

## Homework No.2, 553.793, Due February 11, 2022.

1. This problem studies the local conservation laws of classical molecular fluids.

(a) Derive the local conservation of momentum

$$\partial_t \hat{\mathbf{g}}(\mathbf{x}, t) + \nabla \cdot \hat{\mathbf{T}}(\mathbf{x}, t) = \mathbf{0},$$

where  $\mathbf{T}$  is the stress-tensor given in class and  $(\nabla \cdot \mathbf{T})_i = \partial_j T_{ij}$ . *Hint:* Use Newton's third law, and also use the fundamental theorem of calculus to write

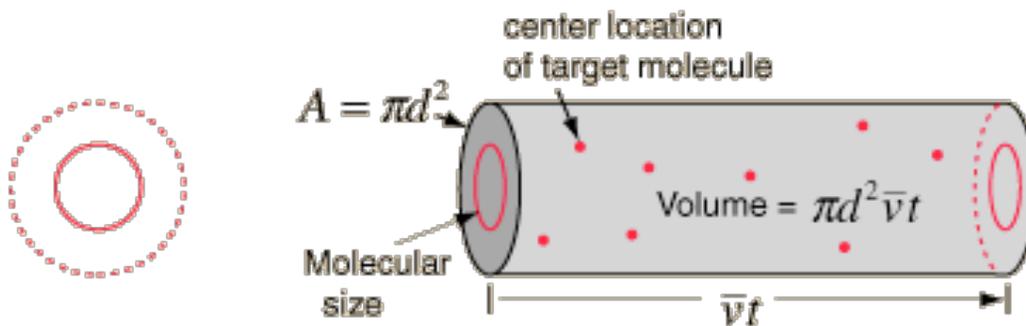
$$(\mathbf{r}_{nm} \cdot \nabla) \int_0^1 ds \delta^3(\mathbf{x} - \mathbf{r}_n + s\mathbf{r}_{nm}) = \delta^3(\mathbf{x} - \mathbf{r}_m) - \delta^3(\mathbf{x} - \mathbf{r}_n).$$

(b) Use a similar argument to derive the local conservation of energy

$$\partial_t \hat{e}(\mathbf{x}, t) + \nabla \cdot \hat{\mathbf{s}}(\mathbf{x}, t) = 0$$

where  $\hat{\mathbf{s}}$  is the energy current given in class.

2. The concept of the *mean free path length* is a very important one in the molecular theory of fluids, which we explore in this problem.



(a) The above figure illustrates the notion of the “collision cylinder” swept out in time  $t$  by a spherical particle of diameter  $d$  moving at speed  $\bar{v}$  in a gas of similar particles at rest. The points in the figure represent the centers of the other particles in the gas. The mean-free-time  $\tau_{mfp}$  is defined to be the time for one collision to occur, i.e. for one particle to reside in the collision cylinder. Show that

$$\tau_{mfp} = \frac{1}{n\pi d^2 \bar{v}}$$

where  $n$  is the density of particles per unit volume. The corresponding distance traveled is  $\lambda_{mfp} = \bar{v}\tau_{mfp} = 1/n\pi d^2$ .

(b) In reality, all of the particles in the fluid are moving with a random velocity chosen from an ensemble with a probability density  $p(\mathbf{v})$ . This will ordinarily be Maxwellian, but we

assume here only that the mean velocity is zero and that distinct particles have statistically independent and identically distributed velocities. Show that the *relative* velocity  $\mathbf{v} - \mathbf{v}'$  of any pair of particles has the root-mean-square value  $v_{rel} = \sqrt{\langle |\mathbf{v} - \mathbf{v}'|^2 \rangle} = \sqrt{2}v_{rms}$  where  $v_{rms}^2 = \int d^3v |\mathbf{v}|^2 p(\mathbf{v})$ . The velocity  $\bar{v}$  in the previous argument should be replaced by  $v_{rel}$ , whereas the distance traveled by the particle in a mean-free-time is  $\lambda_{mfp} = v_{rms}\tau_{rms}$ . Use these ideas to derive

