Some Properties of a Gas with an Ellipsoidal Velocity Distribution Function

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1 Introduction

Increasing the Knudsen number in a monoatomic gas results first in a violation of translational equilibrium. Different translational temperatures in different directions have been evidenced by molecular methods in, e.g., shock waves and jet flows [1].

Transport and relaxation phenomena in gases are related with a collisional time τ_c (or with a translational relaxation time τ). The purpose of this work is to express the collisional time in terms of direction-dependent temperatures T_x, T_y, T_z, rather than in terms of a unique temperature T, when the gas is characterized by an ellipsoidal distribution function. Results on mean thermal velocity, mean relative velocity and mean free path will also be obtained.

Based on these results, the consequences of translational nonequilibrium on the solution of moment equations will be discussed.

2 Relative velocity and thermal velocity

A non isotropic (ellipsoidal) distribution function f_e in cartesian co-ordinates can be written based on different temperatures in the different directions as

$$f_e = \frac{\rho}{(2\pi R)^{3/2}(T_x T_y T_z)^{1/2}} \exp\left(\frac{-c_x{}^2}{2RT_x}\right) \times \exp\left(\frac{-c_y{}^2}{2RT_y}\right) \times \exp\left(\frac{-c_z{}^2}{2RT_z}\right).$$

Using the same technique as used by Bird [1] for a Maxwellian distribution function, the mean relative velocity of gas molecules (1) and (2) is calculated as

$$< c_r > = \rho^{-2} \iint |\vec{c}_1 - \vec{c}_2| \, f_e(\vec{c}_1) \, f_e(\vec{c}_2) \, d\vec{c}_1 \, d\vec{c}_2 =$$

$$\pi^{-3} \iint \sqrt{(c_{x1} - c_{x2})^2 + (c_{y1} - c_{y2})^2 + (c_{z1} - c_{z2})^2}$$

$$\times \exp\left(-\frac{c_{x1}^2 + c_{x2}^2}{2\,R\,T_x}\right) \times \exp\left(-\frac{c_{y1}^2 + c_{y2}^2}{2\,R\,T_y}\right) \times \exp\left(-\frac{c_{z1}^2 + c_{z2}^2}{2\,R\,T_z}\right)$$

$$\times \frac{dc_{x1}}{\sqrt{2\,R\,T_x}} \frac{dc_{x2}}{\sqrt{2\,R\,T_x}} \frac{dc_{y1}}{\sqrt{2\,R\,T_y}} \frac{dc_{y2}}{\sqrt{2\,R\,T_y}} \frac{dc_{z1}}{\sqrt{2\,R\,T_z}} \frac{dc_{z2}}{\sqrt{2\,R\,T_z}},$$

where $\vec{c}$ is the thermal velocity, R is the perfect-gas constant and ρ is the density.

We introduce the variables

$$\frac{c_{xk}}{\sqrt{2RT_x}} = a_{xk}, \qquad \frac{c_{yk}}{\sqrt{2RT_y}} = a_{yk}, \qquad \frac{c_{zk}}{\sqrt{2RT_z}} = a_{zk},$$

where $k = 1, 2$ and $A = 2RT_x, \quad B = 2RT_y, \quad C = 2RT_z$.

To factorize the six-dimensional integral $< c_r >$, we introduce the relative velocity and the velocity of the center of mass of colliding molecules

$$\vec{w}_m = \frac{\vec{a}_1 + \vec{a}_2}{2}, \qquad \vec{w}_r = \vec{a}_1 - \vec{a}_2,$$

where $\vec{a}_k = (a_{xk}, a_{yk}, a_{zk})$, $\vec{w}_m = (w_{mx}, w_{my}, w_{mz})$, $\vec{w}_r = (w_{rx}, w_{ry}, w_{rz})$.

