

The Bhatnagar - Gross - Krook - Welander model collision operator

Inspired by the linearized collision operator, we can write

$$C[f, f] = - \underbrace{\nu(\underline{v}) f(\underline{v})}_{\text{loss term}} + \underbrace{\int d\underline{v}_* \int d\theta d\varphi B(\underline{v}, \theta) f' f_*'}_{\text{gain term}}$$

where the collision frequency is

$$\nu(\underline{v}) = 2\pi \int d\underline{v}_* \int d\theta B(\underline{v}, \theta) f_*.$$

To get a model for $C[f, f]$ we can evaluate ν using $f_*^{(0)}$ and replace $\nu(\underline{v})$ by a constant ν_0 , which is already true for Maxwell molecules ($n=5$).

The loss term becomes $-\nu_0 f$.

We want to model the gain term (the K operator) so that $f \rightarrow f^{(0)}$ under collisions while preserving n, \underline{u}, Θ .

This suggests the BGKW equation

$$\frac{\partial f}{\partial t} + \underline{v} \cdot \nabla f = -\nu_0 (f - f^{(0)}),$$

$$\text{where } f^{(0)}(\underline{v}) = \frac{n}{(2\pi\Theta)^{3/2}} \exp\left(-\frac{|\underline{v} - \underline{u}|^2}{2\Theta}\right).$$

If we choose n, \underline{u}, Θ from f by

$$n = \int d\underline{v} f = \int d\underline{v} f^{(0)}$$

$$\underline{u} = \frac{1}{n} \int d\underline{v} \underline{v} f = \frac{1}{n} \int d\underline{v} \underline{v} f^{(0)}$$

$$\Theta = \frac{1}{3n} \int d\underline{v} |\underline{v} - \underline{u}|^2 f = \frac{1}{3n} \int d\underline{v} |\underline{v} - \underline{u}|^2 f^{(0)}$$

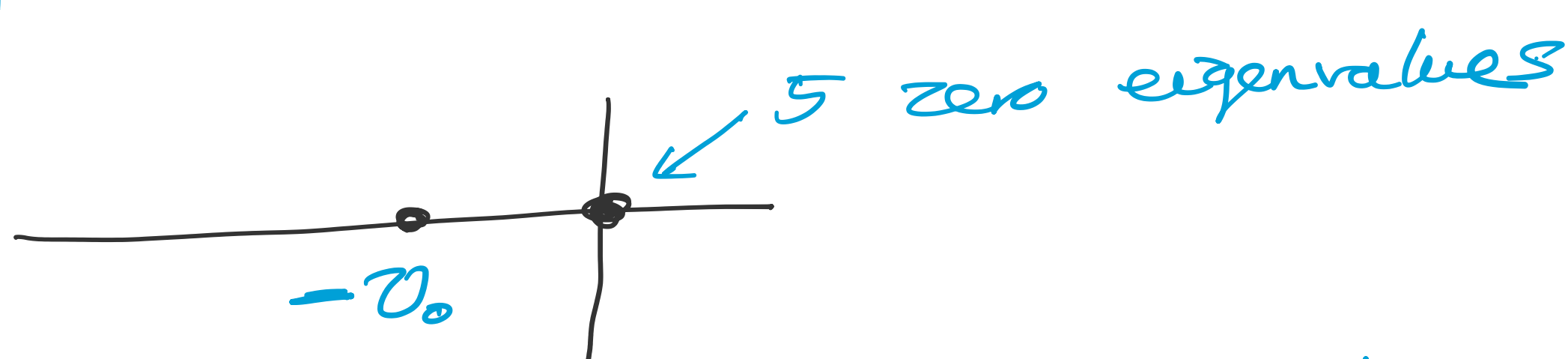
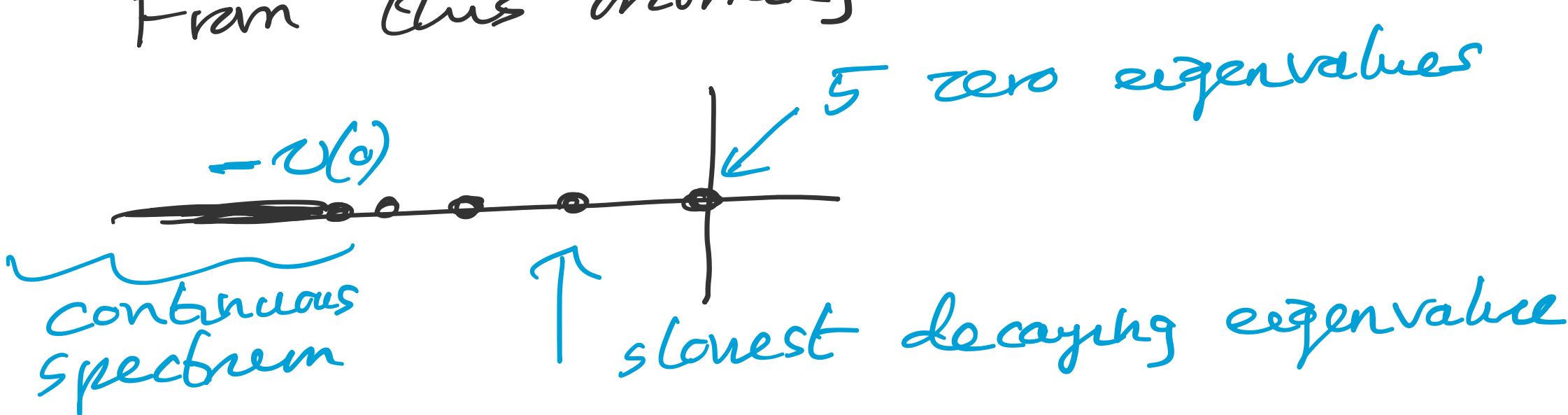
then this model conserves the collision invariants.

