Leuz 2016
TD6_3

1.11 Fluid incompressibility

$$\frac{d\rho}{dt} = \partial_t \rho + (\vec{v}\cdot\vec{\nabla})\rho = 0 \Rightarrow \vec{\nabla}\cdot\vec{v} = 0 \text{ through mass conservation}$$

And this yields

$$\rho\left(\partial_t \vec{v} + (\vec{v}\cdot\vec{\nabla})\vec{v}\right) = \eta \Delta\vec{v} - \vec{\nabla}P$$

where P is now a Lagrange multiplier ensuring incompressibility.

II) Microscopic model: thermal conductivity & shear viscosity

2.1 We denote by $\bar{v}$ the typical velocity $\bar{v} = \left(\frac{kT}{m}\right)^{1/2}$ associated with the temperature.

The mean free path of a gas particle is $\bar{v}\tau$; hence its diffusion coefficient is $D \simeq \bar{v}^2\tau$.

Diffusion $\leftrightarrow$ transport of density $\quad D\partial_x n = \bar{v}^2\tau\,\partial_x n$

Thermal conduct $\leftrightarrow$ transport of T (energy density) $\quad \kappa\partial_x T = \bar{v}^2\tau\,\partial_x(n k_B T)$

Dynamic viscosity $\leftrightarrow$ transport of $\vec{g} \simeq n m \vec{u}$ (linear momentum density) $\quad \eta\partial_x u = \bar{v}^2\tau\,\partial_x(n m u)$

Hence $\quad \kappa \propto \bar{v}^2\tau n k_B \qquad \eta \propto \bar{v}^2\tau n m$

Besides, a dilute gas behaves as an ideal gas when it comes to thermodynamics, hence $c_p \propto \frac{k_B}{m} \Rightarrow Pr = \mathcal{O}(1)$ a constant.

2.2 The kinetic equation to $0^{th}$ order in $\tau$ yields

$$f_1 = -\tau\left[\partial_t + (\vec{v}\cdot\vec{\nabla})\right]f_0$$

$$= -\tau\, v_x(\partial_x f_0) \quad \text{for a stationary, } y \,\&\, z\text{-invariant sys.}$$

And $f_0$ depends on space only through $T(x)$, thus:

$$f_1 = -\tau v_x \cdot \frac{\partial T}{\partial x} \cdot \left.\frac{\partial f_0}{\partial T}\right|_P$$

⚠ the derivative here is not at constant $n$, but instead at constant pressure $P = nT$; indeed, any pressure gradient in the fluid would induce mass transport, of which we assumed there wasn't.

We now turn to the heat flux. It has two pieces

$$J_x^q = \underbrace{J_x^{q(0)}}_{\text{associated w/ } f_0\text{; vanishes by symmetry.}} + \underbrace{J_x^{q(1)}}_{\text{associated w/ } f_1}$$

$$= \frac{m}{2} \int \xi_x \left(\xi^2\right) f_1 \, d\vec{\xi}$$

$$= -\frac{m\tau}{2} \frac{\partial T}{\partial x} \cdot \int v_x^2 \, v^2 \left.\frac{\partial f_0}{\partial T}\right|_P d\vec{v} \quad (\vec{v} = \vec{\xi} \text{ because } \vec{u}\text{:}$$

$$-\kappa \frac{\partial T}{\partial x} = -\frac{m\tau}{2} \frac{\partial T}{\partial x} \frac{\partial}{\partial T}\left[ \int v_x^2 v^2 f_0 \, d\vec{v} \right]$$

And $\displaystyle\int v^4 f_0 \, d\vec{v} = \int \left(v_x^2 + v_y^2 + v_z^2\right) v^2 f_0 \, d\vec{v}$

$$= d \cdot \int v_x^2 \, v^2 f_0 \, d\vec{v}$$

Thus $\displaystyle\int v_x^2 v^2 f_0 \, d\vec{v} = \frac{1}{d} \int v^4 f_0 \, d\vec{v}$

$f_0$ is a Gaussian, we want to compute $\langle v^4 \rangle$

We introduce $\displaystyle g(\alpha) = \frac{1}{(2\pi\sigma^2)^{d/2}} \int e^{-\frac{\alpha x^2}{2\sigma^2}} \, d^d\vec{x}$

$$= \frac{1}{(2\pi\sigma^2)^{d/2}} \cdot \left(\frac{2\pi\sigma^2}{\alpha}\right)^{d/2} = \alpha^{-d/2}$$

