Derivation of a Diffusion Term in Boltzmann Equation

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Abstract

The structure of diffusion terms in Boltzmann equation is analysed and the construction of new macroscopic equations is presented.

1 Introduction

One of the main problems in the modern theory of gases is the general structure of a gradient expansion in the Boltzmann equation, connected with the popular Navier-Stokes (NS) equations [1] – [5]. During last few years a number of variants for corrections to the usual Boltzmann equation were suggested by different authors (see for example the works [16], [17]).

The most reasonable variant for the modification of the Boltzmann equation (BE) was developed recently by Elizarova and Chetverushkin [10] - [14]. This method is very convenient for the numerical calculations, so in the recent work we demonstrate the main physical ideas giving rise to the corresponding diffusion corrections in the BE described by the following formula:

$$f_t + (\vec{v}\nabla)f - (\vec{v}\nabla)\tau(\vec{v}\nabla)f = \mathcal{I}(f). \tag{1.1}$$

Here $f(\vec{x}, \vec{v}, t)$ is the distribution function for monoatomic gas, $\mathcal{I}(f)$ is the collision integral and τ is a local characteristic time due to pair collisions (the local relaxation time).

First of all the modified Boltzmann equation (1.1) have been used for the special methods of numerical calculations for gas flows at large Reynolds numbers. The corresponding numerical methods (Kinetical-Consistent Finite-Difference schemes (KCFD)) are efficient for real computations and are described in details in [10] - [12].

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The equations of hydrodynamics, get by the method of moment averaging in BE (1.1), are named Quasi-Gas-Dynamical equations (QGD) and are more efficient in numerical simulation at moderatly low Knudsen numbers (slip flow regime) in comparison with the popular NS equations. At infinitely small Knudsen numbers QGD and NS numerical calculations give just the same results [14], [15].

In the present work the simple physical model for the interpretation of the corresponding diffusion terms in (1.1) is proposed and the problem of the macroscopic equations for gas flow is analyzed.

2 Diffusion mechanism

The nonlocal character of collision integral $\mathcal{J}(f)$ in real gases gives rise to the corresponding diffusion terms in the BE. It is determined by the effective long-range interactions connected for example with Van-der-Waals forces [6], [7], caused by the electromagnetic fluctuations. As a result the essentially nonlocal structure of the collision integral have the typical form:

$$\mathcal{J}(f) = \int d^3\vec{r^1}\frac{d^3\vec{p^1}}{(2\pi)^3}(W(\vec{p},\vec{p^1},\vec{r}-\vec{r^1})f(\vec{p^1},\vec{r^1},t) - W(\vec{p^1},\vec{p},\vec{r^1}-\vec{r})f(\vec{p},\vec{r},t)) \tag{2.1}$$

The space homogeneous properties of a real gas cause the usual space dependence of the function W on $(\vec{r}-\vec{r^1})$ only.

There are two main types of inter-atomic interactions in real gases giving rise to two parts of a collision integral. The first part is connected with a short-range repulsion leading to a strong "backward" scattering caused by pair collisions. The second part is connected with a long-range attraction giving rise to a weak "forward" scattering leading to the corresponding diffusion terms in the BE.

Note, that together with long-range Van-der-Vaals forces short-range repulsion (the hard-sphere gas model) always takes place in real gases, and gives considerable contribution in its viscosity. Effective nonlocal motion in this case arises due to long-range interactions by means of intermediate molecular scattering.

The complicated structure of a collision integral leads to large difficulties in the separation of these two effective parts, so it is necessary to use the corresponding Fourier transformation in space coordinates $\vec{r}, \vec{r^1}$. As a result the collision integral in (2.1) is factorized and we can separate the diffusion corrections in the framework of the usual relaxation time approximation.

We shall demonstrate this procedure in the simple case of a Brownian motion for heavy particles in the gas of light particles. In this case the additional long-range interaction between heavy particles arises due to the effective hydrodynamic fluctuations [18], so the scattering of light particles

gives rise to this effect. In this case the spatial width of an effective integral kernel $W(\vec{r}-\vec{r^1})$ in (2.1) is determined by the corresponding mean free path l, so the resulting gradient expansion (1.1) takes place in the system.

