Physics 210B

L4b – Transport Coefficients cont'd and Entropy Production, re-visited.

(A)

Recall: Boltzmann Equation + H Theorem

↓

Hydrodynamics (general)

↓

Closure → Chapman – Enskog

↓

Transport Coeffs.

↓

$\boxed{\text{Dissipative Hydrodynamics}}$

→ $\boxed{\text{N-S Eqn}}$

Key calculation: { C-E Expansion

$\Rightarrow f = f_{eq} + \delta f \quad , \quad \frac{\delta f}{f_{eq}} \sim O(l_{mfp}/L)$

$\Leftrightarrow$ $\boxed{\text{Flux – Gradient relation}}$

$\underline{\Pi}_{ij} = -\eta \, \nabla_i V_j \qquad \eta \equiv$ shear viscosity.

$\eta = \# \rho D$

$D = v_{th} l_{mfp}$

$\eta \to$ transport coefficient
(Flux - Gradient proportionality)

Alternative Approach to Transport Coefficients: Moment Closure

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

Relaxation Approx to B.E.

$f_{eq} \downarrow$ local equilibrium distribution

"BGK Eqn."
$\downarrow$
Krook

Approach from moments (macroscopics!) of f, i.e.

for any function A, can define average:

$$\langle A \rangle = \int d\underline{v}\, f(\underline{x}, \underline{v}, t) / \rho$$

$$= \langle A(\underline{x}, t) \rangle$$

Macro.

so

$$\partial_t \rho\langle A\rangle = \int A \frac{\partial f}{\partial t}\, d\underline{v}$$

$$= \int A\left(-\underline{v}\cdot\underline{\nabla} f - \nu(f - f_{eq})\right) d\underline{v}$$

$$= -\underline{\nabla}\cdot\int \underline{v} A f\, d\underline{v} + \int(\underline{v}\cdot\underline{\nabla} A) f\, d\underline{v}$$

$$- \nu\int A(f - f_{eq})\, d\underline{v}$$

so

$$\partial_t \rho\langle A\rangle = -\underline{\nabla}\cdot(\rho\langle\underline{v}A\rangle) + \rho\langle\underline{v}\cdot\underline{\nabla}A\rangle$$

$$- \nu\rho\,(\langle A\rangle - \langle A\rangle_{eq})$$

computed with f_{eq}

check:

- $A = 1$

$$\partial_t \rho = -\underline{\nabla}\cdot(\rho\underline{v}) \quad \text{continuity} \ \checkmark$$

$-A = \underline{v}$

$$\partial_t(\rho \underline{V}) = -\underline{\nabla}\cdot(\rho \langle \underline{v}\,\underline{v}\rangle)$$

then,

(i.e. $\langle \underline{V}\rangle = \langle \underline{v}\rangle_{eq}$)

$$\underline{v} = \underset{\text{macro}}{\underline{V}} + \underset{\text{thermal fluctuation}}{\underline{\tilde{v}}}$$

noting $\langle \tilde{v}\rangle \to 0$,

$$\partial_t(\rho \underline{V}) = -\underline{\nabla}\cdot(\rho \underline{V}\,\underline{V}) - \underset{\text{Reynolds stress}}{\underline{\nabla}\cdot \underline{\underline{T}}}$$

$$\underset{\text{(Micro) stress tensor}}{\underline{\underline{T}}_{ij} = \int \tilde{v}_i \tilde{v}_j f \, d\underline{v}}$$

Caveat: Nomenclature

so for Maxwellian iso.

$$\underline{\underline{T}}_{ij} = \underset{\text{pressure}}{p}\,\delta_{ij} + T_{ij}^{visc}$$

$\longrightarrow$ $\boxed{\text{viscous stress}}$

⇒ $\boxed{\text{How calculate the viscous stress? } \sigma_{ij}^{visc}}$

$(\nabla \cdot \underline{V} = 0)$

Observe: Can calculate moments equations for second, third:

i.e.

