THE BGK MODEL FOR AN IDEAL GAS WITH AN INTERNAL DEGREE OF FREEDOM

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Abstract

The BGK model for an ideal gas with an internal degree of freedom introduces two characteristic times into the Boltzmann equation, accounting for the times between elastic and inelastic collisions, respectively. Moment equations are derived from the Boltzmann equation and the influence of the characteristic times is studied for some processes, such as heating, sound waves and shocks.

1 Introduction

There are two different interaction mechanisms in an ideal gas with an internal degree of freedom:
1.) Elastic collisions ($\mathcal{E}$), which do not change the internal degree of freedom of the particles.
2.) Inelastic collisions ($\mathcal{I}$) which do change the internal degree of freedom and supply or remove energy from the particles.

The present paper examines the influence of these interactions on the behavior of a gas by means of the Boltzmann equation with a BGK collision term.

In the BGK model each interaction mechanism $\alpha = \mathcal{E}, \mathcal{I}$ is characterized by a relaxation time τ_α and an equilibrium phase density f_α. The relaxation time τ_α may be interpreted as the mean time of free flight between collisions of the type α. The equilibrium phase density follows from the maximization of entropy under the constraints of given values for those macroscopic quantities which remain unchanged in collisions of type α.

Integration of the BGK equation leads to moment equations for mass density, momentum density, energy density, pressure tensor and heat flux. These are solved for some simple processes, such as heating, sound waves and shocks. It is shown that the specific heat and the sound speed depend on the ratio of the relaxation times

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$\tau_{\mathcal{I}}/\tau_{\mathcal{E}}$; the same is true for the shock structure. A Maxwellian iteration shows that viscosity and heat conductivity depend on an average characteristic time τ only, which is given by $\frac{1}{\tau}=\frac{1}{\tau_{\mathcal{E}}}+\frac{1}{\tau_{\mathcal{I}}}$.

Although the gas under consideration is not realistic we think that the paper is instructive for two reasons:
1.) It shows how the entropy maximum principle may be used in order to construct BGK collision terms for arbitrary particle interactions.
2.) It provides a simple system where the influence of two distinct characteristic times may be studied by analytical solutions of simple processes.

2 Ideal Gas with an Internal Degree of Freedom

2.1 Phase density

We consider a model gas whose particles are assumed to have an internal degree of freedom which is characterized by a number n, such that $E_n,\ n=0,1,2,\dots$ is the internal energy of the particle.

For detailed calculations we shall assume that the particles are quantum oscillators with

$$E_n=\hbar n\Omega \tag{1}$$

where $\hbar$ is Planck's constant and Ω is a frequency. E_n may be called "vibration energy". Thus the reader may think of a diatomic gas with vibrating molecules. We do not consider the rotation of the molecules.

The phase density f_n of the gas is defined such that $f_n\left(x_i,t,c_i\right)d\mathbf{c}$ gives the number density of particles in the energetic state n with velocities in the range $\left(c_i,c_i+dc_i\right)$ at the point x_i and time t. Once the phase density f_n is known, we may calculate macroscopic quantities by integration over the particle velocities and by summation over the energetic states. Macroscopic quantities with obvious meaning are given below:

$$\begin{aligned}
&\varrho_n=m\int f_n d\mathbf{c} &&\text{mass density of particles in state } n\\
&\varrho=\sum_n\varrho_n &&\text{mass density}
\end{aligned}\tag{2}$$

$\varrho v_i = \sum_n m \int c_i f_n d\mathbf{c}$	momentum density
$\varrho\varepsilon = \sum_n \frac{m}{2} \int C^2 f_n d\mathbf{c}$	density of thermal energy
$\varrho u = \sum_n \int E_n f_n d\mathbf{c} = \sum_n \varrho_n E_n$	density of vibration energy
$p_{ij} = \sum_n m \int C_i C_j f_n d\mathbf{c}$	pressure tensor
$q_i = \sum_n \frac{m}{2} \int C^2 C_i f_n d\mathbf{c}$	heat flux

Here, m denotes the mass of a particle and $C_i = c_i - v_i$ is the peculiar velocity, i.e. the particle velocity measured in a frame which moves with the center of mass velocity v_i.

We shall also need the entropy of the gas which is given by

$$\varrho s = -k \sum_n \int f_n \ln \frac{f_n}{y} d\mathbf{c} \tag{3}$$

where k is Boltzmann's constant and y is the volume of a cell of phase space.

By $(2)_{4,6}$ we find that the trace of the pressure tensor equals twice the energy density. The pressure is given by

$$p = \frac{1}{3} p_{ii} = \frac{2}{3} \varrho\varepsilon \ , \tag{4}$$

so that the pressure tensor may be written as

$$p_{ij} = p\delta_{ij} + p_{\langle ij \rangle} \ , \tag{5}$$

where the brackets denote the symmetric and trace-free part. As usual, temperature is defined by the ideal gas law

$$p = \varrho \frac{k}{m} T \qquad \text{so that} \qquad \varepsilon = \frac{3}{2} \frac{k}{m} T \ . \tag{6}$$

We assume that particles in all states have the same velocity and temperature, i.e.

$$m \int c_i f_n d\mathbf{c} = \varrho_n v_i \qquad \text{and} \qquad \frac{m}{2} \int C^2 f_n d\mathbf{c} = \varrho_n \varepsilon \ . \tag{7}$$

2.2 Boltzmann Equation and Balance Laws

The phase density f_n obeys the Boltzmann equation

$$\frac{\partial f_n}{\partial t} + c_i \frac{\partial f_n}{\partial x_i} = \mathcal{E}_n + \mathcal{I}_n \ , \tag{8}$$

where $\mathcal{E}_n$ and $\mathcal{I}_n$ are collision terms. We have to consider two collision terms because there are two interactions between the particles: $\mathcal{E}_n$ refers to elastic collisions where the energetic states of the particles remain unchanged and $\mathcal{I}_n$ refers to inelastic collisions where the energetic states are changed. Expressions for $\mathcal{E}_n$ and $\mathcal{I}_n$ will be derived in the next subsection.