3 Transformation of Boltzmann equation

The physical sense of diffusion corrections in the Boltzmann equation is connected with the effective friction mechanism giving rise to a diffusion character of a space motion for gas particles.

We shall consider the mixture of heavy and light particles, described by the usual Fokker- Planck approximation [2], [3]. The motion of heavy particles is determined by the BE

$$f_t + (\vec{v}\nabla)f = \mathcal{J}(f), \tag{3.1}$$

where the usual collision integral $\mathcal{J}(f)$ describes both the energy and momentum relaxation processes. These processes are rather different as it is well-known in the theory of electron-hole plasma in semiconductors [8], [9] and in organic conductors [19], [20].

The collision integral in (3.1) can be written down as

$$\mathcal{J} = \mathcal{J}_0 + \mathcal{J}_1, \tag{3.2}$$

where $\mathcal{J}_0$ describes the scattering of heavy particles by light ones and $\mathcal{J}_1$ - their mutual scattering.

The scattering of light particles by the heavy ones is a quasi-elastic process due to the large mass ratio, so the effective energy transfer is small enough and $\mathcal{J}_0(f)$ is described by the Fokker-Planck approximation [2]:

$$\mathcal{J}_0(f) = \frac{\partial}{\partial\vec{p}}(\vec{A}f + \frac{\partial}{\partial\vec{p}}(Bf)), \quad \vec{A} = B\vec{v}/T, \ B = const. \tag{3.3}$$

As a result the usual ballistic motion of heavy particles assumes a diffusion character.

The energy and momentum relaxation for heavy particles is determined by their mutual collisions now, so we can use the usual time-relaxation approximation for $\mathcal{J}_1(f)$:

$$\mathcal{J}_1(f) = (f_0 - f)\tau^{-1}. \tag{3.4}$$

The effective character of the heavy particle mutual collisions strongly depends on long-range Van-der-Waals interaction and on their diffusion motion, so the nonlocal collision integral $\mathcal{J}_1(f)$ takes place in the system. As a result in the Fourier components over $\vec{r}$, t in equation (3.1) we get

$$i(\omega - \vec{k}\vec{v})f = \mathcal{J}_0(f) + \tau^{-1}(\omega, \vec{k})(f_0 - f). \tag{3.5}$$

Taking into account the weak space dispersion for relaxation time $\tau(\omega, \vec{k})$ we get at small $\vec{k} \to 0$:

$$\tau^{-1}(\omega, \vec{k}) = {\tau_0}^{-1}(1 + \tau_0 D_0 k^2), \tag{3.6}$$

where $D_0 \sim 1/3vl \sim 1/3v^2\tau$ is a diffusion coefficient and the symmetry $\tau(-\vec{k}) = \tau(\vec{k})$ is taken into consideration.

As a result the additional diffusion term appears in the collision integral. Passing it to the left-hand side of BE yields an equation similar to Eq. (1.1), where

$$\mathcal{I} = \mathcal{J}_0 + (f_0 - f){\tau_0}^{-1}. \tag{3.7}$$

It is necessary to mention here that the diffusion terms in the Boltzmann equation were described first by Gogolin [19].

The next term in the corresponding gradient expantion in $\vec{k}$ is of the order of k^4. The resulting additional term would differ by a factor $(\tau(v\nabla))^2$ from the last term retained in Eq. 1.1 and could be taken into account for large M and sufficiently large Kn.

The limit case of equal masses for "heavy" and "light" particles gives just the same results because all the diffusion processes are weakly dependent on the effective mass ratio, so even the corresponding numerical coefficients are just the same in the both limit cases [2] (page 60).

4 Macroscopic gas dynamics equations

Using Boltzmann equation in the both forms (1.1) and (3.1) it is possible to get five differential equations for the macroscopic gas parameters connected with the usual conservation laws for mass, momentum and energy [5].