The integral takes the form

$$< c_r > =$$

$$\frac{1}{\pi^3} \int \sqrt{A w_{rx}^2 + B w_{ry}^2 + C w_{rz}^2} \times \exp(-\tfrac{w_{rx}^2}{2}) \exp(-\tfrac{w_{ry}^2}{2}) \exp(-\tfrac{w_{rz}^2}{2}) \, d\vec{w}_r$$

$$\times \int \exp(-2w_{mx}^2) \exp(-2w_{my}^2) \exp(-2w_{mz}^2) \, d\vec{w}_m = \frac{1}{\pi^3} I_1 \times I_2.$$

It differs from the corresponding integral for the case $f = f_0$ by the presence of coefficients $A \neq B \neq C$. Integral I_2 is equal to $I_2 = (\sqrt{\pi}/\sqrt{2})^3$.
To calculate integral I_1, we switch to spherical coordinates

$$x = r\sin\theta\cos\phi, \qquad y = r\sin\theta\sin\phi, \qquad z = r\cos\theta.$$

Accounting for the jacobian of the transformation

$$\frac{D(x, y, z)}{D(r, \theta, \phi)} = r^2 \sin\theta, \quad \text{we get}$$

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$$
\begin{aligned}
I_1 \;=\;& 4 \iiint \sqrt{A\, r^2 \sin^2\theta \cos^2\phi + B\, r^2 \sin^2\theta \sin^2\phi + C\, r^2 \cos^2\theta} \\
& r^2 \sin\theta \exp(-r^2)\, dr\, d\theta\, d\phi = 4 \int_0^\infty r^3 \exp(-r^2) dr \times \\
& \int_0^\pi \sin\theta \left[\int_0^{2\pi} \sqrt{A \sin^2\theta \cos^2\phi + B \sin^2\theta \sin^2\phi + C \cos^2\theta}\, d\phi \right] d\theta.
\end{aligned}
$$

The first integral is equal to $1/2$ and the other one is impossible to calculate in an explicit form. We write

$$
< c_r > = \frac{1}{\pi\sqrt{2\pi}} \times \mathrm{Int}(A, B, C),
$$

where

$$
\mathrm{Int}(A, B, C) = \int_0^\pi \sin\theta \int_0^{2\pi} \sqrt{A \sin^2\theta \cos^2\phi + B \sin^2\theta \sin^2\phi + C \cos^2\theta}\, d\phi\, d\theta.
$$

Similarly we calculate the mean thermal velocity:

$$
\begin{aligned}
< c > =& \frac{1}{\rho} \int c f_e\, d\vec{c} = \frac{1}{\sqrt{\pi^3}} \int \sqrt{c_x^2 + c_y^2 + c_z^2} \\
& \times \exp\left(-\frac{c_x^2}{2RT_x}\right) \exp\left(-\frac{c_y^2}{2RT_y}\right) \exp\left(-\frac{c_z^2}{2RT_z}\right) \frac{dc_x}{\sqrt{2RT_x}} \frac{dc_y}{\sqrt{2RT_y}} \frac{dc_z}{\sqrt{2RT_z}}.
\end{aligned}
$$

After similar transformations we get

$$
< c > = \mathrm{Int}(A, B, C) / \left[2\sqrt{\pi^3} \right].
$$

Thus the ratio between the mean relative velocity and the mean thermal velocity is equal to

$$
< c_r > / < c > = \sqrt{2},
$$

as in an equilibrium gas. This conclusion is interesting in itself and moreover it has a consequence on the mean free path λ in a hard-sphere gas of total collisional cross-section σ_0 and number density n:

$$
\lambda = \frac{< c >}{< c_r >} \times \frac{1}{n\,\sigma_0} = \frac{1}{\sqrt{2}\, n\, \sigma_0}
$$

both for gas with Maxwellian or ellipsoidal distribution functions.

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3   Two-temperature gas

We consider the (extreme) particular nonequilibrium case, with $A = B \neq C$, which corresponds to $T_x = T_y \neq T_z$. Such a situation is encountered, e.g., in the problem of shock wave structure, in the 1D relaxation problem, in the 1D gas expansion problem and in a number of other situations where the flow velocity is directed along the $z-$axis. In these cases the integral $\text{Int}(A, B, C)$ can be found explicitly as

$$\text{Int}(A, C) = 2\pi \int_0^\pi \sin\theta \, \sqrt{A \sin^2\theta + C \cos^2\theta} \, d\theta.$$

For $A < C$ or $T_x = T_y < T_z$, we find

$$\text{Int}(A, C) = 2\pi\sqrt{C} \left(1 + \frac{A}{2\sqrt{C(C-A)}} \ln \frac{\sqrt{C} + \sqrt{C-A}}{\sqrt{C} - \sqrt{C-A}} \right).$$

