ELSEVIER

Physica A 265 (1999) 508–519

PHYSICA A

Electrical current density in a sheared dilute gas

Concepción Marín[a], Vicente Garzó[b,*]

[a] *Departamento de Matemáticas, Universidad de Extremadura, E-06071 Badajoz, Spain*
[b] *Departamento de Física, Universidad de Extremadura, E-06071 Badajoz, Spain*

Received 4 June 1998

Abstract

Electrical current density of charged particles across a rarefied gas of neutral particles under shear flow is analyzed in the limit of small electric fields. The concentration of the charged species is assumed to be much smaller than that of the neutral species so that the interactions of charged–neutral and neutral–neutral type are the dominant ones. The study is made from the exact Boltzmann equation for Maxwell molecules as well as from a kinetic model for general repulsive interactions. By performing a perturbation expansion around a nonequilibrium state, the current density is explicitly evaluated in the first order of the external field. We get a generalized Ohm's law, where an electrical conductivity tensor can be identified. The nonzero elements of this tensor are nonlinear functions of the shear rate, the mass ratio, the force constant ratio, and the interaction parameter.

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

Keywords: Electrical conductivity; Uniform shear flow; Boltzmann equation; Nonlinear transport

1. Introduction

A problem of practical and physical interest is the analysis of transport properties of charged test particles immersed in a rarefied gas of neutral particles and subjected to a constant electric field $\boldsymbol{E}$. The system can be seen as a dilute binary mixture in which the concentration of the charged particles (labelled with the index 1) is much smaller than that of the neutral gas (labelled with the index 2). This implies that one can neglect the effect of collisions among the charged particles themselves on the state of the charged species. In addition, the state of the neutral gas is not disturbed by the presence of the charged particles. In these conditions (*tracer* limit), the interactions of type charged–neutral and neutral–neutral are the dominant ones in the mixture. This

* Corresponding author. Fax: +34-24-275428; e-mail: vicenteg@ba.unex.es.

0378-4371/99/$ – see front matter
PII: S0378-4371(98)00447-6

assumption simplifies enormously the problem since the long-range Coulomb interaction does not need to be considered in the description.

When the neutral gas is at equilibrium, Ohm's law establishes a linear relation between the electrical current density $\boldsymbol{j}_1$ and the electric field $\boldsymbol{E}$ through the electrical conductivity coefficient σ_0 : $\boldsymbol{j}_1 = \sigma_0 \boldsymbol{E}$. Ohm's law is expected to apply when the electric field is weak and the expression of the transport coefficient σ_0 can be obtained, for instance, from the Champman–Enskog method [1]. This situation has been widely studied in the past years in different contexts [2–7]. Nevertheless, much less is known when the rarefied neutral gas is far from equilibrium. This is due basically to the scarcity of exact solutions to the Boltzmann equation in inhomegeneous situations. One of the few exact solutions of the Boltzmann equation for a single gas corresponds to the so-called uniform shear flow, namely, a state macroscopically characterized by a linear velocity field and uniform temperature and density. In the case of Maxwell molecules (repulsive potential of the form r^{-4}), Ikenberry and Truesdell [8,9] derived explicit expressions for the rheological properties of the gas (non-Newtonian shear viscosity and viscometric effects) as functions of the (arbitrary) shear rate. Here, our aim is to get the current density induced by the action of a weak electric field when the background neutral gas is under uniform shear flow. In addition, neutral and charged particles are mechanically different.

According to the assumptions established in the tracer limit, one can avoid the Coulomb interaction and the kinetic equations describing the mixture reduce to a (closed) Boltzmann equation for the velocity distribution function of the neutral particles $f_2(\boldsymbol{r}, \boldsymbol{v}; t)$ plus a Boltzmann–Lorentz equation for the velocity distribution function $f_1(\boldsymbol{r}, \boldsymbol{v}; t)$ of the charged species. We also assume that the mixture is in a strongly shearing state so that the only nonzero gradient is $\partial u_x / \partial y = a = \text{const}$, $\boldsymbol{u}$ being the flow velocity of the mixture. We want to evaluate the influence of the shear rate on the diffusion of charged particles in the limit of small electric fields. In this case, one expects that Ohm's law still holds, but a conductivity tensor σ_{ij} instead of a scalar must be identified. The tensor σ_{ij} will be a nonlinear function of a and the parameters of the system, namely, the mass ratio and the force constant ratio. The derivation of an expression for the conductivity tensor is the main objective of this paper.