$-\nu_0(f - f^{(0)})$ looks linear, but

$f^{(0)}$ depends on f through n, \underline{u}, Θ in a very nonlinear way (much worse than the quadratic nonlinearity in $C[f, f]$).

Exercise: the BGKW equation satisfies the H-theorem.

From this morning



Every other mode decays with rate $-\nu_0$

XII Derivation of hydrodynamics

Multiplying the Boltzmann equation

$$\partial_t f + \underline{v} \cdot \nabla f = C[f, f]$$

by the particle mass m , and one of the collision invariants $1, \underline{v}, \frac{1}{2}|\underline{v}|^2$ and $\int d\underline{v}$ gives

$$\left. \begin{aligned} \partial_t \rho + \nabla \cdot (\rho \underline{u}) &= 0, \\ \partial_t (\rho \underline{u}) + \nabla \cdot \underline{\Pi} &= 0, \\ \partial_t \mathcal{E} + \nabla \cdot \underline{\mathcal{F}} &= 0, \end{aligned} \right\} \text{RHS all vanish because } 1, \underline{v}, \frac{1}{2}|\underline{v}|^2 \text{ are collision invariants.}$$

conservation laws for mass, momentum and energy, where

$$\rho = m \int d\underline{v} f, \quad \rho \underline{u} = m \int d\underline{v} \underline{v} f$$

$$\mathcal{E} = m \int d\underline{v} \frac{1}{2} |\underline{v}|^2 f \\ = \frac{1}{2} \rho |\underline{u}|^2 + \frac{3}{2} \rho \quad (4)$$

The momentum and energy fluxes are

$$\underline{\Pi} = m \int d\underline{v} \underline{v} \underline{v} f,$$

$$\underline{\mathcal{F}} = m \int d\underline{v} \frac{1}{2} |\underline{v}|^2 \underline{v} f.$$

For example, as $\underline{x}, \underline{v}, t$ are independent variables:

$$\underline{v} \partial_t f + \underline{v} \underline{v} \cdot \nabla f = \underline{v} C[f, f]$$

$$m \int d\underline{v} \underline{v} \partial_t f + m \int d\underline{v} \underline{v} \underline{v} \cdot \nabla f = m \int d\underline{v} \underline{v} C[f, f]$$

$$\partial_t \left(m \int d\underline{v} \underline{v} f \right) + \nabla \cdot \left(m \int d\underline{v} \underline{v} \underline{v} f \right) = 0$$

$$\partial_t (\rho \underline{u}) + \nabla \cdot \underline{\Pi} = 0.$$

These macroscopic conservation laws are exact deductions from the Boltzmann equation.

However, we do not know how to calculate the fluxes $\underline{\Pi}$ and $\underline{\mathcal{F}}$.

We don't have any constitutive relations to go with the conservation laws.

We'll try to find these by exploiting the fact that $\underline{\Pi}$ and $\underline{\mathcal{F}}$ naturally evolve on a collisional timescale $\tau \sim 1/\nu_0$ to find equations that hold on a hydrodynamic timescale $T \gg \tau$.

