Exact Non-linear Transport from the Boltzmann Equation [1]

Andrés Santos and Vicente Garzó

Departamento de Física, Universidad de Extremadura, Spain

Abstract

A survey is given of some special problems for which the transport properties can be exactly evaluated from the Boltzmann equation for Maxwell molecules. The solutions refer to the planar Fourier flow and the uniform shear flow for a single gas and the color conductivity problem and the uniform shear flow for a binary mixture. The relevant transport coefficients are obtained in each case by solving the moment equations associated to the Boltzmann equation. They are in general highly non-linear functions of the respective nonequilibrium parameters, namely the thermal gradient, the shear rate and the color field strength. The relevance of exact solutions in far from equilibrium states is discussed.

1 Introduction

The Boltzmann equation [1] represents the starting point for the study of physical phenomena taking place not only in classical dilute gases but also in a wide variety of systems, such as electrons and phonons in solids and elementary excitations in quantum fluids and plasmas. However, the mathematical complexity of its collision term has made difficult the task of finding exact solutions. The knowledge of examples of exact solutions is useful to understand the physical behavior of systems in far from equilibrium states. They are also important as test cases for approximation methods. In this context, the exact solution discovered by Bobylev, Krook and Wu has played a relevant role in the analysis of the relaxation towards equilibrium of spatially homogeneous states [2].

In this paper we offer a brief survey of some examples of nonequilibrium situations for which the transport properties can be exactly derived. These properties are obtained by solving the infinite hierarchy for the moments of the velocity distribution function, in the special case of Maxwell molecules (i.e., particles interacting via a potential $V(r) = \kappa r^{-4}$). For this interaction model, the collision rate is independent of the velocity and, consequently, a

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moment of order k of the collision operator involves only moments of order equal to or less than k. It is worthwhile to remark that we are interested in *non-linear* transport, namely transport taking place beyond the scope of the linear (or Navier-Stokes) regime.

The solutions reviewed here belong to the class of so-called "normal" solutions. This means that the space and time dependence of the velocity distribution function $f(\mathbf{r}, \mathbf{v}; t)$ occurs entirely through a functional dependence on the local conserved densities:

$$f(\mathbf{r}, \mathbf{v}; t) = \mathcal{F}[\mathbf{v}; n(\mathbf{r} + \cdot, t), \mathbf{u}(\mathbf{r} + \cdot, t), T(\mathbf{r} + \cdot, t)], \qquad (1.1)$$

where n, $\mathbf{u}$ and T are the local density, velocity and temperature, respectively. They are defined as the first five moments of f. Solutions to the Boltzmann equation are expected to adopt a normal form in regions far away from the boundaries and in the long-time limit. The well-known Chapman-Enskog method [1,3] provides the normal solution in situations near equilibrium. However, the existence of normal solutions in states arbitrarily far from equilibrium is not well-established.

In standard notation, the Boltzmann equation reads

$$\frac{\partial}{\partial t} f + \mathbf{v} \cdot \nabla f + \frac{1}{m} \frac{\partial}{\partial \mathbf{v}} \cdot (\mathbf{F} f) = \int d\mathbf{v}_1 \int d\Omega g \sigma(g, \theta)(f' f_1' - f f_1)$$
$$\equiv J[f, f]. \qquad (1.2)$$

Here, $\mathbf{F}$ is the external force, which in general can be velocity-dependent. This equation is formally equivalent to an infinite hierarchy of equations for the velocity moments of f. For the sake of convenience, we introduce the moments [3]

$$M_{r\ell m} = \frac{1}{n} \int d\mathbf{v} \Psi_{r\ell m}(\boldsymbol{\xi}) f, \qquad (1.3)$$

where

$$\Psi_{r\ell m}(\boldsymbol{\xi}) = N_{r\ell} \xi^\ell L_r^{(\ell + \frac{1}{2})}(\xi^2) Y_\ell^m(\hat{\boldsymbol{\xi}}), \quad \boldsymbol{\xi} \equiv (m/2k_B T)^{1/2}(\mathbf{v} - \mathbf{u}). \qquad (1.4)$$

The polynomials $\{\Psi_{\mathbf{k}}(\boldsymbol{\xi}), \mathbf{k} \equiv (r, \ell, m)\}$ constitute a complete set of orthonormal functions with the scalar product $\langle \Phi | \chi \rangle = \pi^{-3/2} \int d\boldsymbol{\xi} e^{-\xi^2} \Phi^*(\boldsymbol{\xi}) \chi(\boldsymbol{\xi})$.