The Boltzmann–Lorentz equation of the charged particles is solved by carrying out a perturbative expansion in powers of the external field. The main peculiarity of this expansion is that the reference state (zeroth-order approximation) is not the local equilibrium but a nonequilibrium state with arbitrary values of the shear rate. To first order in the field, an explicit expression for σ_{ij} is obtained. The derivation of such an expression is made from the *exact* Boltzmann equation in the particular case of Maxwell molecules, as well as from a kinetic model for general repulsive interactions. The results show that $\sigma_{xx} = \sigma_{yy} = \sigma_{zz}$ and that the only nonzero off-diagonal element is σ_{xy}. In general, the diagonal elements decrease as the shear rate increases while the off-diagonal element is negative and its magnitude increases with the shear rate.

The paper is organized as follows. In Section 2 we describe the problem and provide a brief account of uniform shear flow in the tracer limit. Section 3 is devoted to the calculation of the electrical conductivity tensor. First, we evaluate it for the Maxwell interaction in the context of the exact Boltzmann equation and then, in order to consider the effect of more general interactions, we get the same quantity by using a kinetic model that incorporates a temperature dependence of the collision frequencies. Finally, in Section 4 the results are discussed and compared with a previous work.

2. Description of the problem

We consider an ensemble of charged test particles (of mass m_1, charge q, and number density n_1) dispersed in a dilute gas of neutral particles (of mass m_2 and number density n_2). We suppose that $n_1 \ll n_2$, so that the interactions of charged–charged type can be neglected in the kinetic equation of f_1. Besides, the state of the neutral gas is not affected by the presence of the charged species. Consequently, only interactions of type 1–2 and 2–2 will be taken into account in the description. Let us assume that the mixture is under uniform shear flow, namely, a state characterized by

$$n_s = \text{const} \ (s = 1, 2) \ , \tag{1}$$

$$\nabla T_s = 0, \tag{2}$$

$$u_{s,i} = u_i = a_{ij} r_j, \quad a_{ij} = a\delta_{ix}\delta_{jy}, \tag{3}$$

where a is the constant shear rate. This parameter measures the departure of the system from equilibrium. Besides, we have introduced the number density n_s, the mean velocity $\boldsymbol{u}_s$, and the temperature T_s of species s defined as

$$\{n_s, n_s \boldsymbol{u}_s, n_s k_B T_s\} = \int d\boldsymbol{v} \{1, \boldsymbol{v}, \tfrac{1}{3} m_s (\boldsymbol{v} - \boldsymbol{u}_s)^2\} f_s \ . \tag{4}$$

The temperature of the mixture T is defined by the relation $nT = n_1 T_1 + n_2 T_2$, where $n = n_1 + n_2$ is the total number density. Shearing motion produces viscous heating and so the temperature increases in time. However, from a computational point of view, it is desirable to measure the rheological properties in a steady state. For this reason, it is usual in molecular dynamics simulations [10] to include an external (nonconservative) force to achieve a constant temperature. The simplest form is $\boldsymbol{F}_s = -m_s \alpha \boldsymbol{V}$, where $V_i = v_i - a_{ij} r_j$. The parameter α, which plays the role of a thermostat, is a function of the shear rate to be determined by consistency. In the case of Maxwell molecules, the presence of the thermostat does not play any role in the results, while a certain influence may exist for other interaction potentials [11–14].

We assume now that we perturb the steady shear flow state by introducing a uniform electric field $\boldsymbol{E}$. Under the geometry established in the shear flow problem, the set of

steady coupled Boltzmann equations becomes

$$-\frac{\partial}{\partial V_i}(a_{ij}V_j+\alpha V_i)f_2=J_{22}[f_2,f_2]\,, \tag{5}$$

$$-\frac{\partial}{\partial V_i}(a_{ij}V_j+\alpha V_i)f_1+\frac{q\boldsymbol{E}}{m_1}\cdot\frac{\partial}{\partial \boldsymbol{V}}f_1=J_{12}[f_1,f_2]\,, \tag{6}$$

where J_{rs} is the Boltzmann collision operator [1], which in standard notation reads

$$J_{rs}[f_r,f_s]=\int d\boldsymbol{v}_1\int d\boldsymbol{k}\,B(\boldsymbol{v}-\boldsymbol{v}_1,\hat{k})[f_r(\boldsymbol{v}')f_s(\boldsymbol{v}_1')-f_r(\boldsymbol{v})f_s(\boldsymbol{v}_1)]\,. \tag{7}$$

Upon writing Eqs. (5) and (6) we have taken into account that the uniform shear flow state becomes spatially homogeneous in the Lagrangian frame moving with the flow velocity $\boldsymbol{u}$. In this new frame, the distribution functions adopt the form $f_s(\boldsymbol{r},\boldsymbol{v})\equiv f_s(\boldsymbol{V})$. We are interested in deriving an expression for the current electrical density $\boldsymbol{j}_1$ when the system is under shear flow in the limit of small electric fields. The current density is defined as

$$\boldsymbol{j}_1=q\int d\boldsymbol{v}\,\boldsymbol{V}f_1(\boldsymbol{V})\,. \tag{8}$$

