

PRELIMINARY COMMUNICATION

Perturbative solution of the BGK equation for very hard particle interaction

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The Hilbert method is applied to the Bhatnagar-Gross-Krook (BGK) model kinetic equation with a velocity dependent collision frequency; we consider the so-called VHP interaction. The pressure tensor and heat flux vector are evaluated to the Navier-Stokes hydrodynamic order.

The Bhatnagar-Gross-Krook (BGK) [1] model kinetic equation is a version of the non-linear Boltzmann equation in which the collision integral is replaced by a simple relaxation term. The details of the interaction potential are modelled by means of an independent-velocity collision frequency ζ . Recently [2], the BGK equation has been solved using the Hilbert perturbative method. Detailed calculations for the momentum and heat fluxes have been achieved up to the Burnett hydrodynamic order. However, if the collision frequency is velocity dependent, the conventional BGK model is not adequate since the collision term does not satisfy the conservation laws. Following Brey and Santos [3], we propose a BGK equation whose reference distribution function is a gaussian function of the velocity. The parameters defining this reference function are determined by requiring the conservation laws to be verified. The purpose of this note is to solve the BGK equation for the so-called very hard particle (VHP) model interaction [4]. Again, we apply the Hilbert method and our analysis is centred on the Navier-Stokes level (first approximation).

We consider a dilute gas whose distribution function $f(\mathbf{r}, \mathbf{v}; t)$ obeys the BGK equation

$$\left(\frac{\partial}{\partial t} + v_j \nabla_j\right) f(\mathbf{r}, \mathbf{v}; t) = -\zeta(\mathbf{r}, \mathbf{v}; t)(f(\mathbf{r}, \mathbf{v}; t) - f_{\mathbf{R}}(\mathbf{r}, \mathbf{v}; t)), \quad (1)$$

where, for the VHP interaction, the collision frequency for molecules of velocity \mathbf{v} , $\zeta(\mathbf{r}, \mathbf{v}; t)$, is defined by

$$\zeta(\mathbf{r}, \mathbf{v}; t) = Cn(\mathbf{r}; t) \left[\frac{3k_{\mathbf{B}}T(\mathbf{r}; t)}{m} + |\mathbf{v} - \mathbf{u}(\mathbf{r}; t)|^2 \right]. \quad (2)$$

Here C is a constant, n is the number density, T is the temperature, \mathbf{u} is the fluid velocity, $k_{\mathbf{B}}$ is the Boltzmann constant and m is the mass of a particle. Also in equation (1) we have considered the reference distribution function [3] $f_{\mathbf{R}}(\mathbf{r}, \mathbf{v}; t)$

$$f_{\mathbf{R}}(\mathbf{r}, \mathbf{v}; t) = a(\mathbf{r}; t) \exp [\mathbf{b}(\mathbf{r}; t) \cdot \mathbf{V}(\mathbf{r}; t) - c(\mathbf{r}; t)V^2(\mathbf{r}; t)], \quad (3)$$

with $\mathbf{V}(\mathbf{r}; t) = \mathbf{v} - \mathbf{u}(\mathbf{r}; t)$, and a , \mathbf{b} and c being determined by imposing the BGK equation (1) to conserve mass, momentum and energy, i.e. $\int d\mathbf{v} \{1, m\mathbf{V}, (m/2)V^2\} \zeta(f - f_{\mathbf{R}}) = 0$. These relations lead to the set of equations (see Appendix A of [3]),

$$\left. \begin{aligned} 6 \frac{nk_{\text{B}}T}{m} &= D \left[\frac{3k_{\text{B}}T}{m} + \frac{b^2}{4c^2} + \frac{3}{2c} \right], \\ 2 \frac{\mathbf{J}}{m} &= \frac{D}{2c} \left[\frac{3k_{\text{B}}T}{m} + \frac{b^2}{4c^2} + \frac{5}{2c} \right] \mathbf{b}, \\ n \left(\frac{3k_{\text{B}}T}{m} \right)^2 + \Phi &= \frac{D}{4c^2} \left[5 \left(\frac{b^2}{c} + 3 \right) + 3 \frac{k_{\text{B}}T}{m} (b^2 + 6c) + \frac{b^4}{4c^2} \right], \end{aligned} \right\} \quad (4)$$

where $D = a \exp(b^2/4c)(\pi/c)^{3/2}$, $\mathbf{J}(\mathbf{r}; t) = \int d\mathbf{v} (m/2)V^2(\mathbf{r}; t)\mathbf{V}(\mathbf{r}; t)f(\mathbf{r}, \mathbf{v}; t)$ is the heat flux vector and $\Phi(\mathbf{r}; t) = \int d\mathbf{v} V^4(\mathbf{r}; t)f(\mathbf{r}, \mathbf{v}; t)$.

