Physics 210B

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

(A)

Recall: Boltzmann Equation + H Theorem

$\downarrow$

Hydrodynamics (general)

$\downarrow$

Closure $\rightarrow$ Chapman-Enskog

$\downarrow$

Transport Coeffs.

$\Downarrow$

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

$\hookrightarrow$ $\boxed{\text{N-S Eqn.}}$

Key calculation: $\left\{\begin{array}{l}\text{C-E} \\ \text{Expansion}\end{array}\right.$

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

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

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

$\eta = \# \rho D$

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

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

Alternative Approach to Transport Coefficients: Moment Closure

Relaxation Approx to B.E.

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

$f_{eq} \downarrow$ 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

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

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

computed with f_{eq}

check:

$- A = 1$

$\partial_t \rho = -\underline{\nabla}\cdot(\rho\underline{V})$ continuity ✓

$-A = \underline{v}$

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

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

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

$\underline{V}$ ↓ Macro; $\underline{\tilde{v}}$ ↓ thermal fluctuation

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

$$\partial_t(\rho \underline{V}) = -\underline{\nabla}\cdot(\rho \underline{V}\,\underline{V}) - \underline{\nabla}\cdot\underline{\underline{\Gamma}}$$

↓ Reynolds stress

$$\underline{\underline{\Gamma}}_{ij} = \int \tilde{v}_i \tilde{v}_j\, f\, d\underline{v}$$

↓ (Micro) stress tensor

Caveat: Nomenclature

so for Maxwellian, iso.

$$\underline{\underline{\Gamma}}_{ij} = P\,\delta_{ij} + \Gamma_{ij}^{visc}$$

P ↓ pressure

$\Gamma_{ij}^{visc} \to \boxed{\text{viscous stress}}$

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

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

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:

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

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

④

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

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, 9 $\quad \theta_0 \to 1$, momentarily

$$\langle \underline{v}\,\underline{v}\,\underline{v}\rangle_{ijk} = \langle \underset{(1)}{(\bar V + \tilde v)_i}\, \underset{(2)}{(\bar V_j + \tilde v_j)}\, \underset{(3)}{(\bar V_k + \tilde v_k)}\rangle$$

$$= \text{[redacted]}\, \bar V_i \underset{(5)}{\bar V_j} \bar V_k + \bar V_i \bar V_j \underset{(6)}{\cancel{\langle \tilde v_k\rangle}} + \bar V_i \underset{(7)}{\cancel{\langle \tilde v_j\rangle}} \bar V_k$$

$$+ \bar V_i \underset{(4)}{\langle \tilde v_j \tilde v_k\rangle} + \bar V_j \underset{(8)}{\langle \tilde v_i \tilde v_k\rangle} + \bar V_k \langle \tilde v_i \tilde v_j\rangle$$

$$+ \cancel{\langle \tilde v_i\rangle} \bar V_j \bar V_k + \langle \tilde v_i \tilde v_j \tilde v_k\rangle$$

(1) → Macroscopic, not viscous
also takes $\nabla\cdot\underline{V} = 0$

(2), (3), (4) → 0 (odd) $\quad$ (8) → 0 (odd)

(5), (6), (7) → contribute.

10

$$T_{ijk\,visc} = -\frac{1}{\text{[redacted]}\, r}\,\nabla\cdot\Big[\, a\, \bar V_i \langle \tilde v_j \tilde v_k\rangle$$

$$+ \bar V_j \langle \tilde v_i \tilde v_k\rangle + \bar V_k \langle \tilde v_i \tilde v_j\rangle \Big]$$

Now

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

so finally;

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

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

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

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

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

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

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

shear viscosity

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

now $\nu = l_{mfp} v_{th}$

$= n\sigma v_{th}$

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

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 $(n, T, V_i \ldots)$

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

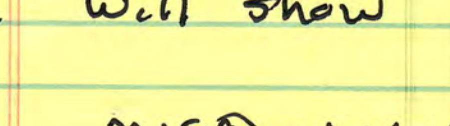
N.B. Will show $\underline{\underline{K}}_{ij} = \underline{\underline{K}}_{j,i}$ for

micro-reversible dynamics

$\Rightarrow$ "Onsager Symmetry".

Observe:

- intuitively, know collisions etc. will relax gradient



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

$\rightarrow$ locally, resulting in

local maximum in entropy

and vanishing local entropy production $\frac{dS}{dt} = 0$

blob:
~ lmfp

DT

— <u>but</u> $f_{max}(n(\underline{x}), T(\underline{x}), \underline{V}(\underline{x}))$ does <u>not</u> satisfy Boltzmann equation $\Rightarrow \delta f$ required.

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

i.e.
$$\left\{\begin{array}{l} \frac{df}{dt} = C(f) \\ C(f_{max}) = 0 \quad \text{but} \\ \frac{d}{dt} f_{max} \neq 0 \end{array}\right.$$

so realize,

$\Rightarrow$ if gradients in thermodynamic quantities $\Rightarrow$ system is not in <u>global</u> maximum entropy state <u>i.e.</u> $\delta f \neq 0$

$\Rightarrow$ to have $\frac{dS}{dt} = 0$ everywhere, system must/will relax gradients.

$\Rightarrow$ Relaxation to maximum entropy state will occur by (collisional, hydro) transport

→ To describe relaxation macroscopically, calculate

flux-induced entropy production

⇒ heating due relaxation of gradients

(in spirit of linear response)

i.e. $\Pi_{\alpha,\beta} = -\underset{(2D)}{\eta} \frac{\partial V_\beta}{\partial x_\alpha}$

viscous momentum transport
⇒ (frictional heating)

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

$\text{hot} \Longrightarrow \text{cold}$

heat bath
(costs)

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

$$\partial_t \mathcal{E}_{Hydro} = \partial_t \int \rho \frac{\underline{V}^2}{2}$$ [rate change of bulk hydro motion

$$= \int d^3x \; \underline{V} \cdot \left(-\underline{\nabla} \cdot \underline{\underline{\Pi}}\right)_{visc}$$ [no contrib. up to S.t. for ideal

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

here

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

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

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

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

So $dE = T\,dS$

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

$\Rightarrow$

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

[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

$1/\tau_{relax} \sim D/L^2$

(diffusion time scale)

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

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

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

$\rightarrow$ long time scale relative to τ_0

so $$\frac{\tau_{relax}}{\tau_0} \sim (L/l_{mfp})^2$$

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

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

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

$$= -\sum_i X_i J_i$$

so for 2×2:

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

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

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

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 $\dfrac{\nabla n}{n} = -\dfrac{\alpha \nabla C}{D}$

sustains steady ∇n with a ∇C

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