Transport equations from the Liu model

V. Garzó[a)]

Laboratorio de Energía Solar, Instituto de Investigaciones en Materiales, Universidad Nacional Autónoma de México, Apartado Postal 34, Temixco 62580, Morelos, Mexico

(Received 6 March 1991; accepted 10 April 1991)

Transport equations are developed by applying the Hilbert method to the Liu model [Phys. Fluids A 2, 277 (1990)]. The pressure tensor and the heat flux vector are calculated to Burnett hydrodynamic order for potentials of the form $r^{-\mu}$. The results are compared with those obtained from the Boltzmann equation.

I. INTRODUCTION

The normal solution of the nonlinear Boltzmann equation provides an adequate way of obtaining transport coefficients for a dilute gas. However, because of the mathematical complexity of the Boltzmann collision operator, it is, in general, very difficult to find explicit results. This problem has motivated the search of mathematically simpler kinetic models that preserve the main physical properties such as the equilibrium solution and the conservation laws. Perhaps one of the most widely used has been the nonlinear model of the Boltzmann equation proposed by Bhatnagar, Gross, and Krook (BGK).[1] The BGK equation has been solved by using the Hilbert perturbative expansion, and constitutive relations for the pressure tensor and the heat flux vector for $r^{-\mu}$ potentials up to the Burnett approximation[2] have been derived. The results have been shown to be identical to those obtained from the Chapman–Enskog method in the hard spheres case.[3]

Although the BGK model has been shown to be very fruitful in the past years, it also presents some insufficiencies. For this reason, Liu has recently suggested a new kinetic model[4] to improve some of the results predicted by the BGK equation. The model is constructed by requiring that, in two limiting cases (viscous flow and molecular flow), solutions obtained from the Liu equation are the same as those of the Boltzmann equation. This requirement leads him to propose a collision term proportional to the Chapman–Enskog first approximation to the distribution function, which is the solution to the linearized Boltzmann equation. Obviously, the Navier–Stokes transport coefficients calculated from the Liu model happen to be the same as those derived from the Boltzmann equation. Now, the question arises as to whether the agreement between the Boltzmann and Liu equations is maintained when higher-order hydrodynamic terms (Burnett, super-Burnett, ...) in the normal solution are retained.

The purpose of this paper is to derive the nonlinear Burnett hydrodynamic equations from the Liu model and to compare them with the ones derived from the Boltzmann equation. In the same way as in the previous BGK results,[2] the Hilbert expansion is used to explicitly evaluate the pressure tensor and the heat flux vector. Then, the transport coefficients that appear in the expansion of the transport fluxes can be compared with those obtained from the Boltzmann equation.[5]

[a)] On leave from Departamento de Física, Universidad de Extremadura, 06071-Badajoz, Spain.

II. NONLINEAR TRANSPORT EQUATIONS

Neglecting external forces, the Liu equation can be conveniently written in the form[4]

$$\frac{\partial f}{\partial t}+\mathbf{v}\cdot\nabla f = -\zeta(f-f_{\mathrm{LE}})f_{\mathrm{LE}}\left(1-\frac{\zeta\eta_{\mathrm{CE}}}{nk_{\mathrm{B}}T}\right) \times\frac{m}{k_{\mathrm{B}}T}(V_iV_j-\tfrac{1}{3}V^2\delta_{ij})\nabla_j u_i +f_{\mathrm{LE}}\left(1-\tfrac{2}{5}\zeta\lambda_{\mathrm{CE}}\frac{m}{nk_{\mathrm{B}}^2T}\right)\left(\frac{mV^2}{2k_{\mathrm{B}}T}-\tfrac{5}{2}\right)V_i\nabla_i\ln T, \tag{1}$$