For example,

$$\begin{aligned} \partial_t \underline{\Pi} + \nabla \cdot (m \int d\underline{v} \underline{v} \underline{v} \underline{v} f) \\ = m \int d\underline{v} \underline{v} \underline{v} C[f, f] \\ \neq 0 \\ \sim -\frac{1}{\tau} (\underline{\Pi} - \underline{\Pi}^{(0)}) \end{aligned}$$

where $^{(0)}$ means a moment of $f^{(0)}$,

$$\text{i.e. } \underline{\Pi}^{(0)} = m \int d\underline{v} \underline{v} \underline{v} f^{(0)}.$$

Moments with respect to peculiar velocity

It's useful to consider moments with respect to the "peculiar" velocity $\underline{w} = \underline{v} - \underline{u}(\underline{x}, t)$.

$$\begin{aligned}\underline{\Pi} &= m \int d\underline{v} \underline{v} \underline{v} f(\underline{x}, \underline{v}, t) \\ &= m \int d\underline{v} (\underline{u} + \underline{w})(\underline{u} + \underline{w}) f \\ &= m \int d\underline{v} (\underline{u}\underline{u} + \underline{w}\underline{u} + \underline{u}\underline{w} + \underline{w}\underline{w}) f \\ &= m \int d\underline{v} (\underline{u}\underline{u} + \underline{w}\underline{w}) f \\ &= \rho \underline{u}\underline{u} + \underline{P} \quad \leftarrow \text{the pressure tensor}\end{aligned}$$

where $\underline{P} = m \int d\underline{v} \underline{w}\underline{w} f$.

All terms with precisely one \underline{w} vanish because $\underline{u} = \frac{1}{n} \int d\underline{v} \underline{v} f$ so $\int d\underline{v} (\underline{v} - \underline{u}) f = 0$.

Beware that $\underline{x}, \underline{w}, t$ are not independent variables, so ∂_t and ∇ don't commute with taking moments with respect to \underline{w} .

The momentum equation becomes

$$\partial_t(\rho \underline{u}) + \nabla \cdot (\rho \underline{u}\underline{u} + \underline{P}) = 0.$$

Evaluating \underline{P} for a Maxwell-Boltzmann distribution gives

$$\begin{aligned}\underline{P}^{(0)} &= m \int d\underline{w} \underline{w}\underline{w} \frac{n}{(2\pi\theta)^{3/2}} e^{-\frac{|\underline{w}|^2}{2\theta}} \\ &= \rho \theta \underline{I} \quad \Rightarrow \text{isotropic}\end{aligned}$$

so we get

$$\partial_t(\rho \underline{u}) + \nabla \cdot (\rho \underline{u}\underline{u} + \rho \theta \underline{I}) = 0,$$

or

$$\partial_t(\rho \underline{u}) + \nabla \cdot (\rho \underline{u}\underline{u}) + \nabla p = 0,$$

with pressure $p = \rho \theta$.

This is the Euler momentum equation for an ideal gas.

We can write this as

$$\rho \frac{D\underline{u}}{Dt} = -\nabla p$$

where $\frac{D}{Dt} = \frac{\partial}{\partial t} + \underline{u} \cdot \nabla$ is the material or Lagrangian time derivative.

We can do the same with the energy density

$$\begin{aligned}\mathcal{E} &= m \int d\underline{v} \frac{1}{2} |\underline{v}|^2 f \\ &= m \int d\underline{v} \frac{1}{2} |\underline{u} + \underline{w}|^2 f \\ &= m \int d\underline{v} \frac{1}{2} |\underline{u}|^2 f + m \int d\underline{v} \frac{1}{2} |\underline{w}|^2 f \\ &= \frac{1}{2} \rho |\underline{u}|^2 + \frac{3}{2} \rho \theta.\end{aligned}$$

The macroscopic energy density is purely kinetic (either bulk or internal) but the contribution from Φ in the original Hamiltonian has been scaled out in the Boltzmann-Grad limit with $nd^3 \rightarrow 0$.

The energy flux becomes

$$\begin{aligned}\underline{F} &= m \int d\underline{v} \frac{1}{2} |\underline{u} + \underline{w}|^2 (\underline{u} + \underline{w}) f \\ &= m \int d\underline{v} \left(\frac{1}{2} \underline{u} |\underline{u}|^2 + \frac{1}{2} \underline{u} |\underline{w}|^2 + \underline{w} \underline{w} \cdot \underline{u} \right. \\ &\quad \left. + \frac{1}{2} \underline{w} |\underline{w}|^2 \right) f\end{aligned}$$

$$= \frac{1}{2} \rho \underline{u} |\underline{u}|^2 + \underline{u} \frac{3}{2} \rho \Theta + \underline{P} \cdot \underline{u} + \underline{q}$$

where $\underline{q} = \frac{1}{2} m \int d\underline{v} \underline{w} |\underline{w}|^2 f$

\Rightarrow the heat flux.

