}{a} \right], \quad (\text{A.8})$$

where we have taken into account that  $F(0) = 1$ . By setting  $\gamma = 1$ , one finally gets

$$\begin{aligned} e^{A+B} g(v_x) &= e^{-\lambda B} e^A e^B g(v_x) \\ &= g[e^a(v_x - \lambda b) + b], \end{aligned} \quad (\text{A.9})$$

where

$$\lambda \equiv e^{-a} \left( 1 + \frac{1}{a} \right) - \frac{1}{a} \quad (\text{A.10})$$

and we have used the identities

$$\exp \left( b \frac{\partial}{\partial v_x} \right) g(v_x) = g(v_x + b), \quad (\text{A.11})$$

$$\exp \left( a v_x \frac{\partial}{\partial v_x} \right) g(v_x) = g(e^a v_x). \quad (\text{A.12})$$

Eq. (19) can be easily obtained from the relation (A.9).

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