In Hilbert theory, the distribution function f and the hydrodynamic variables n , \mathbf{u} and T are expanded in powers of an auxiliary parameter ε which may be set equal to unity at the end of the calculations. Now, in an analogous way we must also consider the expansion of the variables a , \mathbf{b} and c

$$\left\{ \begin{array}{l} a \\ b_i \\ c \end{array} \right\} = \sum_{k=0}^{\infty} \varepsilon^k \left\{ \begin{array}{l} a^{(k)} \\ b_i^{(k)} \\ c^{(k)} \end{array} \right\}, \quad (5)$$

where the parameters $\{a^{(k)}, b_i^{(k)}, c^{(k)}\}$ are, for the moment, left arbitrary. When we insert the corresponding expansions in the BGK equation (1) we obtain the following algebraic equations [2]

$$\left. \begin{aligned} f^{(0)} &= f_{\mathbf{R}}^{(0)}, \\ f^{(1)} &= f_{\mathbf{R}}^{(1)} - \zeta^{(0)-1} \left(\frac{\partial}{\partial t} + v_j \nabla_j \right) f^{(0)}, \\ &\vdots \\ f^{(k)} &= f_{\mathbf{R}}^{(k)} - \zeta^{(0)-1} \left(\frac{\partial}{\partial t} + v_j \nabla_j \right) f^{(k-1)} - \zeta^{(0)-1} \sum_{r=1}^{k-1} \zeta^{(r)} [f^{(k-r)} - f_{\mathbf{R}}^{(k-r)}]. \end{aligned} \right\} \quad (6)$$

At zeroth order, we obtain the function $f_{\mathbf{R}}^{(0)}$ defined from the variables $a^{(0)}$, $\mathbf{b}^{(0)}$ and $c^{(0)}$. In order to obtain these parameters we may consider the definition of the hydrodynamic variables $n^{(0)}$, $\mathbf{u}^{(0)}$ and $T^{(0)}$

$$\left\{ \begin{array}{l} n^{(0)} \\ n^{(0)} u_i^{(0)} \\ \frac{3}{2} n^{(0)} k_{\text{B}} T^{(0)} \end{array} \right\} = \int d\mathbf{v} \left\{ \begin{array}{l} 1 \\ v_i \\ \frac{m}{2} V^{(0)2} \end{array} \right\} f_{\mathbf{R}}^{(0)}. \quad (7)$$

In this way, after some algebra, we get $\mathbf{b}^{(0)} = \mathbf{0}$ (or $\mathbf{J}^{(0)} = \mathbf{0}$), $c^{(0)} = m/2k_{\text{B}}T^{(0)}$ and $a^{(0)} = n^{(0)}(m/2\pi k_{\text{B}}T^{(0)})^{3/2}$. Therefore, $f_{\mathbf{R}}^{(0)}$ corresponds to the conventional local equilibrium function

$$f_{\mathbf{R}}^{(0)} = n^{(0)} \left(\frac{m}{2\pi k_{\text{B}}T^{(0)}} \right)^{3/2} \exp \left[- \frac{mV^{(0)2}}{2k_{\text{B}}T^{(0)}} \right] \quad (8)$$

and the pressure tensor $P_{ij}^{(0)} = \int d\mathbf{v} m V_i^{(0)} V_j^{(0)} f_R^{(0)} = n^{(0)} k_B T^{(0)} \delta_{ij} \equiv p^{(0)} \delta_{ij}$. These results are identical to those given in the Hilbert theory of the conventional BGK equation [2]. On the other hand, it is easy to show that coefficients $a^{(0)}$, $\mathbf{b}^{(0)}$ and $c^{(0)}$ satisfy equations (4) when the expansion of these relations is considered.