where $f(\mathbf{r},\mathbf{v};t)$ is the one-particle distribution function, and $\zeta(\mathbf{r},t)$ is an average collision frequency similar to that of the BGK model. Here, $\mathbf{V}=\mathbf{v}-\mathbf{u}$, and $f_{\mathrm{LE}}(\mathbf{r},\mathbf{v};t)$ is the local equilibrium distribution function defined in terms of the local number density $n(\mathbf{r},t)$, local temperature $T(\mathbf{r},t)$, and local velocity $\mathbf{u},(\mathbf{r},t)$. Furthermore, the Liu equation introduces the coefficients of viscosity $\eta_{\mathrm{CE}}=\frac{5}{8}nk_{\mathrm{B}}T/\nu$, and thermal conductivity $\lambda_{\mathrm{CE}}=\frac{15}{4}k_{\mathrm{B}}\eta_{\mathrm{CE}}/m$ given by the Chapman–Enskog theory. Here, $\nu(\mathbf{r},t)$ is a velocity-independent collision frequency but it can depend upon the density and temperature. In order to carry out explicit calculations, from now on we will consider generic interaction potentials of the form $r^{-\mu}$ for which[5] $\nu=\nu_0nT^{\alpha}$, ν_0 being a constant and $\alpha=\frac{1}{2}-(2/\mu)$. It is clear that a similar dependence on space and time must be taken for ζ. In the same manner as in the BGK equation, Eq. (1) satisfies the conservation laws and has an H theorem. It is noteworthy that, in the particular case where the coefficients η_{CE} and λ_{CE} are substituted by their corresponding BGK values,[2] Eq. (1) reduces to the BGK equation. According to Eq. (1), the Liu model is the BGK equation [first term on the right-hand side of Eq. (1)] plus a single term related with the Chapman–Enskog first approximation. This term depends on the ratio of the collision frequencies ζ/ν, which may be left as arbitrary for the moment. It should be clear that some particular choices of the ratio ζ/ν may simplify the collision term of the starting equation (1). In particular, if one takes $\zeta=\frac{2}{3}\nu$, the term proportional to $\nabla_j u_i$ disappears. Also, if $\zeta=\frac{16}{15}\nu$, the term proportional to $\nabla\ln T$ disappears. As we will see later, such choices lead to a good agreement between Liu and Boltzmann results. Then, an adequate choice of the relation

 0899-8213/91/081980-03$02.00

ζ/ν may allow us to adjust the transport coefficient derived from the Liu model with the corresponding coefficient obtained from the Boltzmann equation. This possibility, using only one collision frequency has been used to compare results derived from the BGK and Boltzmann equations in several transport problems.[6]

Assuming that the distribution function f depends on space and time through the locally conserved variables, we look for normal solutions of Eq. (1) of the form

$$f=\sum_{k=0}^{\infty}\epsilon^k f^{(k)}, \tag{2}$$

where ϵ is an auxiliary parameter that may be set equal to unity at the end of the calculations. Analogously, in the Hilbert theory the hydrodynamic fields must also be expanded in powers of ϵ. Introducing these expansions into Eq. (1) and separating terms of the same order in ϵ, one obtains a set of algebraic equations that may be solved sequentially. Further details of the Hilbert theory can be found in Ref. 2. Here, we will be concerned only with the explicit expressions of the hydrodynamic fluxes. They are defined through

$$P_{ij}=\int d\mathbf{v} m V_i V_j f, \tag{3}$$

$$J_i=\int d\mathbf{v}\frac{m}{2}V^2 V_i f, \tag{4}$$

P_{ij} being the pressure tensor and J_i the heat flux vector. In zeroth order, $f^{(0)}=f^{(0)}_{\mathrm{LE}}$, namely the local equilibrium function defined from the variables $n^{(0)}$,$\mathbf{u}^{(0)}$, and $T^{(0)}$. Then, we immediately find $\mathbf{j}^{(0)}=\mathbf{0}$ and $P^{(0)}_{ij}=p^{(0)}\delta_{ij}$, with $p^{(0)}=n^{(0)}k_{\mathrm{B}}T^{(0)}$. Solving recursively, and using from now on the notation given in Ref. 2, the first approximation to the transport fluxes may be written as

$$P^{(1)}_{ij}=p^{(1)}\delta_{ij}-\eta(2D^{(0)}_{ij}-\tfrac{2}{3}\delta_{ij}D^{(0)}), \tag{5}$$

$$J^{(1)}_i=-\lambda\nabla T^{(0)}_i. \tag{6}$$

Here, $p^{(1)}=n^{(1)}k_{\mathrm{B}}T^{(0)}+n^{(0)}k_{\mathrm{B}}T^{(1)}$, and we have introduced the coefficients of shear viscosity $\eta=\frac{5}{8}p^{(0)}/\nu^{(0)}$ and thermal conductivity $\lambda=\frac{15}{4}k_{\mathrm{B}}\eta/m$ given by the Hilbert theory. The expressions for these coefficients exactly coincide with those given by the Hilbert theory applied to the Boltzmann equation[7] for the particular case of Maxwell molecules ($\alpha=0$). For other types of interactions, the accordance only holds in the first approximation to η and λ.