Since the strength of the electric field $\boldsymbol{E}$ is weak, we will solve the Boltzmann–Lorentz equation (6) by means of a perturbative expansion in powers of $\boldsymbol{E}$. As said in the Introduction, and in contrast to the conventional Chapman–Enskog expansion [1], the reference state retains all the hydrodynamic orders in the shear rate. Therefore, we write $f_1=f_1^{(0)}+f_1^{(1)}+\cdots$, where $f_1^{(k)}$ is of order k in $\boldsymbol{E}$ but it is highly nonlinear in a. In this paper, we will restrict ourselves to the first order in the expansion. The zeroth-order approximation is concerned with a situation where $\boldsymbol{E}=\boldsymbol{0}$, so that the current vanishes. It is described by Eq. (5) and the zeroth-order of (6). This reference state has been widely studied by the authors in the past years from the exact Boltmann equations for Maxwell molecules (repulsive potential of the form $\Phi_{rs}=\kappa_{rs}r^{-4}$) [11,12] as well as from a generalization of the well-known Gross–Krook (GK) kinetic model for $r^{-\ell}$-repulsive interactions [13,14]. This kinetic model is defined in Appendix A. As seen later, in order to get the current density $\boldsymbol{j}_1^{(1)}$ we only need the knowledge of the shear-rate dependence of the thermostat parameter α. The explicit expressions of such a parameter as given from the Boltzmann and GK equations are also quoted in Appendix A.

3. Electrical current density under shear flow

Once the reference state is well characterized, the objective now is to study the effect of the shear flow on the diffusion of charged particles in terms of the shear rate a, the mass ratio $\mu=m_1/m_2$ and the force constant ratio $w=\kappa_{12}/\kappa_{22}$. The analysis will be made from the exact Boltzmann–Lorentz equation for Maxwell molecules and from the GK model for general repulsive interactions.

3.1. Current density from the Boltzmann equation

In the first order of the expansion, the Boltzmann–Lorentz equation (6) becomes

$$-\frac{\partial}{\partial V_i}(a_{ij}V_j+\alpha V_i)f_1^{(1)}+\frac{q\boldsymbol{E}}{m_1}\cdot\frac{\partial}{\partial \boldsymbol{V}}f_1^{(0)}=J_{12}[f_1^{(1)},f_2]\,. \tag{9}$$

At this order, the current electrical density is given by

$$\boldsymbol{j}_1^{(1)}=q\int d\boldsymbol{v}\,\boldsymbol{V}f_1^{(1)}\,. \tag{10}$$

This quantity can be obtained from Eq. (9) by multiplying it by $q\boldsymbol{V}$ and integrating over $\boldsymbol{V}$. Thus, one finds

$$a_{ik}j_{1,k}^{(1)}+\alpha j_{1,i}^{(1)}-\frac{n_1q^2}{m_1}E_i=-\frac{n_2\lambda_{12}}{m_1}j_{1,i}^{(1)}\,, \tag{11}$$

where

$$\lambda_{12}=1.69\pi\left[\kappa_{12}\frac{m_1m_2}{m_1+m_2}\right]^{1/2}\,, \tag{12}$$

and we have used the relation (which only holds for Maxwell molecules) [15,16]

$$\int d\boldsymbol{v}\,\boldsymbol{V}J_{12}[f_1^{(1)},f_2]=-\frac{n_2\lambda_{12}}{m_1q}\boldsymbol{j}_1^{(1)}\,. \tag{13}$$

The solution to Eq. (11) can be recast into the form of a generalized Ohm's law, i.e.,

$$j_{1,i}^{(1)}=\sigma_{ij}E_j\,, \tag{14}$$

where the electrical conductivity tensor is

$$\sigma_{ij}=\frac{n_1q^2}{m_1\tau}\frac{1}{1+\gamma\alpha^*}\left(\delta_{ij}-\gamma\frac{a_{ij}^*}{1+\gamma\alpha^*}\right) \tag{15}$$

with $\tau=n_2\lambda_{12}/m_1$, $a_{ij}^*=a_{ij}/\nu_{22}$, $\alpha^*=\alpha/\nu_{22}$, $\nu_{22}=1.85\pi n_2(\kappa_{22}/m_2)^{1/2}$, and

$$\gamma=\frac{\nu_{22}}{\tau}=1.095\left[\frac{\mu(1+\mu)}{w}\right]^{1/2}\,. \tag{16}$$

