Transport and Chapman - Enskog II

→ have discussed:
- Boltzmann Eqn. and H-Thm.
- fluid equations (macro balance)
- basic transport, Chapman - Enskog, Flux - Force relations

Here, consider more detailed treatment of transport, i.e.:
→ treat B.E. as integral equation
→ note Krook model was a crook model, as violated conservation laws
→ not the full crank...

Recall:

$$\frac{\partial f}{\partial t} + \underline{v} \cdot \underline{\nabla} f = C(f)$$

$$C(f) = \int d\underline{p}_1 \int d\underline{p}' \int d\underline{p}_1' \, w(\underline{p}', \underline{p}_1'; \underline{p}, \underline{p}_1) (f' f_1' - f_1 f)$$

"The solution of the above equation, as we will see shortly, is truly a gruesome task."

- Stewart Harris, "An Intro to the Theory of the Boltzmann Equation"

Now, $f = f_0 + \delta f$

$$\delta f = -\frac{\partial f_0}{\partial \epsilon} \chi(\Gamma)$$

$\Gamma \to$ generic phase space variables

$$= \frac{f_0}{T} \chi(\Gamma)$$

$\hookrightarrow$ re-scaled perturbed dist.

Now, $\chi(\Gamma)$ must satisfy conservation laws / constraints:

number, momentum, energy } conserved $\Rightarrow \int d\Gamma \, \delta f \begin{pmatrix} 1 \\ \underline{p} \\ \epsilon \end{pmatrix} =$

$f = f_0 + \delta f$ values must equal f_0 values $= \int d\Gamma \, f_0 \, \chi \begin{pmatrix} 1 \\ \underline{p} \\ \epsilon \end{pmatrix} = 0$.

Now, for Chapman-Enskog expansion, recall need $C(\delta f)$, i.e.

$$\frac{\partial f}{\partial t} + \underline{v} \cdot \underline{\nabla} f = C(f) = -\nu (f - f_0)$$

l.O. $\quad -\nu(f - f_0) = 0$

$$f^{(0)} = f_{eqbm.}$$

1^{st} O $\quad \underline{v} \cdot \underline{\nabla} f^{(0)} = \underline{v} \cdot \nabla f_{eqbm}$

$$= -\nu(\cancel{f} - f_0)$$

$$= -\nu(\cancel{f_{eqbm}} + \delta - \cancel{f_0})$$

$$= -\nu \delta f$$

Key balance is between:

$$\underline{v}\cdot\underline{\nabla} f^{(0)} = -\nu\, \delta f$$

drive – flux due inhomogeneity

relaxation

so need relaxation of δf!

$$f = f_0 + \delta f = f_0\left(1 + \frac{\chi}{T}\right)$$

$\Rightarrow$

$$C(f) = \int d\underline{p}_1 \int d\underline{p}_1' \int d\underline{p}'\, w' \left(f_0' f_{0,1}' \left(1+\frac{\chi'}{T}\right)\left(1+\frac{\chi_1'}{T}\right) - f_{0,1} f_0 \left(1+\frac{\chi}{T}\right)\left(1+\frac{\chi_1}{T}\right)\right)$$

- expanding to l.o. (linearization)
- noting $f_0' f_{0,1}' = f_{0,1} f_0$

$\Rightarrow$

$$C(\delta f) = f_0 \int d\underline{p}_1 \int d\underline{p}' \int d\underline{p}_1' \frac{w}{T} f_{0,1} \left(\chi' + \chi_1' - \chi_1 - \chi\right)$$

$$\equiv \frac{f_0}{T} I(\chi)$$

defines collisional effect on δf.

$$I(\chi) = \int w' f_{0,1} \left(\chi' + \chi_1' - \chi - \chi_1\right) d\underline{p}_1 \, dp' \, dp_1'$$

observe:

- $\chi = \text{const.}$ $\quad I(\chi) = 0$ ✓

  $\chi = \varepsilon$ $\quad I(\chi) = 0$ ✓

  $\chi = p \cdot \delta V$ $\quad I(\chi) = 0$ ✓

  $\Rightarrow$ $I(\chi)$ consistent with conservation constraints.