The hierarchy of moment equations has the form

$$\frac{\partial}{\partial t} M_{\mathbf{k}} + \sum_{\mathbf{k}'} L_{\mathbf{k}\mathbf{k}'} M_{\mathbf{k}'} = \sum_{\mathbf{k}', \mathbf{k}''} J_{\mathbf{k}\mathbf{k}'\mathbf{k}''} M_{\mathbf{k}'} M_{\mathbf{k}''}. \qquad (1.5)$$

In general, the operator $L_{\mathbf{k}\mathbf{k}'}$ couples moments of order $k = 2r + \ell$ with moments of order $k' = 2r' + \ell' > k$, so that the above hierarchy is not closed. The collision term complicates the coupling further, except in the special case of Maxwell molecules. In this case, the collision rate $g\sigma(g, \theta)$ is only a function of the scattering angle θ and, consequently, $J_{\mathbf{k}\mathbf{k}'\mathbf{k}''}$ vanishes if $k' + k'' \neq k$ [3]. In particular, $J_{\mathbf{k}0\mathbf{k}} = J_{\mathbf{k}\mathbf{k}0} = -\frac{1}{2}\lambda_{r\ell}$, where $\lambda_{r\ell}$ are the eigenvalues of the linearized collision operator [4]. This property is not sufficient to make the hierarchy (1.5) solvable, due to the free-streaming term. Nevertheless, there exist several particular situations for which the hierarchy can be recursively solved. Some of them are reviewed in the next Sections.

2   Planar Fourier flow

This state corresponds to a single gas enclosed between two parallel infinite plates kept at different temperatures. We are interested in the normal solution, namely a stationary solution which applies far from the plates. Asmolov, Makashev and Nosik [5] found such a solution for the case of Maxwell molecules. It is characterized by a constant pressure, a zero flow velocity and a temperature gradient along the direction, say z, perpendicular to the plates of the form

$$T(z) \frac{\partial}{\partial z} T(z) = \text{const.} \qquad (2.1)$$

In this problem, the relevant dimensionless parameter is

$$\epsilon(z) = \frac{1}{\nu(z)} \left(\frac{2k_B T(z)}{m} \right)^{1/2} \frac{\partial}{\partial z} \ln T(z), \qquad (2.2)$$

where $\nu(z) \propto n(z)$ is an effective collision frequency. The parameter ϵ is the relative variation of temperature over a mean free path and measures the departure from equilibrium. In the spirit of a normal solution, all the space dependence of the (dimensionless) moments $M_{r\ell} \equiv M_{r\ell 0}$ appears entirely through ϵ.

In this problem the hierarchy (1.5) becomes [6]

$$\frac{1}{2} \epsilon [\epsilon \frac{\partial}{\partial \epsilon} - (2r + \ell - 1)][A_{r\ell} M_{r, \ell+1} + A_{r, \ell-1} M_{r, \ell-1}$$
$$- B_{r+1, \ell-1} M_{r+1, \ell-1} - B_{r\ell} M_{r-1, \ell+1}]$$
$$+ \epsilon \sqrt{r(r + \ell + \frac{1}{2})} [A_{r-1, \ell} M_{r-1, \ell+1} + A_{r-1, \ell-1} M_{r-1, \ell-1}$$
$$- B_{r, \ell-1} M_{r, \ell-1} - B_{r-1, \ell} M_{r-2, \ell+1}]$$
$$= \frac{1}{\lambda_{11}} (\lambda_{r\ell} M_{r\ell} - \sum_{\mathbf{k}', \mathbf{k}''}{}^\dagger J_{\mathbf{k}\mathbf{k}'\mathbf{k}''} M_{\mathbf{k}'} M_{\mathbf{k}''}), \qquad (2.3)$$

where the dagger in the summation denotes the restrictions $k' + k'' = k$

and $k', k'' > 0$. Here, $A_{r\ell}$ and $B_{r\ell}$ are numerical constants given by

$$A_{r\ell} = (\ell + 1) \left[\frac{r + \ell + \frac{3}{2}}{(2\ell + 1)(2\ell + 3)} \right]^{1/2}, \quad B_{r\ell} = A_{r\ell} \left(\frac{r}{r + \ell + \frac{3}{2}} \right)^{1/2}. \quad (2.4)$$

Notice that eqn. (2.3) still couples moments of order k with moments of order $k + 1$. However, it is straightforward to verify that the hierarchy admits a solution in which the moment $M_{r\ell}$ is a *polynomial* in ϵ of degree $2(r-1) + \ell$ and parity ℓ. Moreover, the first non-zero coefficient in the polynomial corresponds to a power equal to $\max\{\ell, (2r+\ell)/3\}$. In particular, the non-zero moments through fourth order are

$$M_{00} = 1, \ M_{11} = \frac{\sqrt{5}}{2}\epsilon, \ M_{20} = \frac{7\sqrt{30}}{12}\epsilon^2, M_{12} = -\frac{4\sqrt{42}}{21}\epsilon^2. \quad (2.5)$$

The result for M_{11} implies that the heat flux verifies the Fourier law *exactly* for arbitrary values of the thermal gradient and not only in the Navier-Stokes limit ($\epsilon \ll 1$).