Eq. (15) describes the diffusion of charged test particles through a strongly shearing neutral gas in the limit of zero electric field. When $a=0$, $\sigma_{ij}=\sigma_0\delta_{ij}$, where $\sigma_0=n_1q^2/m_1\tau$ is the electrical conductivity coefficient, and one recovers usual Ohm's law [1]. The nonzero elements of σ_{ij} are $\sigma_{xx}=\sigma_{yy}=\sigma_{zz}$ and σ_{xy}. They are nonlinear functions of the shear rate, the mass ratio, and the force constant ratio. For small shear rates, they behave as $\sigma_{ii}/\sigma_0\approx 1-\frac{1}{3}\gamma a^{*2}$, and $\sigma_{xy}/\sigma_0\approx-\gamma a^*(1-\frac{2}{3}\gamma^2a^{*2})$. Since the diagonal elements couple the ith component of the current to the ith component of the field, they can be interpreted as a generalization of the conductivity coefficient σ_0 when the bath is far from equilibrium. The off-diagonal element σ_{xy} measures cross effects in the transport of charge since it gives the current along the x direction due to the component y of the electric field. It is negative and vanishes for zero shear rates. In Figs. 1 and 2, we plot the reduced elements σ_{ii}/σ_0 and $-\sigma_{xy}/\sigma_0$, respectively, as

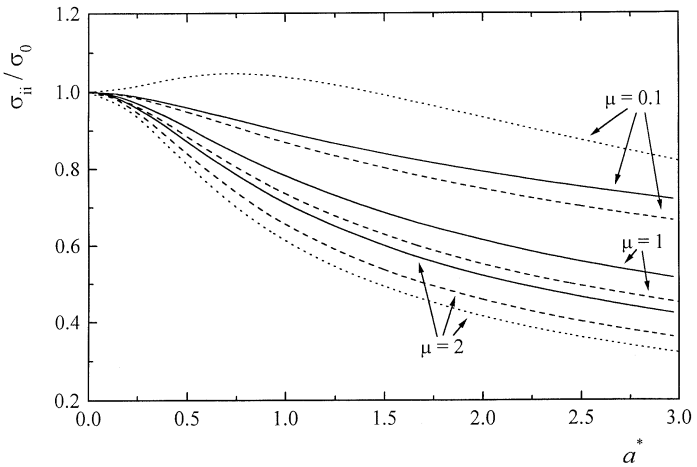

Fig. 1. Plot of the reduced diagonal element σ_{ii}/σ_0 versus the reduced shear rate a^* for several values of the mass ratio $\mu = m_1/m_2$. The force constants have been assumed to be of the form $\kappa_{rs} \propto (m_r m_s)^{1/2}$. The solid lines refer to Boltzmann results for Maxwell molecules while the dashed and dotted lines correspond to kinetic model results for Maxwell molecules and hard spheres, respectively.

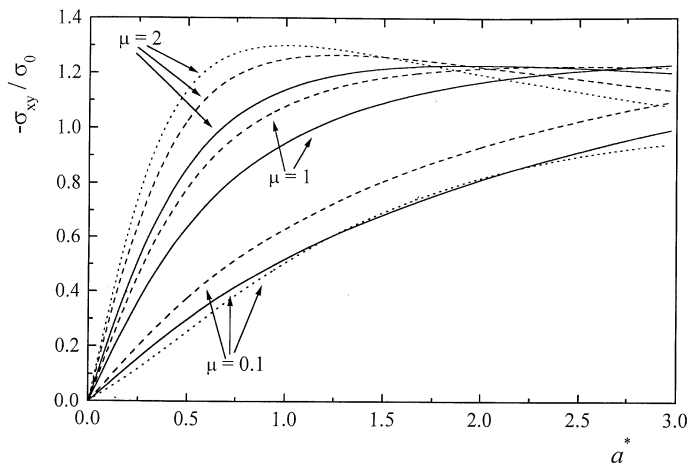

Fig. 2. The same as in Fig. 1 but for the reduced element $-\sigma_{xy}/\sigma_0$.

functions of the reduced shear rate a^* for several values of the mass ratio μ. In both figures, we have assumed that the force constants have a mass dependence of the form $\kappa_{rs} \propto (m_r m_s)^{1/2}$. Such a dependence has been proposed [17] to model the cross section observed in disparate-mass binary mixtures. In the case of the diagonal element, we observe that it decreases as the shear rate increases independently of the mass ratio considered. At a given value of a, the inhibition of σ_{ii} is more significant as the charged particles are heavier than the particles of the neutral gas. With respect to the off-diagonal element, and in the range of shear rates considered, we see that in

general its magnitude increases with the shear rate, although for $\mu > 1$ the opposite happens for large shear rates (say, for instance $a^* \approx 2$).