In the Burnett hydrodynamic order, after some tedious algebra one gets the constitutive relations for the pressure tensor and heat flux vector:

$$\begin{aligned}
P^{(2)}_{ij}=&\,p^{(2)}\delta_{ij}-2\eta(D^{(1)}_{ij}-\tfrac{1}{3}\delta_{ij}D^{(1)})-2\eta(p^{(1)}p^{(0)-1}-\nu^{(1)}\nu^{(0)-1})(D^{(0)}_{ij}-\tfrac{1}{3}\delta_{ij}D^{(0)})\\
&+\zeta^{(0)-1}\delta_{ij}\Big(\tfrac{4}{15}\frac{\lambda}{T^{(0)}}[(\alpha-1)(\nabla T^{(0)})^2-T^{(0)}\nabla^2T^{(0)}]+\tfrac{2}{5}(1-2\alpha)\eta D^{(0)2}\\
&-\tfrac{2}{3}\eta\rho^{(0)-1}p^{(0)-1}(\nabla p^{(0)})^2+\tfrac{2}{3}\eta\rho^{(0)-1}\nabla^2p^{(0)}-\tfrac{2}{3}\eta(D^{(0)}_{kl}D^{(0)}_{kl}+\omega^{(0)}_{kl}\omega^{(0)}_{kl})\\
&+\tfrac{2}{3}\eta\rho^{(0)-1}T^{(0)-1}\nabla p^{(0)}\cdot\nabla T^{(0)}\Big)+\tfrac{4}{5}\zeta^{(0)-1}\lambda(\nabla_i\nabla_jT^{(0)}-(\alpha-1)T^{(0)-1}\nabla_iT^{(0)}\nabla_jT^{(0)})\\
&-\eta\zeta^{(0)-1}\rho^{(0)-1}T^{(0)-1}(\nabla_ip^{(0)}\nabla_jT^{(0)}+\nabla_jp^{(0)}\nabla_iT^{(0)})-2\eta\zeta^{(0)-1}\rho^{(0)-1}(\nabla_i\nabla_jp^{(0)}\\
&-p^{(0)-1}\nabla_ip^{(0)}\nabla_jp^{(0)})+2\eta\zeta^{(0)-1}(D^{(0)}_{ik}D^{(0)}_{kj}+\omega^{(0)}_{ki}\omega^{(0)}_{kj})\\
&-\tfrac{2}{3}(1-2\alpha)\eta\zeta^{(0)-1}D^{(0)}D^{(0)}_{ij}-2\eta\zeta^{(0)-1}(D^{(0)}_{ik}\omega^{(0)}_{kj}+D^{(0)}_{jk}\omega^{(0)}_{ki}),
\end{aligned} \tag{7}$$

$$\begin{aligned}
J^{(2)}_i=&-\lambda(p^{(1)}p^{(0)-1}-\nu^{(1)}\nu^{(0)-1})\nabla_iT^{(0)}-\lambda\nabla_iT^{(1)}+\zeta^{(0)-1}\Big((9-2\alpha)\eta\frac{k_{\mathrm{B}}}{m}+\tfrac{4}{5}\lambda\Big)D^{(0)}_{ik}\nabla_kT^{(0)}\\
&+2\lambda\zeta^{(0)-1}\omega^{(0)}_{ik}\nabla_kT^{(0)}-\zeta^{(0)-1}\Big((2-\tfrac{2}{3}\alpha)\eta\frac{k_{\mathrm{B}}}{m}-(\tfrac{1}{15}+\tfrac{2}{3}\alpha)\lambda\Big)D^{(0)}\nabla_iT^{(0)}\\
&-\zeta^{(0)-1}T^{(0)}\Big(\tfrac{2}{3}\lambda-\tfrac{1}{3}\eta\frac{k_{\mathrm{B}}}{m}\Big)\nabla_iD^{(0)}+\zeta^{(0)-1}\eta\frac{k_{\mathrm{B}}T^{(0)}}{m}\nabla^2u^{(0)}_i\\
&-2\eta\zeta^{(0)-1}\rho^{(0)-1}(D^{(0)}_{ik}-\tfrac{1}{3}\delta_{ik}D^{(0)})\nabla_kp^{(0)},
\end{aligned} \tag{8}$$

where

$$\rho^{(0)}=mn^{(0)},$$

$$p^{(2)}=n^{(0)}_{\mathrm{B}}k_{\mathrm{B}}T^{(2)}+n^{(2)}k_{\mathrm{B}}T^{(0)}+n^{(1)}k_{\mathrm{B}}T^{(1)},$$

and we have expressed the results in terms of the strain rate $D^{(k)}_{ij}$ and the vorticity $\omega^{(k)}_{ij}$. As expected, the Burnett relations consist of terms up to second derivatives in $\mathbf{u}^{(0)}$ and $T^{(0)}$, up to first derivatives in $\mathbf{u}^{(1)}$ and $T^{(1)}$, and combinations of these plus a linear form of the pressure $p^{(2)}$. It must be noticed that no explicit dependence on the collision frequency ζ upon the density and temperature has to be taken in order to derive Eqs. (7) and (8). Moreover, these relations explicitly depend on the ratio ζ/ν.