- now, make progress by relating LHS of Boltzmann Eqn. to macroscopics

i.e. Chapman-Enskog expansion will yield:

$$\frac{\partial f^{(0)}}{\partial t} + \underline{v} \cdot \underline{\nabla} f^{(0)} = C(\delta f)$$

$$= \frac{f_0}{T} I(\chi)$$

now, $$f_0 = \frac{n_0(\underline{x})}{v_{Th}^{3/2}(\underline{x})} \exp\left[\frac{-m(\underline{v} - \underline{V}(\underline{x}))^2}{2T(x)}\right]$$

and use fluid eqns to simplify for n, T, $\underline{V}$ etc.

or, more generally:

$\hookrightarrow$ chemical potential

$$f_0 = \exp\left(\frac{+\mu - \epsilon}{T}\right)$$

after much non-instructive labor
(see Physical Kinetics Pgs. 19–21)

$$\boxed{\left(\frac{\epsilon - c_p T}{T}\right)\underline{v}\cdot\underline{\nabla} T + \left[m v_\alpha v_\beta - \delta_{\alpha,\beta}\frac{\epsilon}{c_v}\right] V_{\alpha,\beta} = I(\chi)}$$

(1) (2)

i.e. – here idea is to "cancel" f_0 on both sides (see attached details)

– $V_{\alpha,\beta} = \frac{1}{2}\left(\frac{\partial V_\alpha}{\partial x_\beta} + \frac{\partial V_\beta}{\partial x_\alpha}\right)$

$\rightarrow$ strain tensor

– $C_v = 3/2\, n\, (k^{-1})$ (spec. heat)

$C_v = (\partial E/\partial T)_v$

$C_p = 5/2\, n\, k^{-1}$ (spec. heat)

$W = C_p T$

$\downarrow$

specific enthalpy

- ① → ∇T effects ⇒ thermal conduction, etc.
  ② → ∇V effects ⇒ viscosity

Now, to calculate thermal conductivity:

- $\underline{Q} = -\underline{\underline{K}} \cdot \nabla T$

heat flux — $\underline{Q}$; conductivity tensor — $\underline{\underline{K}}$; temperature gradient — ∇T

- can take $V_{\alpha,\beta} = 0$

so $\frac{\epsilon - c_p T}{T} \, \underline{v} \cdot \nabla T = I(x)$

$$\delta f = \frac{f_0 x}{T}$$

and

$$Q = \int d^3\underline{v} \; \underline{v} \left(\frac{1}{2} m v^2\right) \left(\cancel{f_0} + \delta f\right)$$

To solve:

- solution must have form:

$x = g \cdot \nabla T$

immediately, $|g| \sim l_{mfp}$

as $\delta f / f_0 = x/T = \frac{l_{mfp}}{L_T} < 1$.

why?

- χ is scalar
- $\underline{\nabla} T$ is thermodynamic force which drives heat flux
- by design, C-E expansion is <u>linear</u> response!

$\Rightarrow$ $\underline{g} = \underline{g}(T)$, indep. of $\underline{\nabla} T$

<u>i.e.</u> χ must be <u>linear</u> in ∇T!

$\Rightarrow$

$$\left(\frac{\epsilon - c_p T}{T}\right) \underline{v} \cdot \underline{\nabla} T = I(\chi)$$

$$= I(\underline{g} \cdot \underline{\nabla} T)$$

$$= I(\underline{g}) \cdot \underline{\nabla} T$$

as ∇T macroscopic - indep. $\underline{v}$ - so <u>outside</u> collision integral.

And, can write:

$$\left(\frac{\epsilon - c_p T}{T}\right) \underline{v} = I(\underline{g})$$

i.e. lifting ∇T from both sides.

→ now, recall χ must satisfy conservation laws:

$$\int d\Gamma \; f_0 \begin{pmatrix} \chi \\ p\chi \\ \epsilon\chi \end{pmatrix} = 0$$

Now, for a number, or energy, perturbation to be finite, would need:

$$\left.\begin{aligned} &\int d\Gamma\, f_0 \underline{g} \neq 0 \\ &\int d\Gamma\, f_0 \epsilon g \neq 0 \end{aligned}\right\} \Rightarrow \text{needs direction}$$

→ but transport eqn has no vector parameters to set direction.

