

§4. Collisional Transport: Qualitative Treatment.

So far we have dealt with homogeneous systems w/o mean flows or density/temp./velocity gradients. (Recall that particles can have nontrivial distribution in space.)

It turns out that, in a coll. system, there will be a tendency to diffuse away all spatial inhomogeneities.

Let me first demonstrate this very roughly, on a qualitative level.

4.1 Diffusion

Let us consider particles carrying some property that distinguishes them from others — colour them (or label — they can be radioactive isotopes e.g.)

Their concentration is n^* . Suppose we set the initial conditions up so that there is a ~~non~~ ∇n^* in some direction \vec{x} .

Say, at time t , we have $n^*(t, \vec{x})$.

Consider now $n^*(t + \Delta t, \vec{x})$ where Δt is a short time during which all particles have moved in straight lines, w/o having an opportunity to be deflected by collisions. Each particle found at position \vec{x} at time $t + \Delta t$ has moved some distance $\Delta \vec{x}$, from position $\vec{x} - \Delta \vec{x}$.

Then $n^*(t+\Delta t, \bar{x}) = \langle n^*(t, \bar{x} - \Delta \bar{x}) \rangle$

↑
avg. because $\Delta \bar{x}$ is random (diff. for different particles)

If $\Delta \bar{x}$ is very small (we'll figure out in a moment what this means), then we can expand:

$$\begin{aligned} n^*(t+\Delta t, \bar{x}) &= \langle n^*(t, \bar{x}) - \Delta \bar{x} \frac{\partial n^*}{\partial \bar{x}} + \frac{\Delta \bar{x}^2}{2} \frac{\partial^2 n^*}{\partial \bar{x}^2} + \dots \rangle \\ &= n^*(t, \bar{x}) - \underbrace{\langle \Delta \bar{x} \rangle}_{\substack{\parallel \\ \circ \text{ assume no mean} \\ \text{motion}}} \frac{\partial n^*}{\partial \bar{x}} + \frac{\langle \Delta \bar{x}^2 \rangle}{2} \frac{\partial^2 n^*}{\partial \bar{x}^2} + \dots \end{aligned}$$

↑ neglect

$$\frac{n^*(t+\Delta t, \bar{x}) - n^*(t, \bar{x})}{\Delta t} = \frac{\langle \Delta \bar{x}^2 \rangle}{2\Delta t} \frac{\partial^2 n^*}{\partial \bar{x}^2}$$

or $\boxed{\frac{\partial n^*}{\partial t} = D \frac{\partial^2 n^*}{\partial \bar{x}^2}}$ diffusion equation

$D = \frac{\langle \Delta \bar{x}^2 \rangle}{2\Delta t}$ (self-) diffusion coefficient.

We can estimate it very roughly by:

$\langle \Delta \bar{x}^2 \rangle \sim \lambda_{mfp}^2$ (particles travelled from their last collision)

$\Delta t \sim \tau_c$

So $\boxed{D \sim \frac{\lambda_{mfp}^2}{\tau_c} \sim v_{th}^2 \tau_c \sim v_{th} \lambda_{mfp}}$

NB: validity:
 $\Delta z \ll L \sim \frac{1}{\frac{1}{n^*} \frac{\partial n^*}{\partial z}}$
 so $\frac{\partial n^*}{\partial z} \ll \frac{1}{\lambda_{mfp}}$

Solutions of the diffusion equation will be discussed in the Maths Methods course.

The basic tendency will be to wipe out inhomogeneities.

E.g. consider an initial sinusoidal distribution:

$$n^*(0, x) = N_0 \sin kx$$

Then the solution is $n^*(t, x) = N(t) \sin kx$

$$\frac{\partial N(t)}{\partial t} = -Dk^2 N(t) \Rightarrow N(t) = N_0 e^{-Dk^2 t} \quad \text{"1/Tdiff"} \quad \text{exp. decay}$$

NB: $T_{diff} = \frac{1}{Dk^2} \sim \frac{L^2}{D} \propto L^2$ (scale of inhomogeneity) (faster for steeper gradients)

~~... ..~~

We can generalise this consideration in several ways

1) Direction x was defined as the direction of the gradient, ∇n^* . So, in 3D (or 2D),

$$\frac{\partial n^*}{\partial t} = D \nabla^2 n^* \quad \text{"Fick's law"}$$

~~... ..~~

2) Just like particles can carry a label, we can loosely think of them as carrying energy and momentum.

Say, on avg, each particle carries $\frac{m\langle v^2 \rangle}{2}$ energy.

Then the energy density is

$$n \frac{m\langle v^2 \rangle}{2} = \frac{3}{2} n k_B T$$

It is a very fundamental property of diffusion that $L \propto t^{1/2}$ - compare to straight unimpeded motion: $L \propto t$ (ballistic)

Let's assume $\eta = \text{const}$ and $T = T(\vec{r})$.