3 Uniform shear flow

This state is macroscopically characterized by a constant density, a spatially homogeneous temperature and a linear profile along the y-direction of the x-component of the velocity, namely

$$u_i(\mathbf{r}) = a_{ij}r_j, \ a_{ij} = a\delta_{ix}\delta_{jy}. \quad (3.1)$$

In this problem the (constant) shear rate a is the nonequilibrium parameter measuring the distance from equilibrium. In the context of normal solutions, we look for solutions that are spatially homogeneous when one refers the velocities to a Lagrangian frame moving with the velocity field $\mathbf{u}(\mathbf{r})$, i.e. solutions of the form $f(\mathbf{r}, \mathbf{v}; t) = f(\mathbf{V}, t)$, where $\mathbf{V} \equiv \mathbf{v} - \mathbf{u}$. In this frame, the Boltzmann equation becomes

$$\frac{\partial}{\partial t}f - \frac{\partial}{\partial V_i}a_{ij}V_j f = J[f, f]. \quad (3.2)$$

In contrast to what happens in the previous example, the free-streaming term does not couple moments of order k to moments of higher order. If, in addition, one considers the case of Maxwell molecules, the associated moment hierarchy can be recursively solved.

About forty years ago, Ikenberry and Truesdell [7,8] obtained the time evolution of the second order moments, i.e. the pressure tensor P_{ij}, for Maxwell molecules. In the long-time limit they behave as $P_{ij}(t) \sim e^{2\alpha\nu t}$,

where ν is again an effective collision frequency and

$$\alpha(a) = \frac{2}{3}\sinh^2[\frac{1}{6}\cosh^{-1}(1 + 9a^{*2})], \ a^* \equiv a/\nu. \quad (3.3)$$

From a rheological point of view, the most relevant transport properties are the (reduced) non-linear shear viscosity η and viscometric functions Φ_1 and Φ_2. They are given by [7,8,9]

$$\eta = -\lim_{t \to \infty} \frac{1}{a^*}\frac{P_{xy}}{p} = \frac{1}{(1 + 2\alpha)^2}, \quad (3.4)$$

$$\Phi_1 = \lim_{t \to \infty} \frac{1}{a^{*2}}\frac{P_{yy} - P_{xx}}{p} = -\frac{2}{(1 + 2\alpha)^3}, \quad (3.5)$$

$$\Phi_2 = \lim_{t \to \infty} \frac{1}{a^{*2}}\frac{P_{zz} - P_{yy}}{p} = 0. \quad (3.6)$$

The parameter α is a monotonically increasing function of a^*. For small shear rates, $\alpha \approx \frac{1}{3}a^{*2}$, while $\alpha \approx 12^{-1/3}a^{*2/3}$ for large shear rates. Thus, according to eqn. (3.4), the non-Newtonian shear viscosity decreases as the shear rate increases. This phenomenon is usually known in the rheological literature as "shear thinning." On the other hand, the expansion of the transport properties in powers of a^* (Chapman-Enskog expansion) happens to be convergent for $|a^*| < \sqrt{2}/3$.

Recently, the time evolution of higher order moments has been analyzed [9,10,11]. According to the concept of normal solution, one would expect that in the long-time limit the reduced moments tend to stationary values dependent on the shear rate. In the uniform shear flow problem, the hierarchy of moments adopts the form

$$\frac{1}{\nu}\frac{\partial}{\partial t}M_{\mathbf{k}} + a^* \sum_{\mathbf{k}', k' \le k} \langle \Psi_{\mathbf{k}'}|\xi_y \frac{\partial}{\partial \xi_x}|\Psi_{\mathbf{k}}\rangle M_{\mathbf{k}'}$$

$$+\alpha \left[kM_{\mathbf{k}} - 2\sqrt{r(r + \ell + \frac{1}{2})}M_{r-1,\ell,m} \right]$$

$$= \frac{1}{\lambda_{11}}(-\lambda_{\mathbf{k}}M_{\mathbf{k}} + \sum_{\mathbf{k}',\mathbf{k}''}{}^\dagger J_{\mathbf{k}\mathbf{k}'\mathbf{k}''}M_{\mathbf{k}'}M_{\mathbf{k}''}). \quad (3.7)$$