Multiplication of the Boltzmann equation with $m, c_i, \frac{m}{2}C^2$ and E_n and subsequent integration and summation yields balance equations for the quantities (2), viz.

$$\begin{aligned}
\frac{\partial \varrho_n}{\partial t}+\frac{\partial \varrho_n v_i}{\partial x_i} &= m\int \mathcal{I}_n d\mathbf{c} \\
\frac{\partial \varrho}{\partial t}+\frac{\partial \varrho v_i}{\partial x_i} &= 0 \\
\frac{\partial \varrho v_i}{\partial t}+\frac{\partial \varrho v_i v_j + p_{ij}}{\partial x_j} &= 0 \\
\frac{\partial \varrho\varepsilon}{\partial t}+\frac{\partial \varrho\varepsilon v_i + q_i}{\partial x_i}+p_{ij}\frac{\partial v_i}{\partial x_j} &= \frac{m}{2}\sum_n\int C^2\mathcal{I}_n d\mathbf{c} \\
\frac{\partial \varrho u}{\partial t}+\frac{\partial \varrho u v_i}{\partial x_i} &= m\sum_n E_n\int \mathcal{I}_n d\mathbf{c}\ .
\end{aligned} \tag{9}$$

Here we have assumed that the elastic collisions do not change the number of particles of state n, nor do they change momentum and thermal energy, so that we have

$$m\int \mathcal{E}_n d\mathbf{c}=0\ ,\qquad m\sum_n\int c_i\mathcal{E}_n d\mathbf{c}=0\ ,\qquad \frac{m}{2}\sum_n\int C^2\mathcal{E}_n d\mathbf{c}=0\ . \tag{10}$$

Inelastic collisions do not contribute to changes in total number, momentum and energy, so that we have

$$\begin{aligned}
& m\sum_n\int \mathcal{I}_n d\mathbf{c}=0 \qquad ,\quad m\sum_n\int c_i\mathcal{I}_n d\mathbf{c}=0\ , \\
& \frac{m}{2}\sum_n\int C^2\mathcal{I}_n d\mathbf{c}+m\sum_n E_n\int \mathcal{I}_n d\mathbf{c}=0\ .
\end{aligned} \tag{11}$$

Note that the flux of internal energy in $(9)_1$ is given by $\varrho u v_i$ - thus the transport of internal energy is purely convective.

2.3 BGK Model

2.3.1 Elastic Collisions

We assume that the collision term for elastic collisions has the BGK form [1]

$$\mathcal{E}_n=-\frac{1}{\tau_{\mathcal{E}}}\left(f_n-f_{\mathcal{E}_n}\right)\ , \tag{12}$$

where $\tau_\mathcal{E}$ is a relaxation time and $f_{\mathcal{E}_n}$ is an equilibrium distribution. In fact $f_{\mathcal{E}_n}$ is *the* equilibrium distribution which maximizes the entropy (3) under the constraint of prescribed values for those macroscopic quantities that are conserved in elastic collisions, i.e. ϱ_n, ϱv_i and $\varrho\varepsilon$. The first step of the maximization process provides

$$f_{\mathcal{E}_n} = y \exp\left\{-1 - \frac{m}{k}\left(\lambda_{\varrho_n} - \lambda_{v_i} C_i - \lambda_\varepsilon \frac{1}{2} C^2\right)\right\} \tag{13}$$

where $\lambda_{\varrho_n}, \lambda_{v_i}$ and λ_ε are Lagrange multipliers which must be determined from the conservation requirements (10). We obtain the Maxwell-Boltzmann phase density

$$f_{\mathcal{E}_n} = \frac{\varrho_n}{m}\sqrt{\frac{3}{4\pi\varepsilon}}^3 \exp\left\{-\frac{3}{4\varepsilon}C^2\right\} = \frac{\varrho_n}{m}\sqrt{\frac{m}{2\pi kT}}^3 \exp\left\{-\frac{m}{2kT}C^2\right\} . \tag{14}$$

The relaxation time $\tau_\mathcal{E}$ should be interpreted as the mean time of free flight of a particle between elastic collisions. $\tau_\mathcal{E}$ accounts for elastic collisions of a particle of energetic state n with all other particles. Thus $\tau_\mathcal{E}$ will depend on the total mass density by the well-known formula $1/\tau_\mathcal{E} = \frac{\varrho}{m}\sigma_\mathcal{E}\bar{g}$ - where $\sigma_\mathcal{E}$ is the cross section for elastic collisions and $\bar{g} = \sqrt{\frac{16}{\pi}\frac{k}{m}T}$ is the mean relative speed. Therefore $\tau_\mathcal{E}$ has the same value for all n.

2.3.2 Inelastic Collisions

We assume that the collision term for elastic collisions has the BGK form

$$\mathcal{I}_n = -\frac{1}{\tau_\mathcal{I}}\left(f_n - f_{\mathcal{I}_n}\right) , \tag{15}$$

where $\tau_\mathcal{I}$ is a relaxation time and $f_{\mathcal{I}_n}$ is an equilibrium distribution. In fact $f_{\mathcal{I}_n}$ is *the* equilibrium distribution which maximizes the entropy (3) under the constraint of prescribed values for those macroscopic quantities which are conserved in inelastic collisions, i.e. ϱ, ϱv_i and $\varrho\varepsilon + \varrho u$. Now the first step of the maximization process provides

$$f_{\mathcal{I}_n} = y \exp\left\{-1 - \frac{m}{k}\left(\lambda_\varrho - \lambda_{v_i} C_i - \Lambda\left(\frac{m}{2}C^2 + E_n\right)\right)\right\} , \tag{16}$$

where $\lambda_\varrho, \lambda_{v_i}$ and Λ are Lagrange multipliers which must be determined from the conservation requirements (11). We obtain

$$f_{\mathcal{I}_n} = \frac{\varrho_{\mathcal{I}_n}}{m}\sqrt{\frac{3}{4\pi\varepsilon_\mathcal{I}}}^3 \exp\left\{-\frac{3}{4\varepsilon_\mathcal{I}}C^2\right\} = \frac{\varrho_{\mathcal{I}_n}}{m}\sqrt{\frac{m}{2\pi kT_\mathcal{I}}}^3 \exp\left\{-\frac{m}{2kT_\mathcal{I}}C^2\right\} , \tag{17}$$

where $\varepsilon_\mathcal{I} = \frac{3}{2}\frac{k}{m}T_\mathcal{I}$ - the thermal energy corresponding to $f_{\mathcal{I}_n}$ - is the solution of