$$\partial_t \rho \langle \underline{v}\,\underline{v} \rangle = -\nabla \cdot \left[\rho \langle \underline{v}\,\underline{v}\,\underline{v} \rangle \right] - \nu \rho \left\{ \langle \underline{v}\,\underline{v} \rangle - \langle \underline{v}\,\underline{v} \rangle_{eq} \right\}$$

$$\partial_t \rho \langle \underline{v}\,\underline{v}\,\underline{v} \rangle = -\nabla \cdot \left[\rho \langle \underline{v}\,\underline{v}\,\underline{v}\,\underline{v} \rangle \right] - \nu \rho \left\{ \langle \underline{v}\,\underline{v}\,\underline{v} \rangle - \langle \underline{v}\,\underline{v}\,\underline{v} \rangle_{eq} \right\}$$

i.e. coupled hierarchy ✓ → $\underbrace{\text{truncation}}$

also observe for steady state:

$$\partial_t \rho \langle \underline{v}\,\underline{v} \rangle \rightarrow 0$$

$$\langle \underline{v}\,\underline{v} \rangle = \underbrace{\langle \underline{v}\,\underline{v} \rangle_{eq}}_{\text{calculated!}} - \frac{1}{\nu \rho} \nabla \cdot \left[\rho \langle \underline{v}\,\underline{v}\,\underline{v} \rangle \right]$$

$\otimes$

$$\langle \underline{v}\,\underline{v} \rangle \equiv \langle \underline{v}\,\underline{v} \rangle_{eq}$$

calculated

$$-\frac{1}{v}\,\frac{\nabla}{\rho}\cdot\left[\rho\langle \underline{v}\,\underline{v}\,\underline{v}\rangle\right]$$

contains viscous stress

$$\rho\langle v_i v_j\rangle = \underbrace{\rho \bar{V}_i \bar{V}_j + P\delta_{ij}}_{\langle \underline{v}\,\underline{v}\rangle_{eq}} + \tau_{vis\;ij}$$

so Remains to calculate triple moment:

$$\underline{v} = \underline{\bar{V}} + \underline{\tilde{v}}$$

Macro fluctuation

and take $\rho = \rho_0$ for simplicity, a $\rho_0 \to 1$, momentarily

$$\langle \underline{v}\,\underline{v}\,\underline{v}\rangle_{ijk} = \langle (V+\tilde{v})_i (V_j + \tilde{v}_j)(V_k + \tilde{v}_k)\rangle$$

$$= \text{[redacted]}\ \underset{(1)}{V_i V_j V_k} + \underset{(2)}{V_i V_j \cancel{\langle \tilde{v}_k\rangle}} + \underset{(3)}{V_i \cancel{\langle \tilde{v}_j\rangle} V_k}$$

$$+ \underset{(5)}{V_i \langle \tilde{v}_j \tilde{v}_k\rangle} + \underset{(6)}{V_j \langle \tilde{v}_i \tilde{v}_k\rangle} + \underset{(7)}{V_k \langle \tilde{v}_i \tilde{v}_j\rangle}$$

$$+ \underset{(4)}{\cancel{\langle \tilde{v}_i\rangle} V_j V_k} + \underset{(8)}{\langle \tilde{v}_i \tilde{v}_j \tilde{v}_k\rangle}$$

(1) → Macroscopic, not viscous
also taking $\nabla\cdot V = 0$

(2), (3), (4) → 0 (odd) (8) → 0 (odd)

(5), (6), (7) → contribute.

b

$$J_{ijk\,visc} = -\frac{1}{\text{[redacted]}\ r}\,\nabla\cdot\Big[a\, V_i \langle \tilde{v}_j \tilde{v}_k\rangle + V_j \langle \tilde{v}_i \tilde{v}_k\rangle + V_k \langle \tilde{v}_i \tilde{v}_j\rangle \Big]$$

Now

$\langle \tilde{v}_i \tilde{v}_j \rangle =$ [redacted] $\frac{T}{m}\,\delta_{ij}$

so finally;

$$\boxed{\sigma_{ij\,visc} = -\frac{1}{\nu}\,\nabla\cdot\left[\rho V_i \frac{T}{m}\,\delta_{jk} + \frac{\rho T}{m} V_j\,\delta_{ik} + \frac{\rho T}{m} V_k\,\delta_{ij}\right]}$$

N.B. — $\nabla\cdot$ contracts an index

so, for n, T homogeneous, $(\nabla\cdot\underline{V} = 0)$

$$\boxed{\sigma_{ij\,visc} = -\frac{nT}{\nu}\left[\frac{\partial V_i}{\partial x_j} + \frac{\partial V_j}{\partial x_i} - \frac{2}{3}\,\delta_{ij}\,\nabla\cdot\underline{V}\right]}$$

(for $\nabla\cdot\underline{V} \neq 0$)

for $\nabla\cdot\underline{V} = 0$,

$$\sigma_{ij\,visc} = -\frac{nT}{\nu}\left[\frac{\partial V_i}{\partial x_j} + \frac{\partial V_j}{\partial x_i}\right]$$

shear viscosity

$$\boxed{\eta = \frac{nT}{\nu}}$$

now $\nu = l_{mfp}^{-1} v_{th}$

$= n\sigma v_{th}$

$$\eta = \frac{\cancel{n} T}{\cancel{n} \sigma v_{th}}$$

η indep n.