→ so no $\begin{pmatrix} \text{number} \\ \text{energy} \end{pmatrix}$ perturbation, as must be.

→ momentum conservation ⇒

$$\int d\Gamma\, f_0\, g \cdot \underline{v} = 0$$

Now,

$$-\delta f = \frac{f_0}{T}\,\chi \,, \qquad \chi = \underline{g} \cdot \underline{\nabla} T$$

so,

$$\underline{Q} = \int d^3v \ \underline{v} \ \epsilon \ \delta f$$

$$= \int d^3v \ \underline{v} \ \epsilon \ \frac{\chi f_0}{T}$$

$$= \int d^3v \ \underline{v} \ \epsilon \ \frac{f_0}{T} \ \underline{g} \cdot \nabla T$$

so

$$\boxed{\begin{aligned} Q_\alpha &= -K_{\alpha\beta} \nabla T_\beta \\ K_{\alpha,\beta} &= -\frac{1}{T} \int f_0 \epsilon v_\alpha g_\beta \, d^3v \end{aligned}}$$

For isotropic gas:

– $K_{\alpha,\beta}$ diagonal

– $K = 1/3 \, K_{\alpha\alpha}$ (sum on rpt).

$$\Rightarrow \boxed{\begin{aligned} \underline{Q} &= -K \underline{\nabla} T \\ K &= -\frac{1}{3T} \int d^3\underline{v} \ f_0 \ \epsilon \ \underline{v} \cdot \underline{g} \end{aligned}}$$

n.b. flux opposite to temp. gradient.

Now, finally;

$$\kappa = \frac{-1}{3T}\int d^3\underline{v}\; f_0\, \epsilon\; \underline{v}\cdot\underline{g}$$

For monatomic gas, g must have form

$$\underline{g} = \frac{\underline{v}}{|v|}\, \underbrace{g(|v|)}_{\text{scalar}}$$, as $\underline{v}$ is only vector 'available' to $\underline{g}$

$\Rightarrow$

$$\kappa = \frac{-1}{3T}\int d^3v\; f_0\, \epsilon\; \frac{\underline{v}\cdot\underline{v}}{|v|}\, g(|v|)$$

What is g? (avoiding useless exercise with Sonine polynomial expansion)

- dimensionally:

$$\delta f/f_0 = \frac{\chi}{T} = \frac{\underline{g}\cdot\nabla T}{T}$$

so

$g \sim$ Length $\sim l_{mfp}$.

- $\delta f/f_0 \sim \frac{l_{mfp}}{L_T} \ll 1$ ✓.

$\Rightarrow \quad g = v_{Th}/\nu \sim \ell_{mfp}$

$\Rightarrow \quad K = c\, n\, \ell_{mfp} v_{Th}$

spec. heat / molecule

$\Rightarrow$ as $\ell_{mfp} \sim 1/n\sigma$

$K \sim \sqrt{T/m} \,/\, \sigma$

Physical Interpretation:

fluxes $\leftrightarrow \int d\Gamma' \, \underline{v} \begin{Bmatrix} \text{moment} \\ v^n \end{Bmatrix} \delta f$

Flux $\rightarrow$ response to fluctuation in f induced by gradient (thermo force)

$\delta f = \dfrac{f_0 x}{T}$

$x = \underline{g} \cdot \underline{\nabla} T$

and correspondence with Krook $\Rightarrow$

$g \sim \ell_{mfp}$.

