Notes 2a.

→ Microscopic Origins of Viscosity

Non-Ideal Fluids, Transport, Chapman- [redacted]
(Viscous) Enskog [redacted] 15

Applications of the Boltzmann Equation [redacted]

→ Chapman-Enskog ⇝ Basics (C-E Light)

- a major application of B.E. is calculation of transport coeffs. Derived Fluid Eqns

- recall, fluid equations [redacted] involve momentum, heat flux

i.e. really $\frac{\partial \underline{v}}{\partial t} = -\nabla \cdot \underline{\underline{\Pi}}$, etc.

continuity form

here:

$$\Pi_{\alpha,\beta} = mn\left(u_\alpha V_\beta + \langle v'_\alpha v'_\beta \rangle\right) +$$

$$\langle v'_\alpha v'_\beta \rangle = \int d^3v \; f \, v'_\alpha v'_\beta$$

if $f = f_{eq} = \frac{n(x)}{(2\pi)^{3/2} v_{Th}(x)^3} \exp\left[-\frac{(\underline{v}-\underline{V}(x))^2}{2 v_{Th}^2}\right]$

⇒

$$\langle v'_\alpha v'_\beta \rangle = \frac{1}{3} \langle v'^2 \rangle \delta_{\alpha,\beta}$$

$$\langle v^2 \rangle = 3T/m$$

but [redacted] is $f = f_{eq}$?!

recall, f satisfies:

$$\partial_t f + \underline{v} \cdot \underline{\nabla} f = C(f)$$

$f_{eq.}$ is soln. to $C(f) = 0$.

$\Rightarrow$ $\boxed{f_{eq} \text{ cannot solve B.E unless } \nabla f_0 = 0}$!

can assign time scales:

$\partial_t f \rightarrow \omega$

$\underline{v} \cdot \underline{\nabla} f \rightarrow v_{th}/L$

$C(f) \rightarrow \nu$;

collisional regime has $\nu > \frac{v_{th}}{L}, \omega$

$d < \bar{r} < l_{mfp} < L$

$\nu = \frac{v_{th}}{l_{mfp}}$ $\quad \frac{v_{th}}{L} < \nu$.

$l_{mfp} = 1/n\sigma$

$\Rightarrow$ $\boxed{f_{eq} \text{ is 0th order solution.}}$

then if f_0 is inhomogeneous $\Rightarrow$ stationary solution has correction!

$f = f_0 + \delta f$

$\hookrightarrow \sim$ inhomogeneity ! $\rightarrow$ more precisely response to inhomogeneity

i.e. $\nabla T, \nabla V$

and $\langle v'_\alpha v'_\beta \rangle = \int d^3v \, (f_0 + \delta f) \, v'_\alpha v'_\beta$

$$= p \, \delta_{\alpha,\beta} + \underbrace{\text{viscous stress}}_{\sim \nabla V}$$

stress vs. rate strain. viscosity $\sim mnD$ $\quad D \sim l_{mfp} v_{th}$

i.e. $mn\langle v'_\alpha v'_\beta \rangle_{visc} = -\eta \dfrac{\partial \langle V_\alpha \rangle}{\partial x_\beta} + \dots$

→ generic form of viscous stress — flux-grad't rel'n.

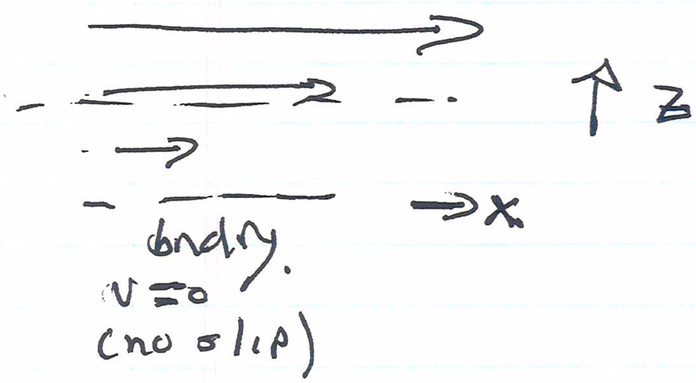
so, need:

- understand viscosity, etc.
- see how calculate df and then transport coeffs (viscosity)

so what is viscosity about?

- simple physics of transport coeffs!