(B) What does it all mean?

$\leftrightarrow$ Connection to entropy production

Recall: $\Pi_{z,x} = -\eta \frac{\partial V_x(z)}{\partial z}$

Example of Fickian Flux - Gradient Relation.

above part of below (i.e. consider multiple gradients)

In general:

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

$\rightarrow$ thermo. forces.

Vector of Fluxes

Onsager Matrix

vector of gradients $(n, T, V_i \ldots)$

$\rightsquigarrow$ $\boxed{\text{Onsager Matrix : matrix of transport coefficients}}$

N.B. Will show $\underline{\underline{K}}_{ij} = \underline{\underline{K}}_{j,i}$ for

micro-reversible dynamics

$\Rightarrow$ "Onsager Symmetry".

Observe:

- intuitively, know collisions etc. will relax gradient

$$\text{hot} \xRightarrow{Q} \text{cold}$$

- f_{max} annihilates C $\rightarrow C(f_{max}) = 0$

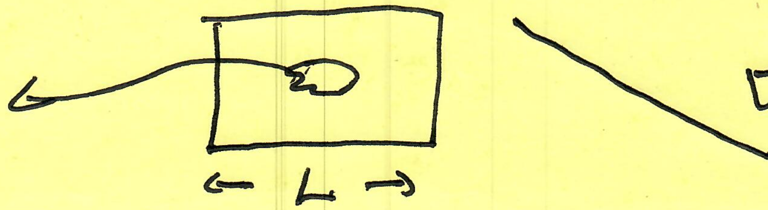
$\rightarrow$ <u>locally</u>, resulting in

<u>local</u> maximum in entropy

and vanishing local entropy

production $\frac{dS}{dt} = 0$

blob: ~ lmfp



∇T

— $\underline{\underline{\text{but}}}$ $f_{max}(n(\underline{x}), T(\underline{x}), \underline{V}(\underline{x}))$

does $\underset{\sim}{\text{not}}$ satisfy Boltzmann

equation $\Rightarrow \delta f$ required.

$$f = f_{Max} + \delta f \qquad \left\{ \begin{array}{l} \underline{\text{i.e.}} \\ \dfrac{df}{dt} = C(f) \\ C(f_{max}) = 0 \ \text{ but} \\ \dfrac{d}{dt} f_{max} \neq 0 \end{array} \right.$$

so realize,

$\Rightarrow$ $\boxed{\text{if gradients in thermodynamic quantities} \Rightarrow \text{system is not in } \underline{\text{global}} \text{ maximum entropy state, } \underline{\text{i.e.}}\ \delta f \neq 0}$

$\Rightarrow$ to have $\dfrac{dS}{dt} = 0$ everywhere,

system must/will relax gradients.

$\Rightarrow$ $\boxed{\text{Relaxation to maximum entropy state will occur by (collisional + hydro) } \underline{\text{transport}}}$

→ To describe relaxation <u>macroscopically</u>, calculate

flux-induced entropy production

⇒ <u>heating</u> due relaxation of

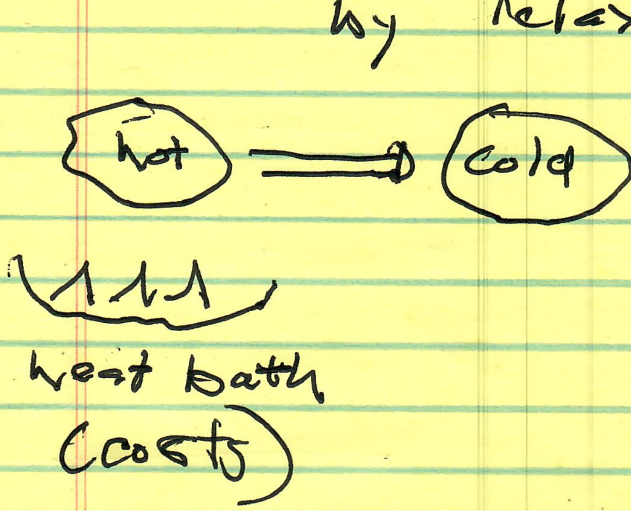
gradients (in spirit of linear response)

i.e. $\Pi_{\alpha,\beta} = -\underset{(\rho D)}{\eta} \frac{\partial V_\beta}{\partial x_\alpha}$

viscous momentum transport

⇒ (frictional heating)