Multiplying Boltzmann equation by the five collision invariants and performing the integration over velocities $\vec{v}$ we can use the typical macroscopic parameters: density, momentum, total energy, internal energy and pressure. In order to get the closed system of macroscopic equations it is necessary to determine also the corresponding viscosity tensor

$$p_{ij} = \int c_i c_j f d\vec{v}$$

and the vector of heat flow

$$q_i = \frac{1}{2} \int c_i \vec{c}^2 f d\vec{v}$$

through the gas parameters. It is necessary to mention the arising of the higher moments of the fourth order in $\vec{c}$:

$$\pi_{ij} = \frac{1}{2} \int c_i c_j \vec{c}^2 f d\vec{v} \tag{4.1}$$

in the case of the modified Boltzmann equation (1.1).

The macroscopic values $p_{i,j}$ and q_i are well defined for the Euler model and for the NS model [4], [5]. The first model is described by the Maxwell distribution function and the second one by the Navier-Stokes one.

The popular NS model makes it possible to get the moment equations from the BE (3.1) using the Chapman-Enskog or Grad expansions for the description of viscous heat-conducting gas [4], [5]. In order to get QGD equations for viscous heat conducting gas it is enough to consider the Euler gas model only. In this case tensor (4.1) is equal

$$\pi_{ij} = \frac{5}{2}\delta_{ij}\frac{p^2}{\rho}. \tag{4.2}$$

The corresponding averaging over velocities for the collision integral in the Boltzmann equation (3.1) gives zero result. For the equation (1.1) just the same situation must take place

$$\int \mathcal{I}\varphi(\vec{v})d\vec{v} = 0$$

according with the structure of the collision integral $\mathcal{I}$ (for example in the mixture of light and heavy particles (3.7)).

With account of these facts we get the following system of QGD equations [13]:

$$\begin{gathered}
\rho_t + div\rho\vec{u} = div\tau(div\rho\vec{u}\otimes\vec{u} + \vec{\nabla}p) \\
(\rho\vec{u})_t + div(\rho\vec{u}\otimes\vec{u}) + \vec{\nabla}p \\
= div\tau(div\rho\vec{u}\otimes\vec{u}\otimes\vec{u} + (\vec{\nabla}\otimes p\vec{u}) + (\vec{\nabla}\otimes p\vec{u})^T) + \nabla\tau div(p\vec{u})
\end{gathered} \tag{4.3}$$

$$\begin{aligned}
E_t + div((E+p)\vec{u}) = {} & div\tau(div(E+2p)\vec{u}\otimes\vec{u} + 0.5\vec{\nabla}p\vec{u}^2) + \\
& \frac{\gamma}{\gamma-1}div\frac{\tau p}{\rho}\nabla p + \frac{\gamma}{Pr(\gamma-1)}div\tau p\nabla\frac{p}{\rho}.
\end{aligned}$$

The system of equations (4.3) is closed with account of the state equations and boundary conditions.

The value of τ in the equations (4.3) is connected with the usual viscosity μ by the relation $\mu = \tau\, p$, so the corresponding analogy between these equations and NS ones is pointed out in [13], [14]. In particular it was shown that QGD and NS systems are closed one to another when $\tau \to 0$ with the accuracy $O(\tau^2)$.

The expressions for dissipative terms in QGD and NS models are different, but in the both cases dissipation is proportional to the mean free-path l, because it is determined by particle collisions. In the dense gases

short-range scattering is greater compared with long-range forces and the differences in QGD and NS systems seems to be small. In rarefied gases due to relatively rare collisions long-range forces are more significant and the difference between QGD and NS models occurs more important. It is proved by the results of numerical calculations [15].

The special exprassions for f based on Grad or Chapman-Enskog expansions are not necessary in the framework of QGD because the corresponding small parameter arises in the system from the collision integral and the usual Euler model with the equilibrium distribution function instead of NS one is sufficient there.

5 Conclusions

In conclusion it is necessary to mention that our theory is not rigorous, so it cannot determine the exact expression for the corresponding diffusion term in Eq. 1.1. The concrete form of diffusion term was successfully chosen by the authors in [10] - [14], because in was good not only for numerical calculations but also give the opportunity to get some theoretical results for QGD system [13], [14].

Having extracted the diffusive part from the collision integral, Eq. 1.1 allows to derive macroscopic equations that include viscosity and heat transfer even for the equilibrium distribution function, instead of introducing a special "Navier-Stokes" expression for f. Local characteristic time τ is then identified as equal to μ/p where μ and p denote dynamic viscosity and pressure, respectively.

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