For $A > C$ or $T_x = T_y > T_z$, we find

$$\text{Int}(A, C) = 2\pi\sqrt{C} \left(1 + \frac{A}{\sqrt{C(A-C)}} \arcsin \frac{\sqrt{A-C}}{A} \right).$$

In both cases, the resulting expression of $< c_r >$ is

$$< c_r >= 2\sqrt{\frac{RT_z}{\pi}} (1 + \mathcal{A}(T_z, T_x)),$$

where

$$\mathcal{A}(T_z, T_x) = \begin{cases} \dfrac{T_x}{2\sqrt{T_z(T_z - T_x)}} \times \ln \dfrac{\sqrt{T_z} + \sqrt{T_z - T_x}}{\sqrt{T_z} - \sqrt{T_z - T_x}} & \text{if } T_x < T_z, \\[4mm] \dfrac{T_x}{\sqrt{T_z(T_x - T_z)}} \times \arcsin\sqrt{\dfrac{T_x - T_z}{T_x}} & \text{if } T_x > T_z. \end{cases}$$

When $T_x \to T_z$, both expressions result in $\mathcal{A} \to 1$, and $< c_r >\to 4\sqrt{RT/\pi}$ which is the mean relative velocity in an equilibrium gas.

Other details can be found in [2].

Mean collisional time and mean thermal velocity

The mean collisional time τ_c and the mean collision frequency ν are given by

$$\tau_c = 1/\nu = 1/(n < \sigma \, c_r >)$$

where σ is the total collisional cross-section.

For the limiting case of **hard-sphere molecules** ($\sigma = \sigma_0 = $ cste)

$$< \sigma c_r > = \sigma_0 < c_r > \qquad \text{and} \qquad \tau_c = 1/(n\,\sigma_0 < c_r >).$$

We calculate the ratio of the collisional times $\tau_{c,e}$ and $\tau_{c,0}$ in gases with ellipsoidal distribution function (temperatures T_x, T_z) and with maxwellian distribution function (temperature $T = (1/3)(T_z + 2T_x)$), respectively:

$$\frac{\tau_{c,e}}{\tau_{c,0}} = \frac{2\sqrt{T}}{\sqrt{T_z}(1 + \mathcal{A}(T_z, T_x))}.$$

The variation of $\tau_{c,e}/\tau_{c,0}$ against $\triangle T/T$ is plotted in Fig.1, where $\triangle T = T_z - T_x$ ($T_x = T - \triangle T/3$, $T_z = T + 2\triangle T/3$).

For $\triangle T = 0$, $T_x = T_z = T$, $\mathcal{A} = 1$ and $\tau_{c,e} = \tau_{c,0}$.

When $\triangle T$ increases ($T_z > T_x$), the value of $\tau_{c,e}$ increases monotonically and reaches a maximum value equal to $1.15\,\tau_{c,0}$ for $\triangle T = 3T$, which corresponds to $T_x = 0$, $T_z = 3T$.

When $\triangle T$ decreases ($T_z < T_x$), the value of $\tau_{c,e}$ increases monotonically again and reaches a maximum value equal to $1.04\,\tau_{c,0}$ for $\triangle T = -(3/2)\,T$, which corresponds to $T_z = 0$, $T_x = (3/2)\,T$.

In the limiting case of **hard-sphere molecules** with an ellipsoidal distribution function, $\tau_{c,e} \geq \tau_{c,0}$ and differs by at most 15 % from an equilibrium gas estimation based on the average temperature T.

In the other limiting case of **Maxwell molecules**, σ is proportional to c_r^{-1} and τ_c does not depend on molecular velocities. We have always $\tau_{c,e} = \tau_{c,0}$.

Thus for realistic gases the mean collisional time always surpasses the equilibrium one and can be estimated from the mean temperature with an accuracy better than 15%.

The variation of mean thermal velocity with nonequilibrium is deduced from the above formulae, remembering that $< c_r > = \sqrt{2} < c >$ for a Maxwellian as well as for an ellipsoidal distribution function:

$$\frac{< c_e >}{< c_0 >} = \frac{< c_{r,e} >}{< c_{r,0} >} = \left(\frac{\tau_{c,e}}{\tau_{c,0}}\right)^{-1} = \frac{\sqrt{T_z}(1 + \mathcal{A}(T_z, T_x))}{2\sqrt{T}}.$$

Thus the mean thermal velocity and the mean relative velocity are smaller when calculated based on direction-dependent temperatures, than based on the mean translational temperature.