$$\begin{aligned} \varrho\varepsilon + \varrho u &= \varrho\varepsilon_\mathcal{I}\left(1 + \frac{\sum_n \frac{E_n}{m\varepsilon_\mathcal{I}} \exp\left\{-\frac{3E_n}{2m\varepsilon_\mathcal{I}}\right\}}{\sum_n \exp\left\{-\frac{3E_n}{2m\varepsilon_\mathcal{I}}\right\}}\right) \\ &= \varrho\frac{k}{m}T_\mathcal{I}\left(\frac{3}{2} + \frac{\sum_n \frac{E_n}{kT_\mathcal{I}} \exp\left\{-\frac{E_n}{kT_\mathcal{I}}\right\}}{\sum_n \exp\left\{-\frac{E_n}{kT_\mathcal{I}}\right\}}\right) \end{aligned} \tag{18}$$

and the density $\varrho_{\mathcal{I}_n}$ is defined by

$$\varrho_{\mathcal{I}_n} = \varrho \frac{\exp\left\{-\frac{3E_n}{2m\varepsilon_{\mathcal{I}}}\right\}}{\sum_n \exp\left\{-\frac{3E_n}{2m\varepsilon_{\mathcal{I}}}\right\}} = \varrho \frac{\exp\left\{-\frac{E_n}{kT_{\mathcal{I}}}\right\}}{\sum_n \exp\left\{-\frac{E_n}{kT_{\mathcal{I}}}\right\}} \; . \tag{19}$$

Insertion of (1) in (18) yields

$$\varrho\varepsilon + \varrho u = \varrho\varepsilon_{\mathcal{I}} + \frac{\varrho}{m} \frac{\hbar\Omega}{\exp\left\{\frac{3\hbar\Omega}{2m\varepsilon_{\mathcal{I}}}\right\} - 1} \tag{20}$$

and this can only be solved analytically for $\varepsilon_{\mathcal{I}}$ if $\frac{\hbar\Omega}{m\varepsilon_{\mathcal{I}}} \ll 1$. We obtain in that approximation

$$\varepsilon_{\mathcal{I}} = \frac{3}{5}\left(\varepsilon + u\right) \qquad \left(\frac{\hbar\Omega}{m\varepsilon_{\mathcal{I}}} \ll 1\right) \; . \tag{21}$$

The last equation may be rearranged for the equilibrium temperature $T_{\mathcal{I}}$,

$$T_{\mathcal{I}} = \frac{3}{5}T + \frac{u}{\frac{5}{2}\frac{k}{m}} \qquad \left(\frac{\hbar\Omega}{kT_{\mathcal{I}}} \ll 1\right) . \tag{22}$$

The relaxation time $\tau_{\mathcal{I}}$ may be interpreted as the mean time free flight of a particle between inelastic collisions. By the same argument as in the elastic case we have $1/\tau_{\mathcal{I}} = \frac{\varrho}{m}\sigma_{\mathcal{I}}\bar{g}$ and $\tau_{\mathcal{I}}$ has the same value for all n.

The proof of the H-Theorem for the Boltzmann equation (8) with BGK interaction terms (12, 15) is given in Section 2.4.

2.3.3 Balance Laws

With the collision terms (12, 15) we may write the right hand sides of $(9)_{4,5}$ as

$$\frac{m}{2}\sum_n \int C^2 \mathcal{I}_n d\mathbf{c} = -\frac{1}{\tau_{\mathcal{I}}}\sum_n \left(\varrho_n\varepsilon - \varrho_{\mathcal{I}_n}\varepsilon_{\mathcal{I}}\right) = -\frac{1}{\tau_{\mathcal{I}}}\varrho\left(\varepsilon - \varepsilon_{\mathcal{I}}\right) \; . \tag{23}$$

The mean free time of elastic collisions will come into play when we consider viscosity and heat conductivity in the next section.

We finish this section with the equations (9) which may now be rewritten as

$$\begin{aligned} \frac{D\varrho}{Dt} + \varrho\frac{\partial v_i}{\partial x_i} &= 0 \\ \frac{Dv_i}{Dt} + \frac{1}{\varrho}\frac{\partial p}{\partial x_i} + \frac{1}{\varrho}\frac{\partial p_{\langle ij\rangle}}{\partial x_j} &= 0 \\ \frac{D\varepsilon}{Dt} + \frac{1}{\varrho}\frac{\partial q_i}{\partial x_i} + \frac{p}{\varrho}\frac{\partial v_i}{\partial x_i} + \frac{p_{\langle ij\rangle}}{\varrho}\frac{\partial v_{\langle i}}{\partial x_{j\rangle}} &= -\frac{1}{\tau_{\mathcal{I}}}\left(\varepsilon - \varepsilon_{\mathcal{I}}\right) \\ \frac{Du}{Dt} &= \frac{1}{\tau_{\mathcal{I}}}\left(\varepsilon - \varepsilon_{\mathcal{I}}\right) \end{aligned} \tag{24}$$

with $\varepsilon_{\mathcal{I}}$ given by (18) and the material derivative defined as $\frac{D}{Dt}=\frac{\partial}{\partial t}+v_i\frac{\partial}{\partial x_i}$.

Note that in total equilibrium $\varrho_n=\varrho_{\mathcal{I}_n}$ and $\varepsilon=\varepsilon_{\mathcal{I}}$ hold. Thus the phase density $f_{\mathcal{I}_n}$ belongs to total equilibrium while the phase density $f_{\mathcal{E}_n}$ belongs to an intermediate state, where the distribution function is isotropic and thermalized, but the partial densities ϱ_n have not yet reached their equilibrium values $\varrho_{\mathcal{I}_n}$.

