Notes 1 : Section V.

Transport and Chapman – Enskog II – Detailed Calculation

→ 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

$\Big\}$ conserved $\Rightarrow \int d\Gamma \, \delta f$ [redacted] $\begin{pmatrix} 1 \\ \underline{p} \\ \epsilon \end{pmatrix} =$

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

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

$$= -\nu(f - f_0)$$

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

$$= -\nu \delta f$$

Key balance is between:

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

$\downarrow$ drive - flux due inhomogeneity

$\downarrow$ 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 $f_0' f_{0,1}' = f_{0,1} f_0$

$\Rightarrow$

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

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

$\downarrow$ defines collisional effect on δf.

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

observe:

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

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

  $\chi = \underline{p} \cdot \delta \underline{V}$ $\qquad I(\chi) = 0$ ✓

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

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

or more generally:

μ chemical potential

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

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

$$\boxed{\left(\frac{\epsilon - c_p T}{T}\right) \overset{1}{\underline{v}\cdot\underline{\nabla} T} + \overset{2}{\left[m v_\alpha v_\beta - \delta_{\alpha,\beta}\frac{\epsilon}{c_v}\right]} V_{\alpha,\beta} = I(\chi)}$$

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:

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

  $\underline{Q}$: heat flux

  $\underline{\underline{K}}$: conductivity tensor

  ∇T: temperature gradient

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

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

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

and

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

To solve:

- solution must have form:

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

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

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

why?

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

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

i.e. χ must be linear 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 outside 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:

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

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 ⇒

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

Now,

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

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 repeated index.)

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

✱

n.b. flux opposite to temp. gradient.

Now, finally;

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

For monatomic gas, g must have form;

$$\boxed{\underline{g} = \frac{\underline{v}}{|v|}\, \underbrace{g(|v|)}_{\text{scalar}}}$$

, 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 : $\hookrightarrow$ see Lifshitz and Pitaevski

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

so

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

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

$\rightarrow \quad g = v_{Th}/\nu \sim l_{mfp}$

$\Rightarrow \quad \kappa = c\, n\, l_{mfp} v_{Th}$

spec. heat / molecule

$\rightarrow$ as $l_{mfp} \sim 1/n\sigma$

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

Physical Interpretation :

Fluxes $\leftrightarrow \int d\Gamma\, \underline{v} \left\{ \begin{matrix} \text{moment} \\ v^n \end{matrix} \right\} \delta f$

Flux → 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 $\Rightarrow$

$g \sim l_{mfp}.$

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

$\Uparrow$ scattering by l_{mfp} $\Rightarrow \delta f$

$\Rightarrow$

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

and can treat viscosity similarly !

see Physical Kinetics, pgs. 24-26.

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

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

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.

$\Rightarrow$ **DETAILS of LHS**

$\Rightarrow$ Now, can make progress by relating Boltzmann equation to macroscopics $\Leftrightarrow$ link to fluid equations *

For gas at rest:

$$f_0 = \exp\left(\frac{\underset{\text{chem. potential}}{\mu} - \epsilon(\Gamma)}{T} \right)$$

[redacted]

energy associated with internal degrees freedom

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

so in moving gas;

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

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. ($W = c_p T$)

$$\underline{\underline{(1)}} \quad \frac{\partial f_0}{\partial t} = \frac{f_0}{T}\left[\left(\frac{\epsilon(\Gamma) - w}{T}\right)\frac{\partial T}{\partial t} + \frac{1}{N}\frac{\partial p}{\partial t} + m\underline{v}\cdot\frac{\partial \underline{V}}{\partial t}\right]$$

and similarly:

$$\underline{\underline{(2)}} \quad \underline{v}\cdot\underline{\nabla} f_0 = \frac{f_0}{T}\left[\left(\frac{\epsilon(\Gamma) - w}{T}\right)\underline{v}\cdot\underline{\nabla} T + \left(\frac{1}{N}\right)\underline{v}\cdot\underline{\nabla} p + m\, v_\alpha v_\beta \bar{V}_{\alpha\beta}\right]$$

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

$$\bar{V}_{\alpha\alpha} = \underline{\nabla}\cdot\underline{V}$$

and used $v_\alpha v_\beta \frac{\partial \bar{V}_\beta}{\partial x_\alpha} = v_\alpha v_\beta \bar{V}_{\alpha\beta}$

As $\frac{\partial f_0}{\partial t} + v\cdot\nabla f_0 = \frac{f_0}{T}(I(\chi))$ will add $\underline{\underline{(1)}}$ and $\underline{\underline{(2)}}$. Observe that

$\underline{\underline{(1)}}$, $\underline{\underline{(2)}}$ add to form fluid equations

[redacted]

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

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

$\left\{ \text{forms emerge from addition} \right.$

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

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

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

as $\left(\frac{\partial s}{\partial T}\right)_\rho = \frac{c_p}{T}$, $\left(\frac{\partial s}{\partial \rho}\right)_T = -\frac{1}{\rho}$

with:

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

$\Rightarrow$ can combine starred equations:

$$\frac{1}{T}\frac{\partial T}{\partial t} = -\frac{1}{c_v}\underline{\nabla}\cdot\underline{V}, \quad \frac{1}{\rho}\frac{\partial \rho}{\partial t} = -\frac{c_p}{c_v}\underline{\nabla}\cdot\underline{V}$$

$$c_p - c_v = 1$$

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

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

w: 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

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

$\underline{Q}$: heat flux

$\underline{\underline{K}}$: conductivity tensor

$\underline{\nabla} T$: temperature gradient