This gives the energy equation

$$\begin{aligned}\partial_t \left(\frac{1}{2} \rho |\underline{u}|^2 + \frac{3}{2} \rho \Theta \right) \\ + \nabla \cdot \left(\frac{1}{2} \rho \underline{u} |\underline{u}|^2 + \frac{3}{2} \rho \underline{u} \Theta + \underline{P} \cdot \underline{u} + \underline{q} \right) = 0\end{aligned}$$

$= \underline{u} \cdot \underline{E}$ $\underbrace{\underline{P} \cdot \underline{u}}_{\text{work done by pressure}}$

Using the known equations for $\frac{\partial \rho}{\partial t}$ and $\frac{\partial \underline{u}}{\partial t}$,

$$\frac{3}{2} \rho \frac{D\Theta}{Dt} + \underbrace{\underline{P} : \nabla \underline{u}}_{= P_{ij} \frac{\partial u_i}{\partial x_j}} + \nabla \cdot \underline{q} = 0$$

Evaluating $\underline{P} = \underline{P}^{(0)} = \rho \Theta \underline{I}$

and $\underline{q} = \underline{q}^{(0)} = 0$ from the Maxwell-Boltzmann distribution gives

$$\frac{3}{2} \rho \frac{D\Theta}{Dt} + \rho \Theta \nabla \cdot \underline{u} = 0,$$

as in the compressible Euler equations

If collisions are so fast ($\tau \ll T$) that $f \approx f^{(0)}(\rho, \underline{u}, \Theta)$ we recover the compressible Euler equations.

Another equation we can write,

for $s = \frac{3}{2} \log(\Theta \rho^{-3/2})$, the gas dynamic entropy, \Rightarrow

$$\rho \Theta \frac{Ds}{Dt} + (\underline{P} - \rho \Theta \underline{I}) : \nabla \underline{u} + \nabla \cdot \underline{q} = 0.$$

$\frac{Ds}{Dt}$ is only nonzero due to deviations from equilibrium.

Evaluating Boltzmann's H-function for a Maxwell-Boltzmann distribution gives

$$H[f^{(0)}] = \int d\underline{v} f^{(0)} \log f^{(0)}$$

$$\begin{aligned}&= \int d\underline{v} \frac{\rho/m}{(2\pi\Theta)^{3/2}} \exp\left(-\frac{|\underline{v} - \underline{u}|^2}{2\Theta}\right) \\ &\quad \left(-\frac{|\underline{v} - \underline{u}|^2}{2\Theta} + \log \rho - \log m - \frac{3}{2} \log \Theta - \frac{3}{2} \log 2\pi \right)\end{aligned}$$

$$= -\frac{3}{2} \rho \left(\log \Theta - \frac{2}{3} \log \rho + \text{constant} \right)$$

$$= -\rho s + \rho \times \text{constant}$$

XIII Beyond the Euler equations

For this we need evolution equations for \underline{P} and \underline{q} .

We know

$$\partial_t \underline{\Pi} + \nabla \cdot (m \int d\underline{v} f(\underline{u} + \underline{w})(\underline{u} + \underline{w})(\underline{u} + \underline{w})) = m \int d\underline{v} \underline{v} \underline{v} C[f, f].$$

Converting into moments with respect to \underline{u} gives

$$\partial_t (\rho u_i u_j + P_{ij}) + \frac{\partial}{\partial x_k} (Q_{ijk} + u_i P_{jk} + u_j P_{ki} + u_k P_{ij} + \rho u_i u_j u_k) = m \int d\underline{v} w_i w_j C[f, f]$$

where $Q_{ijk} = m \int d\underline{v} w_i w_j w_k f$.

We can use $\frac{\partial \rho}{\partial t}$ and $\frac{\partial (P_{ij})}{\partial t}$ to evaluate

$$\partial_t (\rho u_i u_j) = u_i \partial_t (\rho u_j) + \partial_t (\rho u_i) u_j - u_i u_j \partial_t \rho$$

$$= -u_i \partial_k (\rho u_j u_k + P_{jk}) - \partial_k (\rho u_i u_k + P_{ik}) u_j + u_i u_j \partial_k (\rho u_k)$$

There's a lot of cancellation, giving

$$\partial_t P_{ij} + \partial_k (u_k P_{ij} + Q_{ijk}) + P_{ik} \frac{\partial u_j}{\partial x_k} + P_{jk} \frac{\partial u_i}{\partial x_k} = m \int d\underline{v} w_i w_j C[f, f]$$