Solving sequentially, at Navier–Stokes order (first approximation), we obtain the formal solution

$$f^{(1)} = \lim_{n \rightarrow \infty} \left\{ \frac{a^{(1)}}{a^{(0)}} + (2c^{(0)} u_j^{(1)} + b_j^{(1)}) V_j^{(0)} - c^{(1)} V^{(0)2} - \zeta_0^{-1} \sum_{j=0}^n (-1)^j \left(\frac{m}{3k_B T^{(0)}} \right)^j V^{(0)2j} \right. \\ \left. \times \left[V_j^{(0)} \left(\frac{m V^{(0)2}}{2k_B T^{(0)}} - \frac{5}{2} \right) \frac{\nabla_j T^{(0)}}{T^{(0)}} + \frac{m}{k_B T^{(0)}} (V_j^{(0)} V_i^{(0)} - \frac{1}{3} V^{(0)2} \delta_{ij}) \nabla_j u_i^{(0)} \right] \right\} f_R^{(0)}, \quad (9)$$

where $\zeta_0 = 3(C/m)p^{(0)}$ can be considered as the independent velocity collision frequency that appears in the conventional BGK model. The parameters $a^{(1)}$, $\mathbf{b}^{(1)}$ and $c^{(1)}$ can be determined from the relations

$$\left\{ \begin{array}{l} n^{(1)} \\ n^{(1)} u_i^{(1)} \\ \frac{3}{2} p^{(1)} \end{array} \right\} = \int d\mathbf{v} \left\{ \begin{array}{l} 1 \\ V_i^{(0)} \\ \frac{m}{2} V^{(0)2} \end{array} \right\} f^{(1)}, \quad (10)$$

with $p^{(1)} = n^{(1)} k_B T^{(0)} + n^{(0)} k_B T^{(1)}$. When these integrals are performed, we get

$$\left. \begin{array}{l} \frac{a^{(1)}}{a^{(0)}} = \frac{n^{(1)}}{n^{(0)}} - \frac{3}{2} \frac{T^{(1)}}{T^{(0)}}, \\ b_i^{(1)} = -\zeta_0^{-1} \lim_{n \rightarrow \infty} \sum_{j=0}^n (-1)^j \frac{(2j+5)!!}{3^{j+2}} (j+1) \frac{\nabla_i T^{(0)}}{T^{(0)}}, \\ c^{(1)} = -\frac{m}{2k_B T^{(0)}} \frac{T^{(1)}}{T^{(0)}}. \end{array} \right\} \quad (11)$$

From the expression for $f^{(1)}$ we can evaluate the pressure tensor and the heat flux vector in the Navier–Stokes order. Thus, taking into account relations (11) and after some algebra, it is straightforward to show that

$$P_{ij}^{(1)} = \int d\mathbf{v} m V_i^{(0)} V_j^{(0)} f^{(1)} \\ = \delta_{ij} p^{(0)} \left[\frac{a^{(1)}}{a^{(0)}} - 5 \frac{k_B T^{(0)}}{m} c^{(1)} \right] - \frac{p^{(0)}}{\zeta_0} \lim_{n \rightarrow \infty} \frac{1}{15} \sum_{j=0}^n (-1)^j \frac{(2j+5)!!}{3^j} \\ \times [\nabla_i u_j^{(0)} + \nabla_j u_i^{(0)} - \frac{2}{3} \delta_{ij} \nabla_k u_k^{(0)}] \\ = \delta_{ij} p^{(1)} - \eta [\nabla_i u_j^{(0)} + \nabla_j u_i^{(0)} - \frac{2}{3} \delta_{ij} \nabla_k u_k^{(0)}], \quad (12)$$

$$J_i^{(1)} = \int d\mathbf{v} \frac{m}{2} V^{(0)2} V_i^{(0)} f^{(1)} - \frac{5}{2} p^{(0)} u_i^{(1)} \\ = \frac{5}{2} \frac{p^{(0)} k_B T^{(0)}}{m} b_i^{(1)} - \frac{p^{(0)} k_B}{m \zeta_0} \lim_{n \rightarrow \infty} \frac{1}{2} \sum_{j=0}^n (-1)^j \frac{(2j+5)!!}{3^{j+1}} (j+1) \nabla_i T^{(0)} \\ = -\lambda \nabla_i T^{(0)}, \quad (13)$$

where we have introduced the shear viscosity η and the thermal conductivity λ coefficients given by

$$\eta = \eta_0 \lim_{n \rightarrow \infty} \frac{1}{5} \sum_{j=0}^n (-1)^j \frac{(2j+5)!!}{3^{j+1}}, \quad (14)$$