2.4 Entropy and H-Theorem

For the construction of the entropy balance we take the time derivative of (3) and eliminate $\frac{\partial f_n}{\partial t}$ by use of the Boltzmann equation (8). The result reads

$$\frac{\partial \varrho s}{\partial t}+\frac{\partial \phi_k}{\partial x_k}=\sigma \tag{25}$$

where entropy flux ϕ_k and entropy production σ are given by

$$\phi_k=-k\sum_n\int c_i f_n\ln\frac{f_n}{y}d\mathbf{c} \quad , \quad \sigma=-k\sum_n\int\ln\frac{f_n}{y}\left(\mathcal{E}_n+\mathcal{I}_n\right)d\mathbf{c}\ . \tag{26}$$

Now we prove the H-Theorem, i.e. we prove that the entropy production σ is non-negative. By means of the conservation requirements (10, 11) we find that for the equilibrium distributions $f_{\mathcal{E}_n}, f_{\mathcal{I}_n}$ (14, 17) we have

$$-k\sum_n\int\ln\frac{f_{\mathcal{E}_n}}{y}\mathcal{E}_n d\mathbf{c}=0 \quad , \quad -k\sum_n\int\ln\frac{f_{\mathcal{I}_n}}{y}\mathcal{I}_n d\mathbf{c}=0\ . \tag{27}$$

Thus we may write the entropy production as

$$\sigma=-k\sum_n\int\ln\frac{f_n}{f_{\mathcal{E}_n}}\mathcal{E}_n d\mathbf{c}-k\sum_n\int\ln\frac{f_n}{f_{\mathcal{I}_n}}\mathcal{I}_n d\mathbf{c}\ , \tag{28}$$

or - with (12, 15) - as

$$\sigma=\frac{k}{\tau_{\mathcal{E}}}\sum_n\int\ln\frac{f_n}{f_{\mathcal{E}_n}}\left(f_n-f_{\mathcal{E}_n}\right)d\mathbf{c}+\frac{k}{\tau_{\mathcal{I}}}\sum_n\int\ln\frac{f_n}{f_{\mathcal{I}_n}}\left(f_n-f_{\mathcal{I}_n}\right)d\mathbf{c}\geq 0\ . \tag{29}$$

This completes the proof of the H-Theorem.

We proceed with the calculation of the entropies corresponding to the phase densities $f_{\mathcal{E}_n}, f_{\mathcal{I}_n}$. The entropy for the intermediate state $f_{\mathcal{E}_n}$ comes out as

$$s_{\mathcal{E}}=-\frac{k}{\varrho}\sum_n\int f_{\mathcal{E}_n}\ln\frac{f_{\mathcal{E}_n}}{y}d\mathbf{c}=\frac{3}{2}\frac{k}{m}\ln T-\frac{k}{m}\ln\varrho-\frac{k}{m}\sum_n\frac{\varrho_n}{\varrho}\ln\frac{\varrho_n}{\varrho}+s_0 \tag{30}$$

with the entropy constant

$$s_0=\frac{k}{m}\left(\frac{3}{2}+\ln my\sqrt{\frac{2\pi k}{m}}^3\right)\ . \tag{31}$$

$s_{\mathcal{E}}$ has the usual value $\frac{3}{2}\frac{k}{m}\ln T - \frac{k}{m}\ln\varrho + s_0$ for mon-atomic gases with an additional mixing term. The latter is due to the mixing of particles with different states n.

The entropy of total equilibrium follows from (30), if one inserts the equilibrium values of the partial densities (19). This yields

$$s_{\mathcal{I}} = \frac{3}{2}\frac{k}{m}\ln T - \frac{k}{m}\ln\varrho + \frac{k}{m}\sum_n \frac{\frac{E_n}{kT}\exp\left\{-\frac{E_n}{kT}\right\}}{\sum_n \exp\left\{-\frac{E_n}{kT}\right\}} + \frac{k}{m}\ln\sum_n \exp\left\{-\frac{E_n}{kT}\right\} + s_0 \qquad (32)$$

or

$$s_{\mathcal{I}} = \frac{3}{2}\frac{k}{m}\ln T - \frac{k}{m}\ln\varrho + \frac{k}{m}\frac{d}{dT}\left(T\ln\sum_n \exp\left\{-\frac{E_n}{kT}\right\}\right) + s_0 \; . \qquad (33)$$

If E_n is given by (1) with $\frac{\hbar\Omega}{kT} \ll 1$ the equilibrium entropy is given by

$$s_{\mathcal{I}} = \frac{5}{2}\frac{k}{m}\ln T - \frac{k}{m}\ln\varrho + \hat{s}_0 \qquad (34)$$

with the entropy constant

$$\hat{s}_0 = \frac{k}{m}\left(\frac{5}{2} + \ln\frac{myk}{\hbar\Omega}\sqrt{\frac{2\pi k}{m}}^3\right) \; . \qquad (35)$$

3 Heating

We consider a mass M of the gas in the constant volume V, so that

$$M = \int_V \varrho dV \qquad \text{and} \qquad \frac{dM}{dt} = 0. \qquad (36)$$

If the gas is at rest, we obtain from the integration of the balance equations of thermal energy and vibration energy

$$\frac{d\varepsilon}{dt} - \frac{\dot{Q}}{M} = -\frac{1}{\tau_{\mathcal{I}}}\left(\varepsilon - \varepsilon_{\mathcal{I}}\right) \quad , \quad \frac{du}{dt} = \frac{1}{\tau_{\mathcal{I}}}\left(\varepsilon - \varepsilon_{\mathcal{I}}\right) \quad , \qquad (37)$$

where $\dot{Q}$ denotes the heat supply from the outside, given by

$$\dot{Q} = -\int_V \frac{\partial q_j}{\partial x_i} dV = -\int_{\partial V} q_i n_i dA \; . \qquad (38)$$

We use the linear approximation (21) and the abbreviation $\dot{q} = \frac{\dot{Q}}{M}$ to rewrite (37) as two uncoupled equations, viz.

$$\frac{d\left(\varepsilon + u\right)}{dt} = \dot{q} \; , \qquad \frac{d\left(\varepsilon - \frac{3}{2}u\right)}{dt} = \dot{q} - \frac{1}{\tau_{\mathcal{I}}}\left(\varepsilon - \frac{3}{2}u\right) \; . \qquad (39)$$

The solutions for the case of initial equilibrium, i.e. $\varepsilon(t_0) = \frac{3}{2}\frac{k}{m}T_0$, $u(t_0) = \frac{k}{m}T_0$, read

$$\varepsilon + u = \frac{5}{2}\frac{k}{m}T_0 + \int_{t_0}^{t} \dot{q}(t')\, dt' \ , \qquad \varepsilon - \frac{3}{2}u = \int_{t_0}^{t} \dot{q}(t') \exp\left(-\frac{t-t'}{\tau_{\mathcal{I}}}\right) dt' \tag{40}$$

and we find with (6) for the evolution of the temperature

$$T = T_0 + \int_{t_0}^{t} \frac{\dot{q}(t')}{\frac{3}{2}\frac{k}{m}} \left[\frac{3}{5} + \frac{2}{5}\exp\left(-\frac{t-t'}{\tau_{\mathcal{I}}}\right)\right] dt' \ . \tag{41}$$

A gas with constant specific heat c_v obeys the equation

$$c_v \frac{dT}{dt} = \dot{q} \tag{42}$$

with the solution

$$T = T_0 + \int_{t_0}^{t} \frac{\dot{q}(t')}{c_v} dt' \tag{43}$$

and comparison with (41) shows that the ideal gas with internal degree of freedom does not have a constant specific heat. Indeed, the inelastic collisions introduce the term $\dot{q}(t') \exp\left(-\frac{t-t'}{\tau_{\mathcal{I}}}\right)$ into (41) which describes the fading memory of the gas with respect to the heating $\dot{q}(t')$.