Then replace $n^* \rightarrow \frac{3}{2} n k_B T$ and conclude
 ↑ density of labels ↑ density of energy

that temperature gradients are also wiped out in a diffusive way:

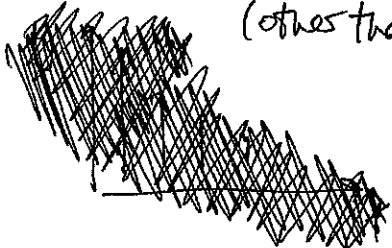
$$\frac{\partial T}{\partial t} = D \nabla^2 T$$

[the Fourier equation]

thermal diffusion equ.
(or heat diffusion)

↑
thermal diffusivity

Similarly, suppose there is a mean flow in some direction ~~other than z~~: say, $u_x = u_x(\vec{r})$
(other than z)



On avg, particles carry momentum $m u_x$ and so momentum density is

$$n m u_x \leftarrow n^* \quad (\text{assup } n = \text{const})$$

We expect then

$$\frac{\partial u_x}{\partial t} = \nu \frac{\partial^2 u_x}{\partial \vec{r}^2}$$

↑
kinematic viscosity ν

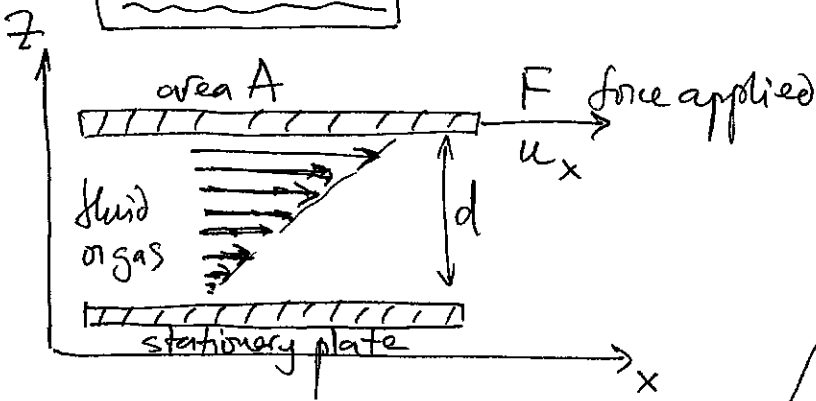
Ex. Work out what will happen if there is a (const) mean flow in \vec{z} direction:
 $\langle \Delta \vec{r} \rangle = u_z \Delta t$

NB: In truth coeff. of self-diffusion, thermal diffusivity and kinematic viscosity are not exactly equal.

They are all $\sim \frac{1}{2} m \lambda_{\text{mfp}}$, but the numerical prefactors are different - this is because there are in fact correlations between, e.g., how much energy a particle carries, and how fast it travels - and, therefore, ~~how far it can carry this energy before colliding~~ how far it can carry this energy before colliding and communicating it to another particle. [but because $f(\vec{v})$ is Maxwellian, this only changes things by factors ~ 1]

I will now give an alternative derivation of viscosity (etc.), which will both shed some further light on what happens physically and clarify where we are failing to do a precise quantitative job.

4.2 Fluxes



We know empirically that for d small enough,

$$\frac{F}{A} = \eta \frac{u_x}{d} = \eta \frac{\partial u_x}{\partial z}$$

shear stress

some coeff. which can be measured exply.
dynamical viscosity

If we do not know the microphysical nature of our substance, all we can do is

parametrise the dependence of F on $\partial u_x / \partial z$.

But we do know something, so let's see if we can calculate η [this physics often prepares]

What happens microphysically?

Upper plate moves, molecules collide with it and get some mean momentum from it

Then they collide with ones further out and communicate this momentum and so on.

Thus, there is a flux of momentum:

[Bored here.]

$$\Pi_z = \frac{\text{momentum}}{\text{unit time} \cdot \text{unit area}} = -\frac{F}{A} = -\eta \frac{\partial u_x}{\partial z}$$

force

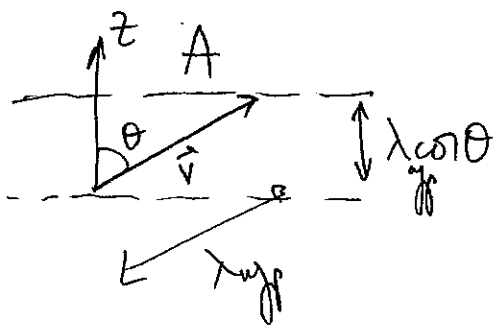
because momentum flows from high to low u_x (Q)

Now let's calculate the same quantity from particle motion.