3.2. Current density from the GK equation

The results derived in the previous section cannot be seen as general, since a model of Maxwell molecules is somewhat limited. Nevertheless, if one wants to derive an explicit expression of the current density for non-Maxwell molecules, one needs to use a kinetic model. As described in Appendix A, here we will start from a generalization of the familiar GK model [18] that incorporates a temperature dependence in the collision frequencies. This allows for the consideration of a general repulsive $r^{-\ell}$-interaction. The reliability of this kinetic model has been assessed in several nonequilibrium problems [19,20] by comparison with exact analytical results [21] as well as with Monte Carlo simulations of the Boltzmann equation [22].

In the context of the GK model [see Eqs. (A.5)–(A.7)], the corresponding Boltzmann–Lorentz equation (9) becomes

$$-\frac{\partial}{\partial V_i}(a_{ij}V_j+\alpha V_i)f_1^{(1)}+\frac{q\boldsymbol{E}}{m_1}\cdot\frac{\partial}{\partial \boldsymbol{V}}f_1^{(0)}=-\nu_{12}(f_1^{(1)}-f_{12}^{(1)})\,, \tag{17}$$

where

$$f_{12}^{(1)}=\frac{m_1}{q}\frac{\mu}{1+\mu}\frac{\boldsymbol{V}\cdot\boldsymbol{j}_1^{(1)}}{n_1k_BT_{12}}f_{12}^{(0)} \tag{18}$$

and

$$f_{12}^{(0)}=n_1\left(\frac{m_1}{2\pi k_BT_{12}}\right)^{3/2}\exp\left(-\frac{m_1}{2k_BT_{12}}V^2\right)\,. \tag{19}$$

Let us introduce the dimensionless moments corresponding to the first-order distribution $f_1^{(1)}$ as

$$M_{k,\ell,m}^{(1)}=\frac{1}{n_1}\left(\frac{2k_BT_2}{m_1}\right)^{-1/2(k+\ell+m)}\int d\boldsymbol{v}\,V_x^kV_y^\ell V_z^m f_1^{(1)}\,. \tag{20}$$

Taking velocity moments in Eq. (17) one gets the hierarchy

$$\delta a^*k\,M_{k-1,\ell+1,m}^{(1)}+[1+\delta\alpha^*(k+\ell+m)]M_{k,\ell,m}^{(1)}=R_{k,\ell,m}\,, \tag{21}$$

where $a^*=a/\nu_{22}$, $\alpha^*=\alpha/\nu_{22}$,

$$\delta=w^{(\eta-1)/2}\left(\frac{2\mu}{1+\mu}\right)^{1/2}\left(\frac{1+\mu}{\mu+\chi}\right)^{\eta/2}\,, \tag{22}$$

$$R_{k,\ell,m}=\delta[kM_{k-1,\ell,m}^{(0)}\varepsilon_x+\ell M_{k,\ell-1,m}^{(0)}\varepsilon_y+mM_{k,\ell,m-1}^{(0)}\varepsilon_z]+\frac{2\mu}{1+\mu}\chi_{12}^{1/2(k+\ell+m-1)}$$
$$\times[A_{k+1,\ell,m}M_{1,0,0}^{(1)}+A_{k,\ell+1,m}M_{0,1,0}^{(1)}+A_{k,\ell,m+1}M_{0,0,1}^{(1)}]\,, \tag{23}$$

and

$$\varepsilon_i=\frac{1}{\nu_{22}}\left(\frac{m_1}{2k_BT_2}\right)^{1/2}\frac{q}{m_1}E_i\,. \tag{24}$$

In the above equations, $\chi \equiv T_1/T_2$, $\chi_{12} \equiv T_{12}/T_2 = (1-2M)\chi + 2M$, $M \equiv m_r m_s/(m_r + m_s)^2, \eta = 1 - 4/\ell$, $M^{(0)}_{k,\ell,m}$ refers to the zeroth-order moments whose expressions are known [19], and

$$A_{k,\ell,m} = \pi^{-3/2}\Gamma\left(\frac{k+1}{2}\right)\Gamma\left(\frac{\ell+1}{2}\right)\Gamma\left(\frac{m+1}{2}\right) \tag{25}$$

if (k,ℓ,m) are even, being zero otherwise. The solution to Eq. (21) can be cast into the form

$$M^{(1)}_{k,\ell,m} = \sum_{q=0}^{k} \delta^q (-a^*)^q \frac{k!}{(k-q)!}[1+\delta\alpha^*(k+\ell+m)]^{-(1+q)} R_{k-q,\ell+q,m}\,. \tag{26}$$