In case that all collisions are elastic we have $1/\tau_{\mathcal{I}} = 0$ and find $c_v = \frac{3}{2}\frac{k}{m}$ as for a usual mon-atomic gas. If there are many inelastic collisions, so that $\tau_{\mathcal{I}} \ll 1$ on the time scale under consideration we find $c_v = \frac{5}{2}\frac{k}{m}$ and the internal degree of freedom contributes with $\frac{k}{m}$ to the specific heat.

We consider constant heating with the rate a during the time Δ,

$$\dot{q} = \begin{cases} a \ , & t \in (0, \Delta) \\ 0 \ , & \mathit{else}, \end{cases} \tag{44}$$

and find from (41)

$$T - T_0 = \begin{cases} \frac{3}{5}\frac{t}{\Delta} + \frac{2}{5}\frac{\tau_{\mathcal{I}}}{\Delta}\left(1 - e^{-\frac{t}{\tau_{\mathcal{I}}}}\right) \ , & t \in (0, \Delta) \\ \frac{3}{5}\frac{t}{\Delta} + \frac{2}{5}\frac{\tau_{\mathcal{I}}}{\Delta}\left(e^{\frac{\Delta - t}{\tau_{\mathcal{I}}}} - e^{-\frac{t}{\tau_{\mathcal{I}}}}\right) \ , & \mathit{else}. \end{cases} \tag{45}$$

Figure 1 shows the result for $\tau_{\mathcal{I}} = \{1000\Delta, 1\Delta, 0.001\Delta\}$. There is a clear relaxation for $\tau_{\mathcal{I}} = 1\Delta$ due to a slow exchange between thermal and vibration energy. For $\tau_{\mathcal{I}} = 1000\Delta$ the heat remains in the thermal part of the energy while in the $\tau_{\mathcal{I}} = 0.001\Delta$ case the heat is distributed immediately between thermal and vibration energy.

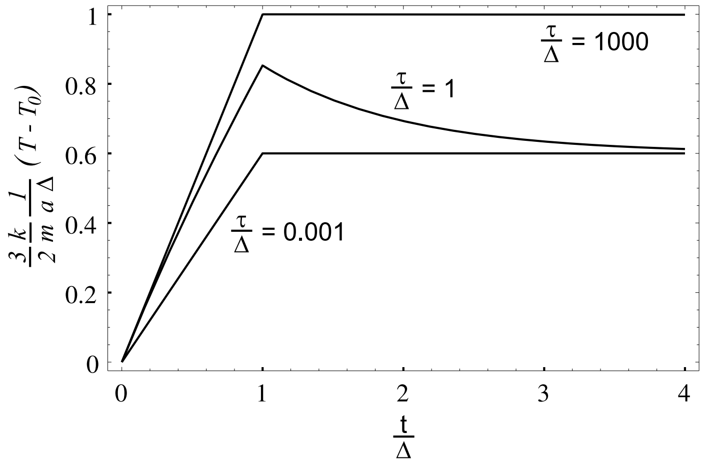

Fig. 1: Heating: Temperature as function of time for various ratios $\frac{\tau_{\mathcal{I}}}{\Delta}$.

4 The Laws of Navier-Stokes and Fourier

Equations (24) do not form a closed set for the quantities $\varrho, v_i, \varepsilon$ and u since they contain the additional quantities $p_{\langle ij\rangle}$ and q_i. The aim of this section is to find simple expressions for these quantities. Multiplication of the Boltzmann equation by $C_{\langle i}C_{j\rangle}$, C^2C_i and subsequent integration and summation gives

$$\begin{aligned}\frac{Dp_{\langle ij\rangle}}{Dt}+p_{\langle ij\rangle}\frac{\partial v_k}{\partial x_k}+\frac{4}{5}\frac{\partial q_{\langle i}}{\partial x_{j\rangle}}+\frac{\partial m_{\langle ijk\rangle}}{\partial x_k}\quad &+2p_{\langle k\langle i\rangle}\frac{\partial v_{j\rangle}}{\partial x_k}+\\ +2p\frac{\partial v_{\langle i}}{\partial x_{j\rangle}}\quad &=-\left(\frac{1}{\tau_{\mathcal{E}}}+\frac{1}{\tau_{\mathcal{I}}}\right)p_{\langle ij\rangle}\end{aligned}\tag{46}$$

$$\begin{aligned}\frac{Dq_i}{Dt}-\left(\frac{5}{3}\varrho\varepsilon\delta_{ij}+p_{\langle ij\rangle}\right)\frac{1}{\varrho}\left(\frac{\partial p}{\partial x_j}+\frac{\partial p_{\langle jk\rangle}}{\partial x_k}\right)+\frac{7}{5}q_i\frac{\partial v_k}{\partial x_k}\quad &+\frac{7}{5}q_k\frac{\partial v_i}{x_k}+\\ +\frac{2}{5}q_k\frac{\partial v_k}{\partial x_i}+\frac{1}{2}\frac{\partial m_{llik}}{\partial x_k}+m_{\langle ijk\rangle}\frac{\partial v_j}{\partial x_k}= &\quad-\left(\frac{1}{\tau_{\mathcal{E}}}+\frac{1}{\tau_{\mathcal{I}}}\right)q_i\end{aligned}\tag{47}$$

with

$$m_{\langle ijk\rangle}=m\sum_n\int C_{\langle i}C_jC_{k\rangle}f_nd\mathbf{c}\ ,\ m_{llik}=m\sum_n\int C^2C_iC_kf_nd\mathbf{c}\ .\tag{48}$$