Can understand this heuristically, via:

$$\delta f = \frac{\partial f}{\partial T}\delta T = -f_0 \frac{\delta T}{T}$$

$$\delta T = T(x - l_{mfp}) - T(x) = -l_{mfp}\, \partial T/\partial x$$

$\Downarrow$ fluctuation in T

$\Downarrow$ scattering by l_{mfp} $\Rightarrow \delta T$

$\Rightarrow$

$$\delta f = \frac{\partial f}{\partial T}\left(-l_{mfp}\frac{\partial T}{\partial x}\right) = \frac{f_0}{T} l_{mfp} \frac{\partial T}{\partial x}.$$

and can treat viscosity similarly!

see Physical Kinetics, pgs. 24–26.

where operator $I(\chi)$ (collisional relaxation of perturbation) is:

$$\boxed{I(\chi) = \int w' f_{0,1} \left(\chi' + \chi_1' - \chi - \chi_1\right) d\Gamma_1 \, d\Gamma' \, d\Gamma_1'}$$

Now, can observe:

if $\chi = \text{const} \Rightarrow I(\chi) = 0$

$\chi = \epsilon \Rightarrow I(\chi) = 0$ as

$$\epsilon' + \epsilon_1' = \epsilon + \epsilon_1 \qquad \text{(energy conservation)}$$

$\chi = \underline{p} \cdot \delta \underline{V} \Rightarrow I(\chi) = 0$ as

$$\underset{\text{boost}}{\delta \underline{V}} \cdot \left(\underline{p}_1' + \underline{p}' = \underline{p} + \underline{p}_1\right) \qquad \text{(momentum conservation)}$$

$I(\chi)$ consistent with conservation constraints.

⇒ DETAILS of LHS

→ Now, can make progress by relating Boltzmann equation to macroscopics ⇒ link to fluid equations

For gas at rest: chem. potential

$$f_0 = \exp\left(\frac{\mu - \epsilon(\Gamma)}{T}\right)$$

energy associated with internal degrees freedom

and $\epsilon(\Gamma) = \frac{1}{2}mv^2 + \epsilon_{int}$

so in moving gas;

$$f_0 = \exp\left[\left(\frac{\mu - \epsilon_{int}}{T}\right)\right] \exp\left[-\frac{m}{2T}\left(\underline{v}-\underline{V}\right)^2\right]$$

as transport coefficients independent $\underline{V}$, can examine in frame where $\underline{V}=0$ (but $\underline{V}' \neq 0$)

so...

$$\frac{1}{f_0}\frac{\partial f_0}{\partial t} = \left[\left(\frac{\partial \mu}{\partial T}\right)_p - \frac{(\mu - \epsilon(\Gamma))}{T}\right]\frac{\partial T}{\partial T} + \left(\frac{\partial \mu}{\partial p}\right)_T \frac{\partial p}{\partial t}$$

$$+ \; m\underline{v}\cdot\frac{\partial \underline{V}}{\partial t}$$

Now, thermo $\Rightarrow$ $\left(\frac{\partial \mu}{\partial T}\right)_p = -S$ (entropy per particle)

$\left(\frac{\partial \mu}{\partial p}\right)_T = 1/N$ (volume per particle)

$\mu = W - TS$ heat fctn. ($W = c_p T$)

(1) $$\frac{\partial f_0}{\partial t} = \frac{f_0}{T}\left[\left(\frac{\epsilon(\Gamma') - W}{T}\right)\frac{\partial T}{\partial t} + \frac{1}{N}\frac{\partial p}{\partial t} + m\underline{v}\cdot\frac{\partial \underline{V}}{\partial t}\right]$$

and similarly:

(2) $$\underline{v}\cdot\underline{\nabla} f_0 = \frac{f_0}{T}\left[\left(\frac{\epsilon(\Gamma') - W}{T}\right)\underline{v}\cdot\underline{\nabla} T + \left(\frac{1}{N}\right)\underline{v}\cdot\underline{\nabla} p + m\, v_\alpha v_\beta V_{\alpha\beta}\right]$$

where $$V_{\alpha\beta} = \frac{1}{2}\left(\frac{\partial V_\alpha}{\partial x_\beta} + \frac{\partial V_\beta}{\partial x_\alpha}\right)$$ → strain tensor

$$V_{\alpha\alpha} = \underline{\nabla}\cdot\underline{V}$$

and used $$v_\alpha v_\beta \frac{\partial V_\beta}{\partial x_\alpha} = v_\alpha v_\beta V_{\alpha\beta}$$

As $$\frac{\partial f_0}{\partial t} + v\cdot\nabla f_0 = \frac{f_0}{T}\left(I(x)\right)$$
will add (1) and (2). Observe that (1), (2) add to form fluid equations

i.e. $\frac{\partial T}{\partial t} + \underline{V} \cdot \nabla T$ - - - - -

$\frac{\partial P}{\partial t} + \underline{v} \cdot \underline{\nabla} P$ - - - - -

{ forms emerge from addition

etc.