⇒ Energy for heating extracted from gradients in termodynamic quantities by relaxation



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

$$\partial_t \mathcal{E}_{Hydro} = \partial_t \int \rho \frac{\underline{V}^2}{2}$$

[rate change of bulk hydro motion]

$$= \int d^3x \; \underline{V}\cdot\left(-\underline{\nabla}\cdot\underline{\underline{\Pi}}\right)_{\text{visc}}$$

[no contrib. up to S.t. for ideal]

$$= \text{S.T.} + \int d^3x \left[\underline{\underline{\Pi}}_{\text{visc}}\cdot\underline{\nabla}\,\underline{V}\right]$$

here

$$\rightarrow \int d^3x \left(-\left(\eta\frac{\partial V_x}{\partial z}\right)\left(\frac{\partial V_x}{\partial z}\right)\right)$$

$$= \int d^3x \left[-\eta\left(\frac{\partial V_x}{\partial z}\right)^2\right]$$

$\underline{\nabla}\cdot\underline{V}=0$

$$\rightarrow \int d^3x \left[-\eta\left(\frac{\partial V_i}{\partial x_j}\right)^2\right] \quad \text{generally}$$

so $\quad dE = T\,dS$

and $\quad \dfrac{d}{dt}\left(\mathcal{E}_K + \mathcal{E}_{Th}\right) = 0$

$\Rightarrow$

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

entropy production due transport - induced relaxation.

Then observe:

$\Rightarrow$ Multiple time scales for Entropy

1) $\rightarrow$ time to form local Maxwellian
$\sim \tau_{coll} \sim \nu^{-1}$

2) time to form global maximum entropy state

$1/\tau_{relax} \sim D/L^3$

(diffusion time scale)

but $\frac{1}{\tau_{relax}} \sim \frac{v_{th}\, l_{mfp}}{L^2}$

$$\sim \frac{v_{th}}{l_{mfp}} \left(\frac{l_{mfp}}{L}\right)^2 \sim \nu \left(\frac{l_{mfp}}{L}\right)^2$$

$$\boxed{\begin{aligned} \tau_{relax} &= (L\nu/l_{mfp})^2 \tau_{coll} \\ &= (L\nu/l_{mfp})^2 \tau_{coll} \end{aligned}}$$

→ long time scale relative to τ_c

so $\frac{\tau_{relax}}{\tau_c} \sim (L/l_{mfp})^2$

More generally: can write,

$$J_i = -\sum_{j=1}^{n} \alpha_{ij}\, X_j$$

J_i: ith flux

α_{ij}: kinetic (transport) coefficient

X_j: jth driving force (gradient)

So define;

$\Psi \equiv$ dissipation function

$$\downarrow \Psi$$

$$\frac{dS}{dt} = \left.\sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_{i,j} X_i X_j \right] \Rightarrow \text{entropy production}$$

$$\frac{dS}{dt} = \Psi$$

$$= -\sum_i X_i J_i$$

so for 2×2:

$$\frac{dS}{dt} = \sum_{i=1}^{2} \sum_{j=1}^{2} \alpha_{ij} X_i X_j$$

$$= \alpha_{1,1} X_1^2 + (\alpha_{1,2} + \alpha_{2,1}) X_1 X_2 + \alpha_{2,2} X_2^2$$

$$\frac{dS}{dt} \geq 0 \quad \Rightarrow \quad \left.\begin{matrix} \alpha_{1,1} \geq 0 \\ \alpha_{2,2} \geq 0 \end{matrix}\right\} \text{diffusion down gradient}$$

and

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

descr

N.B. – off diagonals $\neq 0$
$\alpha_{1,2}$, $\alpha_{2,1}$

– can go < 0 , in some systems

$\Rightarrow$ i.e. – ∇T drive up-gradient particle flux

– chemotaxis: ∇C drives up-gradient particle flux

$$\Gamma = -D\nabla n + Vn$$

$$V = \alpha(\nabla C)$$

$$\Gamma = -D\nabla n + \alpha n \nabla C$$

$\Rightarrow \Gamma = 0$ for $\dfrac{\nabla n}{n} = -\alpha\dfrac{\nabla C}{D}$

sustains steady ∇n with a ∇C

PBLM: Calculate $\Gamma_{\hat{n}}$ driven by ∇T, for $\hat{\nabla} n = 0$.