From this equation, and after some manipulations, it is easy to show that the current density obeys a generalized Ohm's law (14), where the conductivity tensor is given by

$$\sigma_{ij} = \frac{n_1 q^2}{m_1 \tau}\left(\frac{1+\mu}{\mu+\chi}\right)^{\eta/2}\frac{1}{1+\gamma\alpha^*}\left(\delta_{ij} - \gamma\frac{a^*_{ij}}{1+\gamma\alpha^*}\right), \tag{27}$$

where, in the context of the GK equation, $\tau = w^{(1-\eta)/2}[2\mu(1+\mu)]^{-1/2}\nu_{22}$ and

$$\gamma = (1+\mu)\delta = \left[\frac{2\mu(1+\mu)}{w}\right]^{1/2}\left(w\frac{1+\mu}{\mu+\chi}\right)^{\eta/2}. \tag{28}$$

Eq. (27) provides the expression of the electrical conductivity tensor given by the GK model for $r^{-\ell}$-potentials. When $a = 0$, $\sigma_{ij} = \sigma_0\delta_{ij}$, with $\sigma_0 = n_1 q^2/m_1\tau$. For small shear rates, one has $\sigma_{ii}/\sigma_0 \approx 1 - Ba^{*2}$ and $-\sigma_{xy}/\sigma_0 \approx -Ca^*(1-2Ba^{*2})$, where

$$B = \frac{C}{3} + \frac{\eta D}{2(1+\mu)}, \tag{29}$$

$$C = w^{(\eta-1)/2}[2\mu(1+\mu)]^{1/2}, \tag{30}$$

$$D = \frac{1-E}{3ME^2}, \tag{31}$$

$$E = w^{(\eta-1)/2}\left(\frac{1+\mu}{2\mu}\right)^{1/2}. \tag{32}$$

In Figs. 1 and 2, we show the shear-rate dependence of σ_{ii}/σ_0 and $-\sigma_{xy}/\sigma_0$ given by the GK model in the extreme cases of Maxwell molecules ($\eta = 0$) and hard-spheres ($\eta = 1$). Notice that in the case of mechanically equivalent particles ($\mu = 1$), the GK results are universal, independent of the interaction potential. On the other hand, and in order to make a comparison with the Boltzmann results for Maxwell molecules, we have taken for the constant A appearing in Eq. (A.6) the value that gives the same results between the GK and Boltzmann equations in the pure shear flow problem for a single gas [8,9]. With this choice the reduced shear rate a^* is common in both descriptions. We observe that the GK predictions show a quite good agreement with those given from the Boltzmann equation for Maxwell molecules, especially when the charged particles

are lighter than the neutral particles. In general, it is shown that the qualitative trends observed for Maxwell molecules can be extended to non-Maxwell molecules, except for $\mu < 1$ where there is a small region of shear rates in which σ_{ii} increases as a^* increases. This is consistent with the small shear-rate behavior. For $\mu < 1$, given a fixed value of the shear rate, the numerical values of the σ_{ii} and $-\sigma_{xy}$ elements increase as the potential becomes harder while the opposite happens for $\mu \geqslant 1$. This tendency changes in the case of $-\sigma_{xy}$ for large shear rates and mass ratios larger than 1.

4. Discussion

In this paper we have analyzed the diffusion of charged particles in a rarefied neutral gas under the action of a weak electric field. We have assumed that the molar fraction of the charged particles $x_1 = n_1/n_2$ is much smaller than 1 (tracer limit) so that the state of the neutral gas is not perturbed by the presence of the charged particles. In addition, the state of the charged particles is only affected by cross-collisions of type neutral–charged, and consequently the Coulomb interaction does not need to be included in the description of the problem. In the limit of small electric fields $\boldsymbol{E}$ and when the neutral background is at equilibrium, the current density $\boldsymbol{j}_1$ obeys Ohm's law, i.e., $\boldsymbol{j}_1 = \sigma_0 \boldsymbol{E}$, where σ_0 is the electrical conductivity coefficient. These are the usual conditions for measuring the transport properties of ions or electrons in gases. Here, we have generalized the above description to the case in which the neutral gas is under uniform shear flow, namely, a state macroscopically characterized by constant density and temperature and a velocity field given by $u_i = a_{ij} r_j$, where $a_{ij} = a\delta_{ix}\delta_{jy}$, a being the constant shear rate. We have focused our attention on the evaluation of the influence of shear rate on the current density when the electric field is weak. Furthermore, our study is not restricted to specific values of the masses and sizes of the particles of the mixture.