Consider collisional gas:

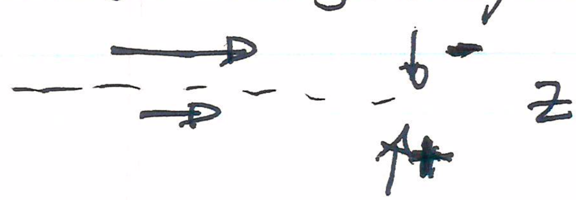


mean flow

$\underline{V} = V(z)\hat{x}$

i.e. shear flow (gradient ⊥ flow)

choose imaginary surface:



Calculate transport of $\hat{x}$ momentum thru surface:

$$\Pi_+ = \int_{v_z>0} d\underline{v}\; m V_x v_z f$$

$$\sim v_{Th} \bar{V} n m_+$$

$$\Pi_- = \int_{v_z<0} d\underline{v}\; m V_x v_z f$$

at first glance, would appear $\Pi_+ = \Pi_-$

so $\Pi_{tot} = 0$?! but!:

l_{mfp}

→ "scale of resolution" for emergin on surface is l_{mfp} ⇒ defines effective thickness.

→ $\boxed{V(z) \text{ has gradient across this!}}$

so

$$\Pi_{tot} = \Pi_- + \Pi_+$$

$$\Pi \cong \overbrace{-nm\,v_{Th}\,\overline{V}\left(z + \frac{l_{mfp}}{2}\right)}^{\Pi_-} \underbrace{+\, nm\,v_{Th}\,\overline{V}\left(z - \frac{l_{mfp}}{2}\right)}_{\Pi_+}$$

expansion smooth $\overline{V}$

$$\cong -nm\,v_{Th}\,l_{mfp}\,\frac{\partial \overline{V}}{\partial z}$$

$\to \sim l_{mfp} v_{Th}$

$$\cong -nm\,D\,\frac{\partial \overline{V}}{\partial z}$$

$$= -\eta\,\frac{\partial \overline{V}}{\partial z}$$

η: viscosity (shear)

$\sim \underline{\rho D}$ $\qquad D \sim v_{Th}\, v$

→ Key Points:

- equal # collisional kicks in +, − direction, but
- more momentum kicked down from above, the velocity gradient.

⇒

- net viscous momentum transport via collisions to relax gradient

How calculate systematically?

$\Rightarrow$ Chapman-Enskog expansion!

now

$$\underbrace{\frac{\partial f}{\partial t}}_{/} + \underbrace{\underline{v}\cdot\underline{\nabla} f}_{v_{Th}/L} = \underbrace{C(f)}_{\nu_{eff.}}$$

{multiple time scales}

$\nu > \frac{v_{Th}}{L}$

f norm ton

and seek:

$$\underbrace{\Pi_{z,x}}_{\text{z direction flux of } \hat{x} \text{ momentum}} = \int d^3v \, \text{[redacted]} \, v_z \left(m v_x f\right)$$

z direction flux of $\hat{x}$ momentum

$$f = f_{eq} + \delta f$$

$$\Pi_{z,x} = \int d^3v \, \text{[redacted]} \, v_z \left(m v_x \left(f_0 + \delta f\right)\right)$$

if $f_{eq} \cong \frac{n_0}{v_{Th}^3} \exp\left[-\frac{\left(\underline{v} - V(z)\hat{x}\right)^2}{2 v_{Th}(x)^2}\right]$

{i.e. local Maxwellian}

→ f_{eq} contribution vanishes by symmetry!

so

$$\Pi_{z,x} = \int d^3v \; v_z \, (m v_x) \, \delta f$$

↑ drives the flux.

How get δf?

⇒ Perturbative solution!?

$$\underline{v} \cdot \nabla f = C(f)$$

→ really an integral equation!

l. O.: $C(f) = 0$

$$f = f_{eq}$$ → Local Maxwellian

1st O.:

$$\underline{v} \cdot \underline{\nabla} f_{eq} = C(\delta f)$$

$$\therefore \quad \delta f = C^{-1}\left[\underline{v} \cdot \underline{\nabla} f_{eq}\right]$$

How?