The results show that the derived Burnett equations happen to be analogous to those obtained from the BGK and Boltzmann equations, although, in principle, the transport

coefficients are different. As a matter of fact, Eqs. (7) and (8) reduce to the BGK results[2] when η and λ are substituted by their explicit values given by the BGK model, namely $\eta^{\mathrm{BGK}} = p^{(0)}/\zeta^{(0)}$ and $\lambda^{\mathrm{BGK}} = \frac{5}{2}p^{(0)}k_{\mathrm{B}}/m\zeta^{(0)}$. As noted above, there exist different ways to choose the relation between ζ and ν. Then, in an attempt to carry out a comparison with the Burnett transport coefficients obtained from the Boltzmann equation, particular values for the ratio ζ/ν must be taken. For instance, if one takes $\zeta = \frac{8}{5}\nu$ (for which $\eta = \eta^{\mathrm{BGK}}$), all the transport coefficients that appear in the pressure tensor (7) coincide exactly with the ones arising from the Boltzmann equation.[5] This means that the contributions to $\mathbf{P}^{(2)}$ coming from Boltzmann collision integrals can be exactly recovered through the use of simple collision frequencies. This is the great usefulness of the kinetic models, since for simple interaction potentials, the dynamics of collisions can be exactly modeled by introducing effective parameters. It must be noticed that the values of the Boltzmann–Burnett coefficients are only exact for Maxwell molecules, although it may be expected that they will not be far from the true values for other molecular models. On the other hand, the above choice defines transport coefficients in the heat flux different to those derived from the Boltzmann equation, even in the Maxwell case. But, now their numerical values are closer to the Boltzmann coefficients (with a discrepancy of around 33%) than the ones reported by the BGK equation. Analogous conclusions are obtained for the heat flux when one chooses $\zeta = \frac{16}{15}\nu$ (for which $\lambda = \lambda^{\mathrm{BGK}}$). In this case, the discrepancy in the pressure tensor coefficients for Maxwell molecules is also around 33%.

In summary, the Liu equation for a dilute gas has been solved using the Hilbert method for $r^{-\mu}$ potentials. In the nonlinear Burnett order, the transport coefficients that appear in the pressure tensor or the heat flux vector are identical to those reported from the Boltzmann equation for some particular values of the ratio of the two collision frequencies. In this way, one may conclude that the results derived from the Liu model improve notably some insufficiencies present in the BGK equation. This conclusion encourages our actual objective of extending to the Liu model some recent results derived from the BGK kinetic equation.[6,8]

ACKNOWLEDGMENTS

The author is grateful to Dr. M. López de Haro for suggestions for the improvement of the manuscript.

This work is supported by the Dirección General de Investigación Científica y Técnica (DGICYT) of the Spanish Government, through Grants No. BE91-102 and No. PS89-0183.

[1] P. L. Bhatnagar, E. P. Gross, and M. Krook, Phys. Rev. **94**, 593 (1954).
[2] V. Garzó, Physica A **149**, 551 (1988).
[3] C. Y. Cha and B. J. McCoy, J. Chem. Phys. **54**, 4369 (1971).
[4] G. Liu, Phys. Fluids A **2**, 277 (1990).
[5] S. Chapman and T. G. Cowling, *The Mathematical Theory of Nonuniform Gases* (Cambridge U.P., Cambridge, 1970).
[6] M. C. Marchetti and J. W. Dufty, J. Stat. Phys. **32**, 255 (1983); R. Zwanzig, J. Chem. Phys. **71**, 4416 (1979); E. S. Asmolov, N. K. Makashev, and V. I. Nosik, Sov. Phys. Dokl. **24**, 892 (1979); A. Santos, J. J. Brey, and V. Garzó, Phys. Rev. A **34**, 5047 (1986).
[7] C. F. Delale, J. Stat. Phys. **28**, 589 (1982).
[8] J. J. Brey, A. Santos, and J. W. Dufty, Phys. Rev. A **36**, 2842 (1987); C. S. Kim, J. W. Dufty, A. Santos, and J. J. Brey, Phys. Rev. A **40**, 7165 (1989).