Under the assumptions established in the tracer limit, the kinetic equation for the distribution function f_2 of the neutral gas reduces to the (closed) nonlinear Boltzmann equation for a single gas while the distribution function f_1 of the charged particles verifies a Boltzmann–Lorentz equation. The current density is obtained by solving the Boltzmann–Lorentz equation from a perturbation expansion in powers of the electric field, taking the pure shear flow state as the reference one. The key point is that an exact description of the zeroth-order approximation (which is characterized by the absence of current but with arbitrary values of a) has been given from the Boltzmann equation for Maxwell molecules [11,12] and from a kinetic model for general repulsive interactions [13,14]. The knowledge of such a solution allows us to get the current density $\boldsymbol{j}_1^{(1)}$ to first order in the external field. We find a generalized Ohm's law, where an electrical conductivity tensor σ_{ij} can be identified. This tensor has really two relevant (independent) elements: one diagonal ($\sigma_{xx} = \sigma_{yy} = \sigma_{zz}$) and one off-diagonal ($\sigma_{xy}$). These elements are nonlinear functions of the reduced shear rate a^*, the mass ratio $\mu = m_1/m_2$, the force constant ratio $w = \kappa_{12}/\kappa_{22}$, and a parameter characterizing the interaction law considered. Our results indicate that the net consequence of the presence of the shear

flow on the diffusion of charge is to inhibit the current density along the y direction. In general, this inhibition is more significant as the mass ratio is larger than 1. With respect to the x direction, $-\sigma_{xy}$ is not a monotonic function of the shear rate and, for a given value of a, its magnitude increases as the mass of the charged particle increases. Concerning the influence of the interaction potential, we conclude that the values of σ_{ii} and $-\sigma_{xy}$ decrease as the potential becomes softer (harder) when the mass ratio is smaller (larger) than 1. Besides, the comparison between the Boltzmann and kinetic model equations in the case of Maxwell molecules shows a good agreement even for large values of a and/or disparate values of μ and w.

Finally, it is interesting to constrast the results presented here with those recently derived for the current density under steady Couette from the GK equation for Maxwell molecules [23]. While in the uniform shear flow problem the system is sheared by applying Lees–Edwards boundary conditions [10], in the Couette flow state the shear flow is generated by more realistic conditions [24]. As a consequence, the density, the temperature, and the shear rate are nonhomogeneous. In the case of the electrical conductivity tensor, comparsion between the results obtained in both states shows that the shear rate dependence of σ_{ii} and σ_{xy} is qualitatively similar. Nevertheless, there are important differences between both problems since in the Couette flow $\sigma_{xx} \neq \sigma_{yy} \neq \sigma_{zz}$ and $\sigma_{yx} \neq 0$ (although it is very small). Besides, at a quantitative level, the numerical discrepancies between both descriptions increase with the shear rate. For instance, for $\mu = 1$ and $a^* \simeq 0.4$, the discrepancies for the trace $(\sigma_{xx} + \sigma_{yy} + \sigma_{zz})/3$ and $-\sigma_{xy}$ are around 7% and 40%, respectively. The comparsion carried out for the conductivity tensor is in the same spirit as the ones previously made for the shear viscosity [25] and for the thermal conductivity tensor [26]. In all the cases, important differences between both states have been found in the nonlinear regime. It is evident that the origin of these discrepancies lies in the fact that both shear flow states are macroscopically different.

Acknowledgements

Partial support from the DGES (Spain) through Grant No. PB97-1501 and from the Junta de Extremadura (Fondo Social Europeo) through Grant No. PRI97C1041 is acknowledged.

Appendix A. Explicit expressions of the thermostat parameter as given by the Boltzmann and GK equations

In the context of the set of Boltzmann equations and for Maxwell molecules, the thermostat parameter is $\alpha = \max(\lambda, \lambda')$, where [11,12]

$$\lambda = \nu_{22}\varphi(a/\nu_{22}) \,, \tag{A.1}$$

$$\lambda' = v_{22}\beta[\varphi(a\beta/v_{22}) - 0.648\mu] \,, \tag{A.2}$$

$$\varphi(x) = \tfrac{2}{3}\sinh^2[\tfrac{1}{6}\cosh^{-1}(1 + 9x^2)] \tag{A.3}$$

and

$$\beta = \left[\frac{2w}{\mu(1+\mu)^3}\right]^{-1/2} \,. \tag{A.4}$$

Beyond the Maxwell interaction, explicit results can only be obtained by using a kinetic model. Here, we use the generalized GK model defined as [19,20]

$$J_{rs}^{\mathrm{GK}} = -\nu_{rs}(f_r - f_{rs}) \,, \tag{A.5}$$

where

$$\nu_{rs} = A(\eta)n_s\left(\kappa_{rs}\frac{m_r + m_s}{m_r m_s}\right)^{(1-\eta)/2}\left(\frac{2k_BT_r}{m_r} + \frac{2k_BT_s}{m_s}\right)^{\eta/2} \tag{A.6}$$