$$\lambda = \lambda_0 \lim_{n \rightarrow \infty} \frac{8}{15} \sum_{j=0}^n (-1)^j \frac{(2j+5)!!}{3^{j+1}} (j+1) \quad (15)$$

and $\eta_0 = p^{(0)}/\zeta_0$, $\lambda_0 = \frac{5}{2} p^{(0)} k_B / m \zeta_0$ can be considered as the shear viscosity and the thermal conductivity coefficients given by the conventional BGK model [2]. The pressure tensor and the heat flux vector expressions (12), (13) are similar to those obtained from the BGK model [2] or the Boltzmann equation [5] using the Hilbert expansion. However, now the limit required in the transport coefficients expressions does not exist and so solution (9) is not uniformly convergent with respect to \mathbf{v} . But we can identify the transport coefficients with well-defined functions having the same asymptotic series. In fact, considering the integral form for the factorials, we can represent the transport coefficients by means of the well-defined functions

$$\eta = \frac{3}{5} \eta_0 \int_0^{\infty} dt \exp(-t) \exp(-t^2/6), \quad (16)$$

$$\lambda = \frac{8}{5} \lambda_0 \left[1 - \int_0^{\infty} dt \exp(-t) (t + t^3/6) \exp(-t^2/6) \right]. \quad (17)$$

We take equations (16) and (17) as the proper definitions of coefficients η and λ . In this way, η and λ can be understood as the Laplace transform $f(s)$ of the functions $t \exp(-t^2/6)$ and $(t + t^3/6) \exp(-t^2/6)$ evaluated at $s = 1$. In accordance with Laplace transform theory, we get the results

$$\eta = \frac{3}{5} \eta_0 \left[1 - \sqrt{\left(\frac{3\pi}{2}\right)} \exp\left(\frac{3}{2}\right) \operatorname{Erfc}\left(\sqrt{\frac{3}{2}}\right) \right], \quad (18)$$

$$\lambda = 9 \lambda_0 \left[5 - 6 \sqrt{\left(\frac{3\pi}{2}\right)} \exp\left(\frac{3}{2}\right) \operatorname{Erfc}\left(\sqrt{\frac{3}{2}}\right) \right], \quad (19)$$

where $\operatorname{Erfc}(x)$ is the complementary error function whose series representation is given by [6]

$$\operatorname{Erfc}(x) = 1 - \frac{2}{\sqrt{\pi}} \exp(-x^2) \sum_{k=0}^{\infty} 2^k \frac{x^{2k+1}}{(2k+1)!!}. \quad (20)$$

Therefore, the transport coefficients can be represented by the convergent expansions

$$\begin{aligned} \eta &= \frac{3}{5} \eta_0 \left[1 - \sqrt{\left(\frac{3\pi}{2}\right)} \exp\left(\frac{3}{2}\right) + 3 \sum_{j=0}^{\infty} \frac{3^j}{(2j+1)!!} \right] \\ &= 0.3418(7) \eta_0, \end{aligned} \quad (21)$$

$$\begin{aligned} \lambda &= \frac{1}{5} \lambda_0 \left[96 \sqrt{\left(\frac{3\pi}{2}\right)} \exp\left(\frac{3}{2}\right) - 76 - 288 \sum_{j=0}^{\infty} \frac{3^j}{(2j+1)!!} \right] \\ &= 0.3533(3) \lambda_0. \end{aligned} \quad (22)$$

Finally, we remark that the results obtained in this approximation are totally consistent again with relations (4).

The author wishes to thank A. Casanovas for assistance on the computational work.

References

- [1] CERCIGNANI, C., 1975, *Theory and Applications of the Boltzmann Equation* (Scottish Academic Press).
- [2] GARZO, V., and DE LA RUBIA, J., 1987, *Chem. Phys. Lett.*, **135**, 143. GARZO, V., *Physica A* (in the press).
- [3] BREY, J. J., and SANTOS, A., 1984, *J. statist. Phys.*, **37**, 123.
- [4] ERNST, M., 1981, *Phys. Rep.*, **78**, 117.
- [5] DELALE, C. F., 1982, *J. statist. Phys.*, **28**, 589.
- [6] GRADSHTEYN, I. S., and RYZHIK, I. M., 1980, *Table of Integrals, Series and Products* (Academic Press).