Clearly $g(\alpha = 1) = 1$

Now $\displaystyle\left\langle -\frac{x^2}{2\sigma^2} \right\rangle = g'(1) = -\frac{d}{2}$

$$\left\langle \left(\frac{x^2}{2\sigma^2}\right)^2 \right\rangle = g''(1) = \left(-\frac{d}{2}\right) \cdot \left(-\left(1 + \frac{d}{2}\right)\right) = \frac{d\,(d+2)}{4}$$

Thus $\langle x^4 \rangle = (2+d)\,d\,\sigma^4$

And here $\langle v^4 \rangle = d(2+d) \cdot n \left(\frac{k_B T}{m}\right)^2$

remember $f_0 = n \times$ (a normalized Gaussian)

Finally:

$$\kappa = \frac{m\tau}{2} \frac{\partial}{\partial T} \left[ (2+d) \left(\frac{k_B}{m}\right)^2 \cdot n T^2 \right] \Big|_{nT = \text{const.}}$$

$$= \frac{m\tau}{2} (2+d) \left(\frac{k_B}{m}\right)^2 n T \cdot \frac{\partial}{\partial T} T$$

$$\underline{\kappa = \left(1 + \frac{d}{2}\right) \cdot \frac{n k_B^2 T \tau}{m}}$$ compatible w/ our dimensional argument.

Applying this result to hard spheres requires that we notice that $\tau$ depends on $T$. Letting $l$ be the mean free path, we have $l \propto \frac{1}{n \sigma^2}$ sphere radius.
Then $\bar{v} \propto \frac{l}{\tau} \Rightarrow \tau \propto \frac{1}{n\sigma^2} \sqrt{\frac{m}{k_B T}} \Rightarrow \kappa \propto \frac{k_B^{3/2} T^{1/2}}{m^{1/2} \sigma^2}$ indep't of $n$

2.3 We remember

$$P_{ij} = -\eta\, \partial_j u_i + -\tilde{\eta}\, \delta_{ij} \underbrace{\partial_k u_k}_{=0 \text{ here}} + \rho\, u_i u_j + \delta_{ij} P$$

$$P_{12} = -\eta\, \partial_2 u_1 = -\eta\, \partial_y u_x = -\eta a$$

Now

$$f_1 = -\tau\, v_y \cdot \partial_y f_0$$

And since $f_0$ depends on $y$ only through $u_x$:

$$f_1 = -\tau\, v_y \cdot \frac{\partial u_x}{\partial y} \cdot \frac{\partial f_0}{\partial u_x}$$

$$= -\tau\, v_y \cdot a \cdot \left( - \frac{m(u_x - v_x)}{k_B T} \right) \cdot f_0$$

$$= -\frac{m a \tau}{k_B T} \underbrace{(v_x - u_x)}_{\xi_x} \underbrace{v_y}_{\xi_y} \cdot f_0$$

From this we compute

$$P_{xy} = P_{xy}^{(1)} = -\frac{m^2 a\tau}{k_B T}\int \xi_x^2 \xi_y^2 f_0 \, d\vec{\xi}$$

$$-\eta a = -\frac{m^2 n a \tau}{k_B T}\cdot\left(\frac{k_B T}{m}\right)^2$$

$$\underline{\eta = n\cdot\tau\cdot k_B T}$$

2.4 Our gas is an ideal gas from the point of view of thermodynamics; thus its free energy is simply the kinetic energy:

$$F(T,V) = \frac{N d k_B T}{2}$$

$$\Rightarrow C_V = \left.\frac{\partial F}{\partial T}\right|_V = \frac{N d k_B}{2}$$

$$\Rightarrow c_V = \frac{C_V}{Nm} = \frac{d k_B}{2m}$$

And the enthalpy reads $G(T,P) = F + PV$ w/ $P = \frac{N k_B T}{V}$

$$\Rightarrow G(T,P) = N k_B T\left(1+\frac{d}{2}\right)$$

$$\Rightarrow C_p = \left.\frac{\partial G}{\partial T}\right|_p = N k_B\left(1+\frac{d}{2}\right)$$

$$\Rightarrow c_p = \frac{C_p}{Nm} = \frac{k_B(1+d/2)}{m}$$

Therefore $\underline{Pr} = \frac{\eta c_p}{K} = \frac{n\tau k_B T}{n k_B^2 T\tau/m \times (1+\frac{d}{2})}\cdot\frac{k_B(1+d/2)}{m} = \underline{1}$

The error in the determination of Pr resides in the single relaxation time hypothesis.