Now we perform a so-called Maxwell iteration [2] in these equations, i.e. we insert the equilibrium values of the moments in the left hand sides of (46, 47). This procedure is justified in case that a typical process frequency is small compared to the total collision frequency

$$\frac{1}{\tau}=\frac{1}{\tau_{\mathcal{E}}}+\frac{1}{\tau_{\mathcal{I}}}\ .\tag{49}$$

If a typical process frequency is small in comparison with the collision frequency $\frac{1}{\tau_{\mathcal{I}}}$ of inelastic collisions we may use the total equilibrium density $f_{\mathcal{I}_n}$ for the determination of the moments of the left hand side. If on the other hand, the amount of elastic collisions exceeds the amount of inelastic collisions we have to use the phase density of intermediate equilibrium, $f_{\mathcal{E}_n}$, given by (14). This gives the moments as

$$p_{\langle ij\rangle|\mathcal{E}} = 0 \ , \ q_{i|\mathcal{E}} = 0 \ , \ m_{\langle ijk\rangle|\mathcal{E}} = 0 \ , \ m_{llik|\mathcal{E}} = \frac{20}{9}\varrho\varepsilon^2\delta_{ik} \tag{50}$$

and (46, 47) reduce to the laws of Navier-Stokes and Fourier,

$$p_{\langle ij\rangle} = -2\mu\frac{\partial v_{\langle i}}{\partial x_{j\rangle}} \qquad , \qquad q_i = -\kappa\frac{\partial T}{\partial x_i} \tag{51}$$

where viscosity η and heat conductivity κ are given by

$$\mu = \tau p \qquad , \qquad \kappa = \frac{5}{2}\tau p\frac{k}{m} \ , \tag{52}$$

so that viscosity and heat conductivity are determined by the total free time τ. As always in the BGK model with constant relaxation time [3] we find for the Prandtl number $Pr = \frac{\kappa}{\mu} = \frac{5}{2}\frac{k}{m}$.

5 Euler Equations

5.1 Equations, Range of Validity

In the remaining part of the paper we consider the Euler case of the balance equations (24), i.e. we set $p_{\langle ij\rangle} = 0$, $q_i = 0$. Moreover we consider only the case $\frac{\hbar\Omega}{m\varepsilon_{\mathcal{I}}} \ll 1$, which means that (21) holds,

$$\varepsilon_{\mathcal{I}} = \frac{3}{5}\left(\varepsilon + u\right) \qquad \text{or} \qquad T_{\mathcal{I}} = \frac{3}{5}T + \frac{u}{\frac{5}{2}\frac{k}{m}} \quad . \tag{53}$$

and obtain the Euler equations for the gas with internal degree of freedom

$$\begin{aligned}
\frac{D\varrho}{Dt} + \varrho\frac{\partial v_i}{\partial x_i} &= 0 \\
\frac{Dv_i}{Dt} + \frac{1}{\varrho}\frac{\partial p}{\partial x_i} &= 0 \\
\frac{D\varepsilon}{Dt} + \frac{p}{\varrho}\frac{\partial v_i}{\partial x_i} &= -\frac{1}{\tau_{\mathcal{I}}}\left(\frac{2}{5}\varepsilon - \frac{3}{5}u\right) \\
\frac{Du}{Dt} &= \frac{1}{\tau_{\mathcal{I}}}\left(\frac{2}{5}\varepsilon - \frac{3}{5}u\right) \quad .
\end{aligned} \tag{54}$$

First we have to discuss the range of validity of the equations (54). Indeed, by (49) - (51), we may set $p_{\langle ij\rangle} = 0$, $q_i = 0$ only if the total free time τ is very small in comparison to the time scale of the process under consideration. In (54) we find the free time $\tau_{\mathcal{I}}$ only which may be written by (49) as

$$\frac{1}{\tau_{\mathcal{I}}} = \frac{\alpha}{\tau} \qquad \text{with} \qquad \alpha = \frac{1}{1 + \frac{\tau_{\mathcal{I}}}{\tau_{\mathcal{E}}}} \tag{55}$$

The coefficient α assumes values between $\alpha = 0$ - when only elastic collisions occur - and $\alpha = 1$ for inelastic collisions. In the latter case we have $\tau_{\mathcal{I}} = \tau$ and - since τ is extremely small in the time scale under consideration - we conclude from $(54)_{3,4}$ that

$$\varepsilon - \varepsilon_{\mathcal{I}} = 0 \qquad \text{or} \qquad T_{\mathcal{I}} = T \qquad (\alpha \to 1)\ . \tag{56}$$

This is the equilibrium case where the gas is in local equilibrium at every instant. By (53) we have $u = \frac{2}{3}\varepsilon_{\mathcal{I}} = \frac{k}{m}T$ in this case.

The case $\alpha = 0$ corresponds to a frozen non-equilibrium where both ε and u are conserved quantities due to the fact that all collisions are elastic and the energetic states of the particles remain unchanged.

5.2 Isentropic Laws

The equations (54) may be combined to give an equation for the total energy $\varepsilon + u$, viz.

$$\frac{D(\varepsilon + u)}{Dt} - \frac{p}{\varrho^2}\frac{D\varrho}{Dt} = 0 \tag{57}$$

If $\alpha = 1$ holds we have total equilibrium with $\varepsilon = \frac{3}{2}u = \frac{3}{2}\frac{k}{m}T$ and (57) reduces to the isentropic law

$$\frac{T^{\frac{5}{2}}}{\varrho} = const. \tag{58}$$

- the equilibrium entropy (34) is constant.

If $\alpha = 0$ holds $(54)_{1,3}$ reduce to the isentropic law

$$\frac{T^{\frac{3}{2}}}{\varrho} = const. \tag{59}$$

corresponding to constant entropy (30).

Thus we have different isentropic coefficients in the two cases. Processes for values of α between 0 and 1 are not isentropic since there is production of entropy due to the inelastic collisions.