is an effective collision frequency for molecules interacting through repulsive potentials of the form $\kappa_{rs}r^{-\ell}$ ($\ell = 4, \ldots, \infty$), $\eta = 1 - 4/\ell$, and $A(\eta)$ is a constant for a given potential. Besides, f_{rs} is given by

$$f_{rs} = n_r\left(\frac{m_r}{2\pi k_BT_{rs}}\right)^{3/2}\exp\left[-\frac{m_r}{2k_BT_{rs}}(\boldsymbol{v} - \boldsymbol{u}_{rs})^2\right], \tag{A.7}$$

with $\boldsymbol{u}_{rs} = (m_r\boldsymbol{u}_r + m_s\boldsymbol{u}_s)/(m_r + m_s)$, and $T_{rs} = T_r + 2M[T_r - T_s + (m_s/6k_B)(\boldsymbol{u}_r - \boldsymbol{u}_s)^2]$. In the context of the GK model, the thermostat is again $\alpha = \max(\lambda, \lambda')$ where λ is also given by Eq. (A.1) but now λ' is the largest real root obtained numerically from the following coupled equations [13,14]:

$$a^2\nu_{12}(1 - 2M) = 3(\nu_{12} + 2\alpha)^2(M\nu_{12} + \alpha) \,, \tag{A.8}$$

$$\chi = \frac{T_1}{T_2} = \frac{M\nu_{12}[2a^2 + 3(\nu_{12} + 2\alpha)^2]}{3(M\nu_{12} + \alpha)(\nu_{12}2\alpha)^2 - a^2\nu_{12}(1 - 2M)} \,. \tag{A.9}$$

In the special case of Maxwell molecules ($\eta = 0$), ν_{12} does not depend on the temperature ratio χ and Eq. (A.9) reduces to a closed cubic equation for α. Nevertheless, its real solution does not coincide with the one obtained from the Boltzmann equation, i.e., Eq. (A.2).

References

[1] S. Chapman, T.G. Cowling, The Mathematical Theory of Nonuniform Gases, Cambridge University Press, Cambridge, 1970.
[2] L. Ferrari, Physica A 93 (1978) 531.
[3] L. Ferrari, Physica A 101 (1980) 491.
[4] L. Ferrari, Physica A 133 (1985) 103.
[5] E.A. Mason, E.W. McDaniel, Transport Properties of Ions in Gases, Wiley, New York, 1988.
[6] L.C. Woods, An Introduction to the Kinetic Theory of Gases and Magnetoplasmas, Oxford University Press, Oxford, 1993.

[7] A.S. Clarke, B. Shizgal, Phys. Rev. E 49 (1994) 347.
[8] E. Ikenberry, C. Truesdell, J. Rat. Mech. Anal. 5 (1956) 55.
[9] C. Truesdell, R. Muncaster, Fundamentals of Maxwell's Kinetic Theory of a Simple Monoatomic Gas, Ch. 5, Academic Press, New York, 1980.
[10] D.J. Evans, G.P. Morriss, Statistical Mechanics of Nonequilibrium Liquids, Academic Press, London, 1990.
[11] C. Marín, V. Garzó, A. Santos, Phys. Rev. E 52 (1995) 3812.
[12] C. Marín, A. Santos, V. Garzó, Europhys. Lett. 33 (1996) 599.
[13] C. Marín, V. Garzó, Phys. Fluids 8 (1996) 2756.
[14] C. Marín, V. Garzó, A. Santos, Phys. Rev. E 56 (1997) 2291.
[15] L.H. Holway, Phys. Fluids 9 (1966) 1658.
[16] E. Goldman, L. Sirovich, Phys. Fluids 10 (1967) 1928.
[17] E.A. Johnson, Phys. Fluids 21 (1978) 1239.
[18] E.P. Gross, M. Krook, Phys. Rev. 102 (1956) 593.
[19] V. Garzó, M. López de Haro, Phys. Fluids 7 (1995) 478.
[20] C. Marín, J.M. Montanero, V. Garzó, Physica A 225 (1996) 235.
[21] C. Marín, V. Garzó, A. Santos, J. Statist. Phys. 75 (1994) 797.
[22] C. Marín, J.M. Montanero, V. Garzó, Mol. Phys. 88 (1996) 1249.
[23] V. Garzó, Phys. Rev. E 57 (1998) 4186.
[24] S.Y. Liem, D. Brown, J.H.R. Clarke, Phys. Rev. A 45 (1992) 3706.
[25] A. Santos, V. Garzó, J.J. Brey, Phys. Rev. A 46 (1992) 8018.
[26] V. Garzó, Phys. Rev. E 48 (1993) 3589.