→ lengthy calculation

→ Krook (crook) Model !

$$C(f) = -\nu (f - f_{eq})$$

↓ collisional decay to local Maxwellian

caveat Emptor!

or

$$\underline{v} \cdot \underline{\nabla} f = C(f) = -\nu (f - f_{eq})$$

$$f = f_{eq} + \delta f$$

$$\underline{v} \cdot \underline{\nabla} (f_{eq} + \delta f) = -\nu (f - f_{eq})$$

l.o.: $-\nu (f - f_{eq}) = 0$

$$f = f_{eq}$$

1st order:

$$\underline{v} \cdot \underline{\nabla} f_{eq} = -\nu \, \delta f$$

$$\delta f = -\frac{\underline{v} \cdot \underline{\nabla}}{\nu} f_{eq}$$

↓

perturbative correction to f_{eq}; $\quad O\left(\frac{v_{Th}}{L\nu}\right)$

So

$$\Pi_{z,x} = \int d^3v \; v_z \, m v_x \, \delta f$$

$$= \int d^3v \; v_z \, m v_x \left(- \frac{v_z}{\nu} \frac{\partial}{\partial z} f_{eq} \right)$$

$$\vec{V} = V(z)\,\hat{x}$$

now
$$f_{eq} \cong \frac{n(\underline{x})}{v_{Th}^3(\underline{x})} \exp\left[- \frac{(v - V(z)\,\hat{x})^2}{2 v_{Th}^2(\underline{x})} \right]$$

$$= \frac{n}{v_{Th}^3} \exp\left[- \frac{(v - V(z))^2}{2 v_{Th}^2} \right]$$

$$\frac{\partial f_{eq}}{\partial z} = \frac{n}{v_{Th}^3} \frac{v_x}{v_{Th}^2} \frac{\partial V(z)}{\partial z} \exp[\;\;]$$

linear respons.

$$- 2 \frac{V(z)}{v_{Th}^2} \frac{\partial V(z)}{\partial z} \exp[\;\;]$$

dropped ⇒ interested in only linear response of flux to gradient.

see next

$$\Rightarrow \frac{\partial f_0}{\partial z} = f_{eq} \frac{v_x}{v_{Th}^2} \frac{\partial V(z)}{\partial z}$$

Note:

→ here seek linear relation between flux and gradient

→ presumes weak distortion from Maxwellian, i.e.

$$f_{eq} = \frac{n}{v_{Th}^3} \exp\left[-\frac{(v - V(x)\hat{x})^2}{2 v_{Th}^2} \right]$$

$$= \frac{n}{v_{Th}^3} \exp\left[-\frac{(v^2 - 2 v V + V^2)}{2 v_{Th}^2} \right]$$

$$= \frac{n}{v_{Th}} \exp\left[\frac{-v^2}{2 v_{Th}^2} \right] \left[1 + \frac{v_x V}{v_{Th}^2} \right]$$

e.o. factor on expansion

$$= f_{eq}^0 \left(1 + \frac{v_x V}{v_{Th}^2} \right)$$

yields result.

up-coming → "Linear Response Theory"

Green-Kubo Relation

so

$$\Pi_{z,x} = \int d^3\cancel{x}\, v \; v_z \, m v_x \left(-\frac{v_z}{\nu} \frac{v_x}{v_{Th}^2} \right) \times f_{eq} \frac{\partial V(z)}{\partial z}$$

$$= -\# \frac{mn}{\nu} v_{Th}^2 \frac{\partial V(z)}{\partial z}$$

$$= -\# \, mn \underbrace{\left(\frac{v_{Th}}{\nu}\right)}_{l_{mfp}} v_{Th} \frac{\partial V(z)}{\partial z}$$

$$D = v_{Th} \, l_{mfp}$$

$$\boxed{\begin{aligned} \Pi_{z,x} &= -\# \, mn D \frac{\partial V(z)}{\partial z} \\ &= -\# \rho D \frac{\partial V(z)}{\partial z} \end{aligned}}$$

$$\eta = -\# \rho D$$

⇒ basic result for collisional shear viscosity

can get #

Note form of result:

$$\Pi_{zx} = -\underbrace{\#nm\lambda}_{\text{microscopics}} \frac{\partial V_x(z)}{\partial z}$$

Π_{zx} ↓ flux

microscopics ↓ transport coefficient

$\frac{\partial V_x(z)}{\partial z}$ → gradient of thermo. quantity (dist.) ↓ thermodynamic force.

⇒ example of thermodynamic flux – force relation.

⇒ $\boxed{\text{constitutive relation}}$. proportionality is transport coefficient

In general, have vector relation:

$$\underline{\Gamma} = -\underline{\underline{K}} \cdot \underline{\nabla} C$$

$\underline{\Gamma}$ ↓ vector of fluxes

$\underline{\nabla} C$ ↓ vector of gradients

$\underline{\underline{K}}$ ↓ matrix of transport coefficients – $\boxed{\text{Onsager matrix}}$)

(n.b. Onsager symmetry ⇒ $\underline{\underline{K}}$ symmetric)

⇒ Observe:

- $f_{\substack{Max \\ eq}}$ annihilates collision operator.
  and corresponds to $\frac{dS}{dt} = 0$
  state ⇒ maximal entropy.