5.3 Dispersion Relation

We consider the Euler equations (54) for small deviations from a global equilibrium and one dimensional processes, i.e. we set

$$\varrho = \varrho_0 + \hat{\varrho}(x,t)\ ,\ v_i = (\hat{v}(x,t), 0, 0)_i\ ,\ \varepsilon = \varepsilon_0 + \hat{\varepsilon}(x,t)\ ,\ u = \frac{2}{3}\varepsilon_0 + \hat{u}(x,t) \tag{60}$$

and ignore all quadratic terms in the non-equilibrium contributions $\hat{\varrho}$, $\hat{v}$, $\hat{\varepsilon}$ and $\hat{u}$,

$$\begin{aligned}
\frac{\partial\hat{\varrho}}{\partial t}+\varrho_0\frac{\partial\hat{v}}{\partial x} &= 0\\
\frac{\partial\hat{v}}{\partial t}+\frac{2}{3}\frac{\partial\hat{\varepsilon}}{\partial x}+\frac{2}{3}\frac{\varepsilon_0}{\varrho_0}\frac{\partial\hat{\varrho}}{\partial x} &= 0\\
\frac{\partial\hat{\varepsilon}}{\partial t}+\frac{2}{3}\varepsilon_0\frac{\partial\hat{v}}{\partial x} &= -\frac{\alpha}{\tau}\left(\frac{2}{5}\hat{\varepsilon}-\frac{3}{5}\hat{u}\right)\\
\frac{\partial\hat{u}}{\partial t} &= \frac{\alpha}{\tau}\left(\frac{2}{5}\hat{\varepsilon}-\frac{3}{5}\hat{u}\right)\ .
\end{aligned} \tag{61}$$

For this linear system we assume plane wave solutions

$$\hat{\varphi}=\bar{\varphi}\exp i\left(\omega t-kx\right)\ , \tag{62}$$

where ω is the frequency of the wave, k denotes the wave number and $\bar{\varphi}$ is the complex amplitude. Introducing this ansatz into (61) yields the homogeneous algebraic system

$$\begin{bmatrix}
i\omega & -ik\varrho_0 & 0 & 0\\
-ik\frac{2}{3}\frac{\varepsilon_0}{\varrho_0} & i\omega & -ik\frac{2}{3} & 0\\
0 & -ik\frac{2}{3}\varepsilon_0 & i\omega+\frac{2}{5}\frac{\alpha}{\tau} & -\frac{3}{5}\frac{\alpha}{\tau}\\
0 & 0 & -\frac{2}{5}\frac{\alpha}{\tau} & i\omega+\frac{3}{5}\frac{\alpha}{\tau}
\end{bmatrix}
\begin{bmatrix}\bar{\varrho}\\ \bar{v}\\ \bar{\varepsilon}\\ \bar{u}\end{bmatrix}=0 \tag{63}$$

which has non-trivial solutions if the determinant vanishes, i.e. if

$$\frac{1}{k}=\pm\frac{1}{\omega}\sqrt{\frac{5}{3}\frac{p_0}{\varrho_0}}\sqrt{1-\frac{4}{25}\frac{1}{1+\frac{i\omega\tau}{\alpha}}} \tag{64}$$

holds. Equation (64) is the dispersion relation which implies the phase velocity $v_{ph}=\frac{\omega}{\operatorname{Re}k}$ and the damping coefficient $\eta=-\operatorname{Im}k$. Figure 2 shows v_{ph} and η for given τ,ω as functions of α. The phase velocity has the value $v_{ph}=\sqrt{\frac{5}{3}\frac{p_0}{\varrho_0}}$ for $\alpha=0$ and becomes $v_{ph}=\sqrt{\frac{7}{5}\frac{p_0}{\varrho_0}}$ for $\alpha=1$ while the damping vanishes in both cases. We repeat that the Euler equations may only be used if τ is small, i.e. if $\omega\tau\ll 1$. The value $\omega\tau=0.1$ in Figure 1 is not small enough to ensure $\eta\left(\alpha=1\right)=0$; it was chosen in order to give a clear picture. In the intermediate region, $0<\alpha<1$, phase speed and the non-vanishing damping depend on the frequency ω.

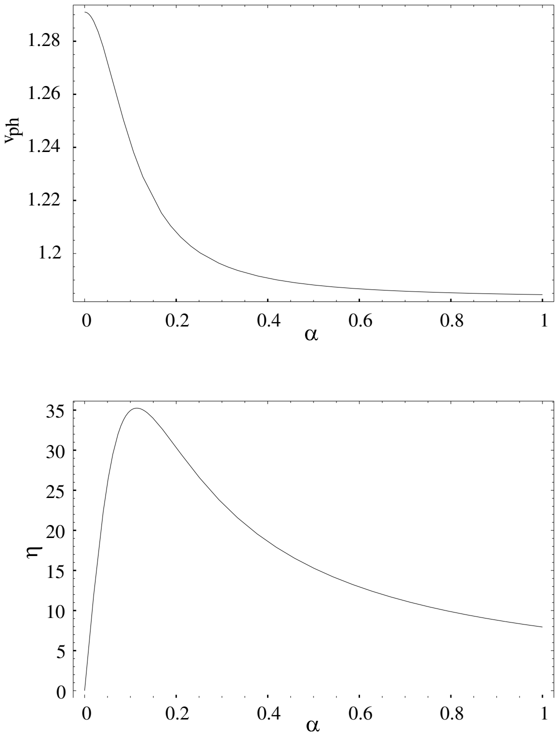

Fig. 2: Phase speed v_{ph} and damping ηas functions of α $\left(\tau = 0.0001\frac{1}{s}, \omega = 1000\frac{1}{s}\right)$.

5.4 Shock Structure

Now we consider a stationary one dimensional shock wave for which the Euler equations (54) reduce to

$$\begin{aligned} \frac{d}{dx}\left(\varrho v\right) &= 0 \\ \frac{d}{\partial x}\left(\varrho v^2 + p\right) &= 0 \\ \frac{d}{\partial x}\left(\varrho v\left(\varepsilon + \frac{p}{\varrho} + u + \frac{1}{2}v^2\right)\right) &= 0 \\ \frac{d}{dx}\left(\varrho u v\right) &= \frac{\alpha}{\tau}\varrho\left(\frac{2}{5}\varepsilon - \frac{3}{5}u\right) \end{aligned} \tag{65}$$

v is the velocity in x-direction and - as always - $\varepsilon = \frac{3}{2}\frac{k}{m}T$. We denote the fields before the shock by ϱ_0, v_0, T_0, u_0 and assume that the gas is in equilibrium before the shock, such that $u_0 = \frac{k}{m}T_0$. The first three equations $(65)_{1-3}$ may be integrated to give

$$\varrho v = \varrho_0 v_0 \ , \ v + \frac{k}{m}\frac{T}{v} = v_0 + \frac{k}{m}\frac{T_0}{v_0} \ , \ \frac{5}{2}\frac{k}{m}T + u + \frac{1}{2}v^2 = \frac{7}{2}\frac{k}{m}T_0 + \frac{1}{2}v_0^2 \ . \tag{66}$$