The evolution of the moments of order $k = 2r + \ell$ is governed by the eigenvalues of the matrix

$$\mathcal{L}_{\mathbf{k}\mathbf{k}'} = (\lambda_{\mathbf{k}} + k\alpha)\delta_{\mathbf{k}\mathbf{k}'} + a^*\langle \Psi_{\mathbf{k}'}|\xi_y \frac{\partial}{\partial \xi_x}|\Psi_{\mathbf{k}}\rangle, \ k' = k. \quad (3.8)$$

The moments reach stationary values if all the eigenvalues are positive. The explicit shear-rate dependence of the stationary fourth-order moments has been derived in Ref. [9]. Quite surprisingly, if the reduced shear rate is larger than the critical value $a_c^* \simeq 6.845$, one of the eigenvalues associated to fourth-order moments becomes negative. This implies that those moments diverge in time beyond the critical shear rate [10]. The same qualitative behavior is found for higher-order moments [11]. The corresponding values of a_c^* decrease as the order increases. In fact, the results suggest that $a_c^* \rightarrow 0$ as $k \rightarrow \infty$.

4 Color conductivity problem

The previous cases refer to a single gas. In the case of a binary mixture, the description is in general much more complicated, since new parameters (such as the molar fractions and the mass ratio) must be taken into account. For this reason, it is worthwhile to consider specific tractable situations. Perhaps, one of the simplest problems where non-linear transport takes place in a mixture is the so-called "color" conductivity problem. It can be described as follows [12]. In a binary mixture of mechanically different particles, "color charges" are assigned to particles of different species. By the action of a constant external field **E**, particles of each color are accelerated along opposite directions. As a consequence, mass fluxes are generated across the system in a spatially homogeneous state. In order to achieve a steady state, a drag force is introduced.

In this problem one has to deal with the set of two coupled Boltzmann equations:

$$-\frac{\partial}{\partial \mathbf{v}} \cdot \left(\frac{k_B T}{m_1 x_1} \mathbf{E} + \alpha \mathbf{v} \right) f_1 = J_{11}[f_1, f_1] + J_{12}[f_1, f_2], \qquad (4.1)$$

$$-\frac{\partial}{\partial \mathbf{v}} \cdot \left(-\frac{k_B T}{m_2 x_2} \mathbf{E} + \alpha \mathbf{v} \right) f_2 = J_{21}[f_2, f_1] + J_{22}[f_2, f_2]. \qquad (4.2)$$

Here, $x_s \equiv n_s/n$ is the molar fraction of species s and α is a drag coefficient whose dependence on the field **E** must be determined by consistency. The relevant transport coefficient is the so-called color conductivity σ, which is defined as the ratio between the mass flux and the field strength, namely

$$\mathbf{j}_{1,2} = \mp \frac{m_1 m_2 n^2}{\rho} \sigma \mathbf{E}, \qquad (4.3)$$

where ρ is the total mass density. According to the original motivation of the color field method in molecular dynamics simulations [12], σ reduces to the conventional mutual diffusion coefficient D in the zero-field limit. The interesting problem addressed in this Section is to analyze the non-linear response of the system as measured by the dependence of σ on **E**.

As happened in the two previous Sections, the hierarchy of moments can be recursively solved if one restricts oneself to Maxwell molecules. In particular, the expression for the color conductivity coefficient is [13]

$$\frac{\sigma}{D} = E^{*-2} \left(\sqrt{1 + 2E^{*2}} - 1 \right), \qquad (4.4)$$

where E^* is a reduced field strength. We observe that, in terms of convenient reduced units, the color conductivity exhibits a universal dependence on the color field, in the sense that all the influence of the ratios of mass, concentration and force constants has been scaled out. The expansion of σ in powers of E^* is convergent for $E^{*2} < 1/2$. The ratio σ/D monotonically deceases from 1 (zero-field limit) to $\sqrt{2}|E^*|^{-1}$ (large-field limit). The latter result means that the mass fluxes reach saturation values $\mathbf{j}_{1,2}^{sat}$ in the limit of large field strengths. In this limit, the system behaves as a collisionless gas, so that the velocity distribution functions become delta-distributions [13]:

$$\lim_{|E^*| \rightarrow \infty} f_{1,2}(\mathbf{v}) = n_{1,2} \delta(\mathbf{v} - \frac{\mathbf{j}_{1,2}^{sat}}{\rho_{1,2}}). \qquad (4.5)$$

Other physically interesting quantities, such as the pressure tensor, have been evaluated exactly as functions of the field strength [13,14].