Now, use:

$$\frac{\partial \underline{V}}{\partial t} = \frac{-1}{\rho} \underline{\nabla} P = -\frac{1}{Nm} \underline{\nabla} P \qquad \text{(Euler)}$$

$$\frac{\partial N}{\partial t} = -N \, \underline{\nabla} \cdot \underline{V} \qquad \text{(Continuity)}$$

As $N = P/T$ for gas,

$$\frac{1}{N} \frac{\partial N}{\partial t} = \frac{1}{P} \frac{\partial P}{\partial t} - \frac{1}{T} \frac{\partial T}{\partial t} = -\underline{\nabla} \cdot \underline{V}$$

Also, entropy conservation $\Rightarrow$

$$\frac{\partial s}{\partial t} + \underline{V} \cdot \underline{\nabla} s = 0$$

and $\underline{V} = 0 \Rightarrow \partial s / \partial t = 0$

$$\frac{\partial s}{\partial t} = 0 = \frac{\partial}{\partial t}\left(\left(\frac{\partial s}{\partial T}\right)_p T + \left(\frac{\partial s}{\partial p}\right)_T p\right)$$

$$0 = \frac{C_p}{T}\frac{\partial T}{\partial t} - \frac{1}{p}\frac{\partial p}{\partial t} \qquad (*)$$

as $\left(\frac{\partial s}{\partial T}\right)_p = \frac{C_p}{T}$, $\left(\frac{\partial s}{\partial p}\right)_T = -\frac{1}{p}$

with:

$$\frac{1}{p}\frac{\partial p}{\partial t} - \frac{1}{T}\frac{\partial T}{\partial t} = -\underline{\nabla}\cdot\underline{V} \qquad (*)$$

$\Rightarrow$ can combine starred equations:

$$\frac{1}{T}\frac{\partial T}{\partial t} = \frac{-1}{C_v}\,\underline{\nabla}\cdot\underline{V}, \quad \frac{1}{p}\frac{\partial p}{\partial t} = -\frac{C_p}{C_v}\,\underline{\nabla}\cdot\underline{V}$$

$$C_p - C_v = 1$$

So, can add results for $\partial f_0/\partial t$, $\underline{v}\cdot\underline{\nabla} f_0$ and exploit macroscopic relations to obtain:

$$\frac{\partial f_0}{\partial t} + \underline{v} \cdot \underline{\nabla} f_0 = \frac{f_0}{T} \left\{ \frac{\epsilon(\Gamma) - w}{T} \, \underline{v} \cdot \underline{\nabla} T + m v_\alpha v_\beta \, \nabla_{\alpha\beta} \right.$$

$$\left. + \left(\frac{w - T c_p - \epsilon(\Gamma)}{c_v} \right) \underline{\nabla} \cdot \underline{V} \right\}$$

enthalpy

with $W = c_p T$, can re-write Boltzmann equation for gas as:

$$\boxed{\left(\frac{\epsilon(\Gamma) - c_p T}{T} \right) \underline{v} \cdot \underline{\nabla} T + \left[m v_\alpha v_\beta - \delta_{\alpha\beta} \frac{\epsilon(\Gamma)}{c_v} \right] \nabla_{\alpha\beta} = I(\chi)}$$

→ Boltzmann eqn. in Chapman-Enskog expansion, expressed in macro-scopics.

→ drive on LHS linked to macroscopics.

→ Application: Calculating the Thermal Conductivity .... — Rigorously

Now, → need determine $\underline{\underline{K}}$ s/t

$$\underline{Q} = -\underline{\underline{K}} \cdot \underline{\nabla} T$$

heat flux

temperature gradient

conductivity tensor.