It is straightforward to derive similar results for a 3-temperature gas. They involve the integral $\text{Int}(A, B, C)$ which cannot be expressed explicitely, but can be tabulated for practical applications.

4 Transport properties and consequences

When considering moment equations for a 3-temperature gas, the problem arises of expressing scalar quantities such as the viscosity coefficient μ and the pressure p in terms of temperature(s).

The present work was undertaken to treat this question for the Quasigas-dynamic (QGD) equations [2, 3]. These equations involve a translational relaxation time τ.

In the particular case of small Knudsen number with a unique translational temperature, QGD equations reduce to Navier-Stokes equations and τ coincides with μ/p. Thus we can relate τ with the mean collision time τ_c. We model the actual molecules by Variable Hard Sphere (VHS) molecules, characterized by $\mu \propto T^\omega$, intermediate between hard-sphere ($\omega = 1/2$) and Maxwell ($\omega = 1$) molecules. According to Bird [1], we have

$$\tau_c = \frac{1}{\nu} = \frac{\mu}{p} \times \frac{(7 - 2\omega)(5 - 2\omega)}{30} = \tau \times \frac{(7 - 2\omega)(5 - 2\omega)}{30}$$

and it is clear that the ratio τ/τ_c is of the order of unity and depends only on ω, i.e. on the intermolecular potential. It seems reasonable to assume that the ratio of these two scalar quantities is not affected by the anisotropy of the distribution function and we can derive the expressions of $\tau(T_x, T_y, T_z)$ from the expressions for τ_c. Thus τ differs by at most 15% from its value based on the average temperature.

The classical problems of 1-D translational relaxation and shock wave structure in a monoatomic gas have been solved on the basis of three-temperature QGD equations [2, 3]. A DSMC calculation was used as a reference. Here we consider the "worst case" of hard-sphere molecules and we compare the results obtained when τ is expressed as a fonction of the average translational temperature T or as a function of the two temperatures T_x and T_z. The profiles of macroscopic flow parameters were compared. The differences in the results were found to be negligibly small and could not be distinguished in the figures.

5 Conclusion

- Expressions for mean relative velocity, mean thermal velocity and mean collisional time have been obtained for a gas characterized by an ellipsoidal velocity distribution function.

- Explicit forms of these expressions were found in the particular case of a two-temperature gas.
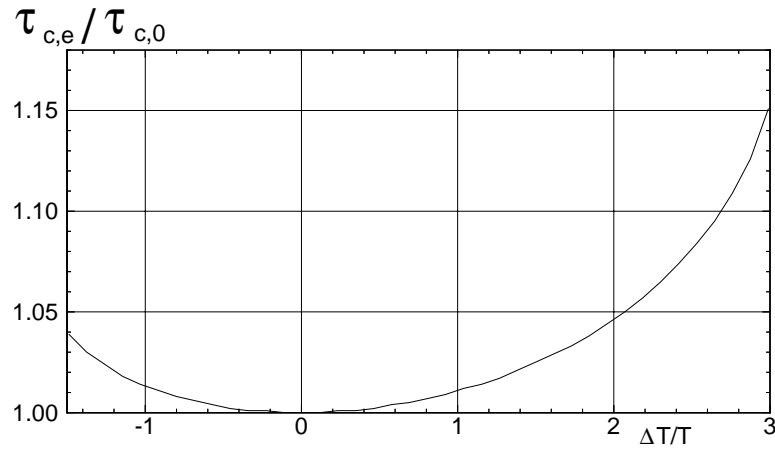
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Figure 1: Variation of collisional time with translational nonequilibrium (hard-sphere molecules)

- These quantities differ by at most 15% from the values estimated on the basis of the average translational temperature.

- An expression for the translational relaxation time involved in the Quasigasdynamic equations was obtained.

- When applied to the problems of 1-D translational relaxation and of shock wave structure, this expression introduced negligible difference on the results, compared with the expression based on the average translational temperature. Thus for practical application, τ may be calculated based on the average temperature.

References

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