Recall from p. 19, # of particles with velocity \vec{v} that hit ~~area~~ a unit area per unit time:

$$dN(\vec{v}) = v_z n f(\vec{v}) d^3\vec{v} = n v^3 \overset{\text{Max.}}{f(v)} \cos\theta \sin\theta dv d\theta dp$$

$\theta \in [0, \pi/2]$



But these molecules have travelled distance $\approx \lambda_{mfp}$ since last collision, so they came from $\Delta z = \lambda_{mfp} \cos\theta$ away

They bring in some extra momentum (ve if they come from smaller z):

$$\Delta p = -m \frac{\partial u_x}{\partial z} \Delta z = -m \frac{\partial u_x}{\partial z} \lambda_{mfp} \cos\theta$$

2 minus signs in them

+ the same from ones that came from opp. side $\theta \in [\pi/2, \pi]$

Note: Boyle's experiment: pump gas from a vessel - η const
Breaks down when $\lambda_{mfp} \sim L$ (Q)

Then flux of momentums is

$$\begin{aligned} \Pi_z &= 2 \int \Delta p \, dN(\vec{v}) = \\ &= -2nm \frac{\partial u_x}{\partial z} \lambda_{mfp} \int_0^\infty dv v^3 f(v) \int_0^{\pi/2} d\theta \cos^2 \theta \sin \theta \int_0^{2\pi} d\phi \\ &= -\frac{1}{3} \lambda_{mfp} \frac{\partial u_x}{\partial z} 4\pi n \int_0^\infty dv v^3 f(v) \end{aligned}$$

~~scribble~~ $= -\frac{1}{3} nm \lambda_{mfp} \langle v \rangle \frac{\partial u_x}{\partial z}$

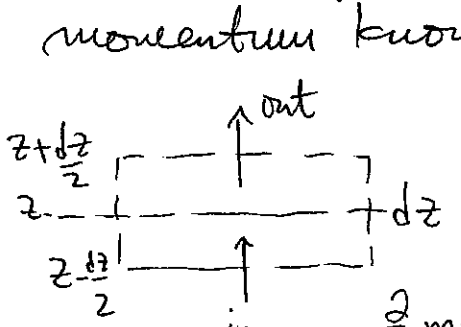
So we have for

$$\boxed{\eta = \frac{1}{3} nm \lambda_{mfp} \langle v \rangle}$$

$$\sim nm \frac{1}{n\sigma} \sqrt{\frac{T}{m}}$$

So, no dependence on density (= on pressure @ const T)

Note that if we want to calculate the change in momentum knowing the flux, we get:



$$\frac{\partial}{\partial t} mn u_x(t, z) = \left[\Pi_z(z - \frac{dz}{2}) - \Pi_z(z + \frac{dz}{2}) \right] A$$

So $\frac{\partial}{\partial t} mn u_x = -\frac{\partial}{\partial z} \Pi_z(z) = \frac{\partial}{\partial z} \eta \frac{\partial u_x}{\partial z}$

Assump $\eta = \text{const}$, $\frac{\partial u_x}{\partial t} = \left(\frac{\eta}{mn} \right) \frac{\partial^2 u_x}{\partial z^2}$

~~scribble~~
~~scribble~~
~~scribble~~
 $\frac{\eta}{mn} = \frac{1}{3} \lambda_{mfp} \langle v \rangle$ kinematic viscosity $\sim D$ as before.

We can do exactly the same for the flux of energy (\equiv particle heat).

(Ex)

Set up a temperature gradient $\frac{\partial T}{\partial z}$.

Again, empirically, heat flux $J_z = -\kappa \frac{\partial T}{\partial z}$

Microscopically where, by def.,

thermal conductivity

$$J_z = \frac{\text{energy}}{\text{time} \cdot \text{area}}$$

Particles bring extra energy:

(2)
$$\Delta E = -\frac{\partial}{\partial z} \left(\frac{3}{2} k_B T \right) \cdot \Delta z = -\frac{3}{2} k_B \frac{\partial T}{\partial z} \lambda_{mfp} \cos \theta$$

+ same from above.

$$J_z = 2 \int \Delta E dN(\vec{v}) = -\frac{1}{3} n \lambda_{mfp} \langle v \rangle \cdot \frac{3}{2} k_B \frac{\partial T}{\partial z}$$

$$= -\frac{1}{3} C_V \lambda_{mfp} \langle v \rangle \frac{\partial T}{\partial z}$$

$$) C_V = \frac{3}{2} n k_B$$

heat capacity per unit volume

(will encounter it later)

$$\boxed{\kappa = \frac{1}{3} C_V \lambda_{mfp} \langle v \rangle}$$

and again
$$\frac{\partial}{\partial t} \left(\frac{3}{2} n k_B T \right) = -\frac{\partial J_z}{\partial z} = \frac{\partial}{\partial z} \kappa \frac{\partial T}{\partial z}$$

$$\frac{\partial T}{\partial t} = \left(\frac{\kappa}{C_V} \right) \frac{\partial^2 T}{\partial z^2}$$

These derivations are basically equivalent to what I did before. They look more quantitative, but in fact are not

" $\frac{1}{3} \lambda_{mfp} \langle v \rangle \sim D$ heat diffusivity (thermal)"

They look more quantitative, but in fact are not

What is wrong with them?