If $\alpha = 0$, all collisions are elastic such that, by $(65)_4$, $u = u_0 = const.$ In this case (66) reduce to the well-known Rankine-Hugoniot relations of a mon-atomic gas, viz.

$$\varrho v = \varrho_0 v_0 \ , \ v + \frac{k}{m}\frac{T}{v} = v_0 + \frac{k}{m}\frac{T_0}{v_0} \ , \ \frac{5}{2}\frac{k}{m}T + \frac{1}{2}v^2 = \frac{5}{2}\frac{k}{m}T_0 + \frac{1}{2}v_0^2 \tag{67}$$

If $\alpha = 1$, all collisions are inelastic and we have $u = \frac{2}{3}\varepsilon = \frac{k}{m}T$ since the Euler equations are only valid for $\tau \to 0$ and the right hand side of $(65)_4$ must be finite. In this case (66) reduce to the Rankine-Hugoniot relations

$$\varrho v = \varrho_0 v_0 \ , \ v + \frac{k}{m}\frac{T}{v} = v_0 + \frac{k}{m}\frac{T_0}{v_0} \ , \ \frac{7}{2}\frac{k}{m}T + \frac{1}{2}v^2 = \frac{7}{2}\frac{k}{m}T_0 + \frac{1}{2}v_0^2 \ . \tag{68}$$

Both cases correspond to discontinuous shock waves. Smooth shock structures are only possible for intermediate values of α. The values of the fields behind the shock -where we have equilibrium again - are the solutions of (68),

$$\varrho_1 = \frac{\varrho_0}{1 + \frac{7}{\hat{v}_0^2}} \ , \ T_1 = \frac{T_0}{36}\left(34 - \frac{7}{\hat{v}_0^2} + 5\hat{v}_0^2\right) \ , \ \hat{v}_1 = \frac{1}{6}\left(\frac{7}{\hat{v}_0^2} + \hat{v}_0\right) \tag{69}$$

with the dimensionless speed $\hat{v} = v \Big/ \sqrt{\frac{k}{m}T_0}$.

Equations (66) serve to eliminate ϱ, T and u from $(65)_4$ which - after some rearrangements - reads

$$\frac{d\hat{v}}{d\hat{x}} = -\frac{3\hat{v} + \left(\frac{7}{2} + \frac{\hat{v}_0^2}{2}\right)\frac{1}{\hat{v}} - \frac{7}{2}\left(\hat{v}_0 + \frac{1}{\hat{v}_0}\right)}{4\hat{v} - \frac{5}{2}\left(\hat{v}_0 + \frac{1}{\hat{v}_0}\right)} \tag{70}$$

where we have introduced the dimensionless space variable $\hat{x} = \frac{\alpha}{\tau}\frac{3x}{5\sqrt{\frac{k}{m}T_0}}$. The numerator of the right hand side vanishes for $\hat{v} = \hat{v}_0 = \sqrt{\frac{7}{5}}$ so that a gas moving with the speed $\sqrt{\frac{7}{5}\frac{k}{m}T_0}$ will not develop a shock structure. No shock will be observed if $\hat{v}_0 < \sqrt{\frac{7}{5}}$ which corresponds to $\hat{v}_1 < \hat{v}_0$, $\varrho_1 < \varrho_0$, $T_1 < T_0$.

For $\hat{v}_0 \geq \sqrt{\frac{5}{3}}$ the denominator vanishes in the interval (v_0, v_1) and the shock will be discontinuous.. Thus we will find a continuous shock structure only, if $\hat{v}_0$ lies in the interval $\left(\sqrt{\frac{7}{5}}, \sqrt{\frac{5}{3}}\right)$.

Figure 3 shows $\hat{v}, \hat{T} = \frac{T}{T_0}$ and $\hat{u} - \hat{T} = \frac{u}{\frac{k}{m}T_0} - \frac{T}{T_0}$ as functions of the dimensionless length $\hat{x}$ for $\hat{v}_0 = 1.01\sqrt{\frac{7}{5}}$. The shock thickness depends on the fraction of inelastic collisions α: the shock broadens with increasing α.

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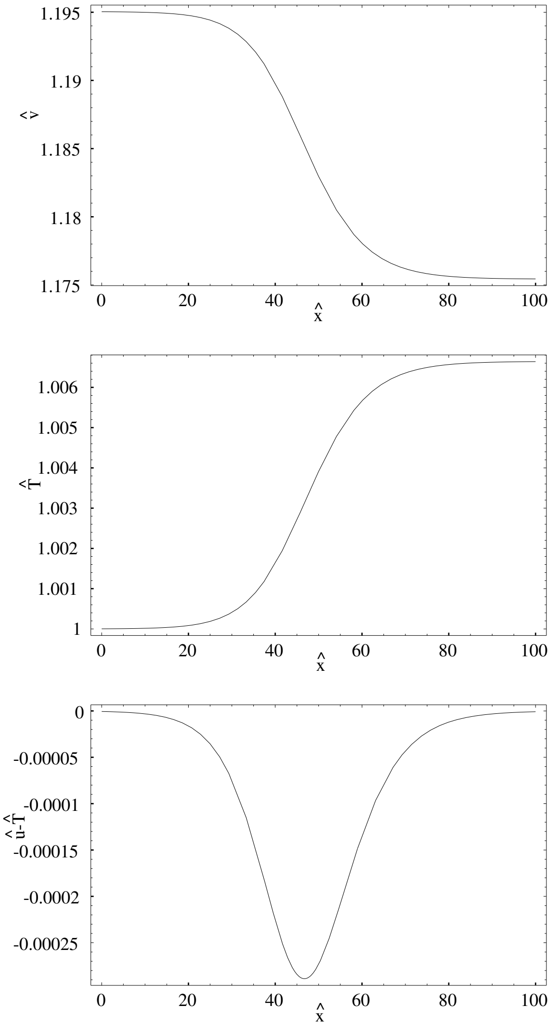

Fig. 3: Shock structure for $\hat{v}_0 = 1.01\sqrt{\frac{7}{5}}$.

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