5 Other transport problems in binary mixtures

In §3 we described the solution of the Boltzmann equation for a single gas under uniform shear flow. An interesting problem is to extend the above solution to a binary mixture [15]. The solution corresponds to a state characterized by constant number densities, a uniform temperature and identical linear profiles for the flow velocities of both species. Consequently, no mutual diffusion appears. By solving the set of coupled Boltzmann equations by means of the moment method one gets the momentum fluxes of each species and the total pressure tensor. This tensor defines the non-linear shear viscosity and viscometric functions. In the same way as in the case of a single gas, they are functions of the shear rate, but now they also depend on the parameters characterizing the mixture, namely the molar fractions and the ratios of mass and force constants. Obviously, the results discussed in §3 are recovered in the limit of identical particles. Further, the expressions previously derived in the tracer limit [16] are reobtained in a non-trivial way from the solution found in Ref. [15].

Let us assume now that we assign a color charge to the mixture subjected to uniform shear flow. If a color field is applied in an analogous way as in §4, mutual diffusion is generated. Thus, momentum and mass fluxes are coupled, so that both the shear viscosity and the color conductivity coefficients are functions of the shear rate and the field strength. This problem has been exactly analyzed in the case of mechanically equivalent particles

[17]. The results indicate that both transport coefficients are smaller than their Navier-Stokes values. Further, competition between the shearing and the color field produces inhibition of mass and momentum transport: the shear flow gives rise to a decrease of the color conductivity and the color field induces a decrease of the shear viscosity.

6 Discussion

In this paper we have offered a brief review of some special nonequilibrium states for which the transport properties can be exactly evaluated from the Boltzmann equation for Maxwell molecules. More specifically, we have considered the planar Fourier flow, the uniform shear flow, the color conductivity problem and the coupling between the latter two. In all the cases, one can identify a nonequilibrium parameter (or two in the case of the coupling color-shear) which controls the degree of departure from equilibrium. The solutions belong to the class of normal solutions, i.e. they apply outside the boundary layers and for long times. The goal is to get the relevant transport coefficients of the problem (thermal conductivity, shear viscosity, color conductivity, ...) as functions of the corresponding nonequilibrium parameter. In fact, the expansion in powers of that parameter is equivalent to the Chapman-Enskog expansion and turns out to be convergent (usually with a finite radius). In general, the non-linear response of the system, as measured by the transport coefficient, is weaker than the one corresponding to the linear regime (Navier-Stokes order). An exception is the thermal conductivity coefficient, since it exactly coincides with its Navier-Stokes value, even in the non-linear regime. It must be stressed that the above analyses do not provide the corresponding velocity distribution function.

The knowledge of exact solutions is of a great interest. Although they usually correspond to idealized (non-trivial) situations, exact solutions allow one to progress in the understanding of complex transport mechanisms taking place in more realistic situations. For instance, the exact verification of the Fourier law for Maxwell molecules supports the known fact that deviations from the Fourier law are hardly observable [18]. In addition, the exact shear viscosity derived for a dilute Maxwell gas exhibits shear-thinning effects also present in many complex fluids (e.g. polymers, dense colloidal dispersions and micellar solutions) [19]. On the other hand, some caution is needed before extrapolating some features present in particular exact solutions. For example, the convergent character of the Chapman-Enskog expansion is probably not a general property [20] and the Fourier law does not apply for non-planar geometries [5].

A second reason for which exact solutions are important is as a tool to test approximate methods, such as Grad's method and kinetic models [1]. In this context, the reliability of the BGK equation to get transport

properties is supported by the fact that its solution for the planar Fourier flow [21] has the same structure as that of the Boltzmann equation and by the fact that it gives the same expression for the pressure tensor as the Boltzmann equation in the uniform shear flow [22]. However, the latter agreement is not maintained in the case of fourth order moments [23]. More information about the relationship between Boltzmann and BGK solutions can be found in Ref. [24].

Finally, we think that the search for exact solutions of the Boltzmann equation is still an open subject. As a matter of fact, one could explore whether some known exact solutions of the BGK equation can also be extended to the Boltzmann equation for Maxwell molecules. In particular, the combined heat and momentum flow [25] is a good candidate for a new exact solution.

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