1) I treated velocities as having a distribution for the purposes of ~~angular~~ angle integrals and fluxes of particles ($v_z n f(\vec{v}) d^3\vec{v}$) - but assumed that all particles travelled exactly the same distance λ_{mfp} ~~and carried exactly the same momentum or energy (but by mean momentum and energy)~~ - but surely ~~there~~ ~~depend~~ depend on each particle's specific velocity as well?

2) I used homogeneous Maxwellian distributions derived on the assumption that there are no special dependencies and no mean flows - but now there are!

~~...~~
This might be OK if mean flows are small ($\ll v_{th}$) and gradients not very steep ($\ll \frac{1}{\lambda_{\text{mfp}}}$) - but I have not set this approximation up carefully.

I am going to do a better job of it in the next section. But now let me first comment on some ^{further} uses of diffusion equations.

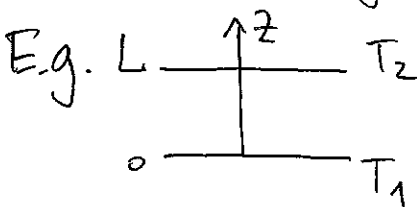
4.3. Steady States.

It is a typical situation that some gradient in the system (shear flow, temp. ~~and~~ difference) is maintained forcibly, e.g. by moving boundaries or heating/cooling them - mathematically, via imposing boundary conditions. Then we expect a steady state:

$$\frac{\partial T}{\partial t} = D \frac{\partial^2 T}{\partial z^2} = 0 \quad \frac{\partial^2 T}{\partial z^2} = 0$$

(more generally, $\nabla^2 T = 0$ Laplace equation)

We can solve if we know the boundary conditions.



$$T = A + Bz = T_1 + (T_2 - T_1) \frac{z}{L}$$

$$T(0) = A = T_1$$

$$T(L) = A + BL = T_2 \Rightarrow B = \frac{T_2 - T_1}{L}$$

Things can be a bit more complicated (but still 1D) if we work in spherical or axisymmetry.

Ex.



What is $T(r) = ?$

NB: Work out ∇^2 in cylindrical symmetry.

Sometimes you may know not the temp. on boundary but heat flux through it - e.g. if you ^{are} generating energy inside at a known rate.

Then it is hardy to write the equation so:

$$\frac{3}{2} k_B n \frac{\partial T}{\partial t} = - \frac{\partial J_z}{\partial z} = 0$$

$$J_z = - \kappa \frac{\partial T}{\partial z} = \text{const} = J_0 \text{ flux through boundary}$$

$$T = - \frac{J_0}{\kappa} z + \text{const}$$

↑ calculate this if you know $T(0)$ or $T(L)$

Ex. Do the same for a cylinder or a sphere.

↳ ended here

Note. Vector flux: obviously, $\vec{J} = - \kappa \nabla T$

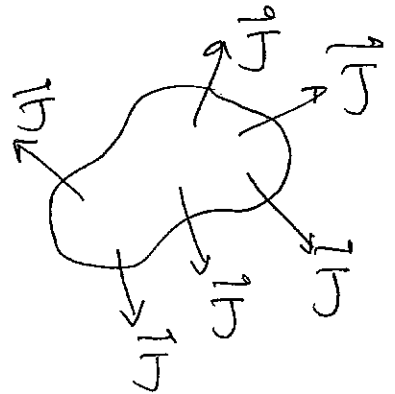
if we postulate this, this applies more generally to gas.

A more general derivation of the thermal diffusion equation is

$$\frac{\partial}{\partial t} \int_V d^3x \frac{3}{2} k_B n T = - \int_{\partial V} dS \cdot \vec{J}$$

↑ some volume
↑ boundary

change of energy inside
flux out



$$= - \int_V d^3x \nabla \cdot \vec{J} \quad \text{Gauss theorem}$$

Since this is true for any volume,

$$\frac{3}{2} n k_B \frac{\partial T}{\partial t} = - \nabla \cdot \vec{J} = \kappa \nabla^2 T$$

+ generation terms if applicable (e.g. $\text{m}^2 \text{J}^{-2}$ Joule heat)

Note. You will learn to solve time-dependent problems involving heat diffusion eqn in the Math. Methods course.