$$\lambda_{mfp} = \frac{1}{n\sqrt{2}\pi d^2}.$$

(d) Estimate the mean-free-path length of air at atmospheric pressure  $P = 1.1013 \times 10^5$  Pa and  $T = 300^\circ\text{K}$ . Use the ideal gas law  $P = nk_B T$  to obtain the density  $n$  and estimate  $d = 2R$  where  $R = 1.55 \times 10^{-10}$  m is the van der Waals radius of molecular nitrogen. Calculate the ratio  $\epsilon = R/\lambda_{mfp}$ , which is the relevant small parameter for the validity of the Boltzmann kinetic equation.

3. (a) Using the mass and momentum equations of the compressible Navier-Stokes system, derive the balance equation for kinetic energy:

$$\partial_t \left( \frac{1}{2} \rho v^2 \right) + \nabla \cdot \left[ \left( \frac{1}{2} \rho v^2 + P \right) \mathbf{v} + \mathbf{T}^{(1)} \cdot \mathbf{v} \right] = -Q + P(\nabla \cdot \mathbf{v})$$

where  $Q = -\mathbf{T}^{(1)} : \nabla \mathbf{v} = 2\eta S^2 + \zeta D^2 \geq 0$  is the rate of kinetic energy dissipation per unit volume, with  $D = \nabla \cdot \mathbf{v}$  the velocity-divergence/dilatation and  $\mathbf{S} = \frac{1}{2} [\nabla \mathbf{v} + (\nabla \mathbf{v})^\top - (2/3)D\mathbf{I}]$  the velocity strain-rate tensor.

*Hint:* It is useful to show first that

$$\rho D_t \mathbf{v} + \nabla P + \nabla \cdot \mathbf{T}^{(1)} = 0$$

with  $D_t = \partial_t + \mathbf{v} \cdot \nabla$  the Lagrangian or material time-derivative.

(b) Use part (a) and conservation of total energy to derive the balance equation for internal energy density:

$$\partial_t u + \nabla \cdot [u\mathbf{v} + \mathbf{q}] = Q - P(\nabla \cdot \mathbf{v}),$$

where  $\mathbf{q} = -\kappa \nabla T$  is the heat transport vector due to thermal conduction, or, alternatively,

$$D_t u + u(\nabla \cdot \mathbf{v}) + \nabla \cdot \mathbf{q} = Q - P(\nabla \cdot \mathbf{v}),$$

(c) Use the balance equation for conservation of mass to show that the velocity-divergence is given by

$$\nabla \cdot \mathbf{v} = -D_t \rho / \rho = D_t \mathcal{V} / \mathcal{V}$$

where  $\mathcal{V} = 1/n$  is the *specific volume*, or volume per particle. Use this result to show that the pressure-dilatation term is given by

$$P(\nabla \cdot \mathbf{v}) = -\frac{1}{\mathcal{V}} D_t W$$

where  $D_t W \doteq -P D_t \mathcal{V}$  is the rate at which work is performed by the velocity field acting against pressure to compress the fluid.

(d) The entropy per volume  $s(u, \rho)$  is a thermodynamic function which satisfies the first law of thermodynamics in the form

$$ds = (du - \mu d\rho)/T$$

where  $T(u, \rho)$  is the absolute temperature and  $\mu(u, \rho)$  is the chemical potential per mass. These thermodynamic state functions also satisfy the *homogeneous Gibbs relation*

$$u + P = sT + \mu\rho.$$

Using these standard facts from thermodynamics and the system of compressible Navier-Stokes equation, derive the balance equation for entropy density

$$\partial_t s + \nabla \cdot [s\mathbf{v} + \mathbf{q}/T] = \frac{Q}{T} + \frac{\kappa|\nabla T|^2}{T^2} \geq 0.$$

This equation is a precise statement of the *second law of thermodynamics* for a single-component compressible fluid.

*Hint:* It is helpful to use the relation

$$D_t s = (1/T)D_t u - (\mu/T)D_t \rho$$

that follows from the first law of thermodynamics.