<u>but</u>

- $f_{Max}[n(\underline{x}), T(\underline{x}), V(\underline{x})]$ does <u>not</u> satisfy Boltzmann eqn. ⇒ δf needed.

<u>i.e.</u> $\underline{v} \cdot \underline{\nabla} f = C(f)$

$$\Rightarrow \quad f = f_{Max} + \delta f$$

why?: ⟶ $\boxed{\text{gradients in thermodynamic quantities} \Rightarrow \text{system is not in maximum entropy state i.e. } \delta f \neq 0}$

- so $\delta f \sim \underline{\nabla} C$, ⇒ relaxation to maximum entropy state will occur by <u>collisional</u> <u>transport</u>.

- can describe relaxation macroscopically, i.e.

$$\underset{\text{flux}}{\Pi_{\alpha,\beta}} = -\rho D \underset{\text{force}}{\frac{\partial V_\beta}{\partial x_\alpha}}$$

$$\frac{\partial \rho v}{\partial t} = -\nabla \cdot \underline{\underline{\Pi}}$$

$$-\frac{\partial V_\beta}{\partial x_\alpha} \Pi_{\alpha,\beta} = \rho D \left(\frac{\partial V_\beta}{\partial x_\alpha}\right)^2 \qquad \partial_t \int \mathcal{E}_{v_1} = \int \underline{\Pi} \cdot \underline{\nabla V}$$

$$\Rightarrow \boxed{\frac{dS}{dt} = \frac{\rho D}{T} \left(\frac{\partial V_\beta}{\partial x_\alpha}\right)^2}$$

– entropy production due transport-induced relaxation

Note time scales:

i.) to form local Maxwellian, H-thm $\Rightarrow \tau_{coll} \sim \nu^{-1}$

ii.) to form global maximum entropy state:

$$1/\tau_{relax} \sim D/L_v^2 \sim \nu \frac{l_{mfp}^2}{L_v^2} \qquad L_v^{-1} = \frac{1}{V}\frac{\partial V}{\partial x}$$

$$\tau_{relax} \sim \left(L_v / l_{mfp} \right)^2 \tau_{coll}.$$

$\Rightarrow$ entropy production / relaxation is multiple time scale process!.

More generally, can write:

$$\underbrace{J_i}_{i\text{th flux}} = - \sum_{j=1}^{n} \underbrace{\alpha_{ij}}_{\text{kinetic coefficient}} \underbrace{X_j}_{\text{driving force}}$$

$$\frac{dS}{dt} = \psi = \text{"Dissipation Function"}$$

$$\Rightarrow \quad \frac{dS}{dt} = \sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_{i,j} X_i X_j$$

$\alpha_{ij} = \alpha_{ji}$ if basic interaction time reversible.

Onsager Symmetry

i.e. $$\frac{dS}{dt} = - X_j J_i$$

so, for 2x2:

$$\frac{dS}{dt} = \sum_{i=1}^{2} \sum_{j=1}^{2} \alpha_{1,1} X_1^2 + (\alpha_{1,2} + \alpha_{2,1}) X_1 X_2 + \alpha_{2,2} X_2^2$$

clearly need:

$$\alpha_{1,1} \geq 0 \qquad \rightarrow \text{ i.e. diffusion}$$
$$\alpha_{2,2} \geq 0 \qquad \quad \text{down gradient}$$

and $\alpha_{1,1}\,\alpha_{2,2} - \frac{1}{4}\left(\alpha_{1,2} + \alpha_{2,1}\right)^2 \geq 0.$

(i.e. descr $\Rightarrow$ diag.)

N.B. Off-diagonals?!

i.e. Can ∇T drive a density flux?

$$\Gamma = \int d^3v \; \underline{v}\; \delta f$$

$$\delta f = -\frac{1}{\nu}\, \underline{v} \cdot \nabla f_0$$

$$\Rightarrow \Gamma = \int d^3v \; \underline{v} \left(-\frac{1}{\nu} v_x \frac{\partial}{\partial x} \left(\frac{n_0}{v_{th}(x)^3} \exp\left[-\frac{m v^2}{2T(x)} \right] \right) \right)$$

clearly can get contribution to Γ_x.
$\rightarrow$ Thermal diffusion.

Message: Gradient in distribution function is the key! --- but integration symmetries matter.