Using either the BEKW model or the linearized Boltzmann collision operator for Maxwell molecules gives

$$m \int d\underline{v} w_i w_j C[f, f] = -\frac{1}{\tau} (P_{ij} - P_{ij}^{(0)})$$

so we end up with

$$\partial_t P_{ij} + \partial_k (u_k P_{ij} + Q_{ijk}) + P_{ik} \frac{\partial u_j}{\partial x_k} + P_{jk} \frac{\partial u_i}{\partial x_k} = -\frac{1}{\tau} (P_{ij} - P_{ij}^{(0)})$$

We can deal with $\partial_t P_{ij}$ by

writing $\underline{P} = \underline{P}^{(0)} - \underline{T}$ in terms of a deviatoric stress \underline{T} , and $\underline{P}^{(0)} = p \underline{\mathbb{I}}$,

to obtain

$$\begin{aligned} \partial_t T_{ij} + \partial_k (u_k T_{ij} - Q_{ijk} + \frac{1}{3} Q_{ulk} \delta_{ij}) \\ - p \mathbb{A} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3} \delta_{ij} \frac{\partial u_k}{\partial x_k} \right) \\ + T_{ik} \frac{\partial u_j}{\partial x_k} + T_{jk} \frac{\partial u_i}{\partial x_k} \\ - \frac{2}{3} (T_{kl} \frac{\partial u_k}{\partial x_l}) \delta_{ij} = -\frac{1}{\tau} T_{ij}. \end{aligned}$$

This is exact (though horrible).

Something very similar arises for describing elastic liquids with dissolved polymers (like shampoo).

Now expand the non-conserved moments, as series in τ ,

$$\begin{aligned} \underline{T} &= \underline{T}^{(0)} + \tau \underline{T}^{(1)} + \dots \\ \underline{Q} &= \underline{Q}^{(0)} + \tau \underline{Q}^{(1)} + \dots \end{aligned} \quad \left. \begin{aligned} \underline{T}^{(0)} &= 0 \\ \underline{Q}^{(0)} &= 0 \end{aligned} \right\}$$

To evaluate the above exact equation to $O(1)$

we need $\underline{T}^{(1)}$ on the RHS

as the $-\frac{1}{\tau}$ cancels the τ ,

but only $\underline{T}^{(0)} = 0$ and

$\underline{Q}^{(0)} = 0$ on the LHS, leaving

$$\tau p \mathbb{A} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3} \delta_{ij} \frac{\partial u_k}{\partial x_k} \right) = \tau T_{ij}^{(1)}$$

This is the stress tensor for a compressible Newtonian fluid.

The LHS is a traceless symmetric tensor, traceless because $\text{Tr } \underline{\Pi} = 2E$, and E is conserved under collisions.

This gives the Navier-Stokes momentum equation

$$\partial_t (\rho \underline{u}) + \nabla \cdot (\rho \underline{u} \underline{u} + \mathbb{A} \rho \underline{T} - \tau p \mathbb{A} \underline{E}) = 0$$

where $\underline{E} = (\nabla \underline{u}) + (\nabla \underline{u})^T - \frac{2}{3} \underline{T} \nabla \cdot \underline{u}$

is the symmetric & traceless strain rate,

the dynamic viscosity is $\mu = \tau p \mathbb{A}$.

The bulk viscosity is zero, because energy is conserved under collisions.

Applying the same approach to derive an exact evolution equation for the heat flux vector \underline{q} defined by $q_k = \frac{1}{2} Q_{ik}^i$, then substituting all the non-equilibrium moments at leading order, gives

$$\tau \underline{q}^{(1)} = -\frac{5}{2} \tau p \mathbb{A} \nabla \mathbb{A}.$$

This is Fourier's Law with thermal conductivity $\kappa = \frac{5}{2} \tau p \mathbb{A}$.

In these units the specific heat at constant pressure $c_p = 5/2$ so the thermal diffusivity $k = \frac{\kappa}{\rho c_p} = \tau \mathbb{A}$

is the same as the kinematic viscosity $\nu = \mu / \rho = \tau \mathbb{A}$.

The kinetic theory Prandtl

number $Pr = \frac{\nu}{\kappa} = 1$. This is an artifact of the BEKW collision operator.

Real monatomic gases have $Pr \approx 2/3$ since the heat flux involves the $|\underline{u}|^3$ moment is carried more predominantly by faster particles than the $O(|\underline{u}|^2)$ momentum flux.

We would get $Pr = 2/3$ exactly using the linearized Boltzmann collision operator for Maxwell molecules.