

TD6: Connecting the microscopic and the macroscopic in fluid flows

Statistical Mechanics – iCFP M2

Here we illustrate the complementariness of generalized hydrodynamics and microscopic approaches through the study of viscous fluid using both approaches. Sec. 1 thus derives the fluid's hydrodynamic equations up to a single phenomenological coefficient (in the incompressible limit at least), which we then determine in Sec. 2.

1 Phenomenological theory: the Navier-Stokes equation

We consider a fluid with two conserved quantities, namely its momentum density $\mathbf{g}(\mathbf{r}, t)$ and its mass density $\rho(\mathbf{r}, t)$. The conservation equations for these two quantities read

$$\partial_t g_i = -\partial_j P_{ij} \quad (1a)$$

$$\partial_t \rho = -\partial_i J_i \quad (1b)$$

$$(1c)$$

Here $P_{ij} = -\sigma_{ij}$, with σ_{ij} the usual total stress tensor.

- 1.1 What are the symmetries of \mathbf{g} and ρ under spatial symmetries and time-reversal?
- 1.2 In this section we consider an isothermal system. What is the proper thermodynamic potential f per unit volume to use in this situation? Define the thermodynamic conjugates A_i^g and A^ρ as derivatives of this potential. Assuming that f is the sum of a kinetic energy and a static part, relate A_i^g and A^ρ to the fluid velocity and chemical potential. What are their spatial symmetries?
- 1.3 Write the dissipative currents of \mathbf{g} and ρ , first giving the couplings in their most general tensorial form. We will only keep the first-order terms in A_i^g and A^ρ , implying that we place ourselves in a state that only weakly deviates from a motionless fluid (an approximation valid at low Reynolds number) with constant density ρ_0 . Include gradient terms up to first order.
- 1.4 Rotational invariance imposes that these tensors commute with any rotation, implying that they are isotropic tensors. Here we give the most general form of an isotropic tensor with up to four indices in three dimensions:

$$T_{ij} = a\delta_{ij} \quad (2a)$$

$$T_{ijk} = a\epsilon_{ijk} \quad (2b)$$

$$T_{ijkl} = a\delta_{ij}\delta_{kl} + b\delta_{ik}\delta_{jl} + c\delta_{il}\delta_{jk}, \quad (2c)$$

where a , b and c are arbitrary constants, δ_{ij} is the Kronecker delta. The completely antisymmetric tensor ϵ_{ijk} is defined by $\epsilon_{123} = 1$ and the fact that it is antisymmetric with respect to any permutation of its indices. Apply these results to reduce the number of unknown dissipative phenomenological coefficients down to five.

- 1.5 Insert the dissipative currents into the conservation equations and use inversion symmetry to reduce the number of independent unknown dissipative coefficients to three.
- 1.6 Now write the dissipative currents, keeping only the zeroth order in gradients. Use rotational symmetry to reduce the number of unknown reactive phenomenological coefficients to two.
- 1.7 What is the relationship between these coefficients dictated by Onsager symmetry?

- 1.8 Write the full equations of motion. Use Galilean invariance to show that the reactive mass current is exactly equal to \mathbf{g} . Deduce from this the value of all reactive coefficients.
- 1.9 We now seek to relate these phenomenological equations to the usual form of the Stokes equation. Write the free energy F of a macroscopic system with volume V and its thermodynamic derivative, and infer from these that $\rho\delta\mu = \delta P$, where P is the usual fluid pressure. There are only two dissipative coefficients left. What is their sign? What is their physical meaning?
- 1.10 Write the full equations of motion. We are missing the advection term to recover the full Navier-Stokes equation. Further considerations related to Galilean invariance can be used to show that beyond the linear terms considered here, the reactive pressure tensor has a nonlinear term equal to $\rho A_i^g A_j^g$. We also neglect the dissipative mass current to lowest order in gradients. Using this additional information, recover the full flow equation for a compressible fluid.
- 1.11 Finally, impose the incompressibility of the fluid to recover the Navier-Stokes equation. What is the status of P in this case?

2 Microscopic model: thermal conductivity and shear viscosity

While the hydrodynamic considerations developed above give the full form of the equations of motion associated with a fluid flow, they cannot by themselves provide the value of the kinetic coefficients that they involve. Once the hydrodynamic equations are known, these coefficients can be obtained by studying a microscopic model in a convenient simple flow geometry.

In this section, we consider one such model drawn from the kinetic theory of gases. The fluid considered has a conserved energy density, mass density and momentum density, and is thus in principle described by a more complicated hydrodynamic theory than that of Sec. 1. However in practice we will only discuss this fluid in two simple situations: the zero-momentum case (where its hydrodynamics is described by the two-component fluid of the main lecture), and the isothermal case (where the description of Sec. 1 applies).

Transport phenomena in a dilute gas can be described by the Boltzmann equation, which governs the probability density $f(\mathbf{r}, \mathbf{v}, t)$ of finding a particle with velocity \mathbf{v} at a position \mathbf{r} at time t . The overall form of the Boltzmann equation is

$$\left(\frac{\partial}{\partial t} + \mathbf{v} \cdot \nabla\right) f(\mathbf{r}, \mathbf{v}, t) = I_c, \quad (3)$$

where the left-hand-side represents the fact that the probability is advected by the velocity \mathbf{v} , and the term I_c on the right-hand side is a collision operator that acts as a source of probability, converting particles of a given velocity into particles with another velocity depending on the local density of the fluid (and thus on the collision probability).

Unfortunately, the Boltzmann equation involves many relaxation time scales and is all in all difficult to tackle theoretically. Here we instead consider a simplified collision operator involving only one relaxation time scale τ , an approximation known in the literature as the ‘‘BGK model’’ (Bhatnagar, Gross, Krook):

$$\left(\frac{\partial}{\partial t} + \mathbf{v} \cdot \nabla\right) f(\mathbf{r}, \mathbf{v}, t) = -\frac{f - f_0}{\tau}, \quad (4)$$

where the distribution f_0 is associated with the local thermodynamic equilibrium:

$$f_0(\mathbf{r}, \mathbf{v}, t) = n \left(\frac{m}{2\pi kT}\right)^{3/2} \exp\left[-\frac{m(\mathbf{v} - \mathbf{u})^2}{2kT}\right]. \quad (5)$$

Here m is the particle mass, kT the thermal energy, n the particle density. We assume a spatial dimension $d = 3$, although our approach can be extended to other dimensions without any additional difficulty. The local equilibrium solution also involves the local velocity field $\mathbf{u}(\mathbf{r}, t)$ and the local temperature field $T(\mathbf{r}, t)$, which we define through

$$n\mathbf{u} = \int \mathbf{v} f \, d\mathbf{v} = \int \mathbf{v} f_0 \, d\mathbf{v} \quad \text{and} \quad \frac{3nk}{m}T = \int (\mathbf{v} - \mathbf{u})^2 f \, d\mathbf{v} = \int (\mathbf{v} - \mathbf{u})^2 f_0 \, d\mathbf{v}. \quad (6)$$

Once Eq. (4) has been solved for a given set of initial and boundary conditions, the heat flux \mathbf{J}^q and the pressure tensor P_{ij} can be obtained through

$$J_i^q = \frac{m}{2} \int \xi_i(\xi^2) f d\xi \quad (7a)$$

$$P_{ij} = m \int \xi_i \xi_j f d\xi, \quad (7b)$$

where we define $\boldsymbol{\xi} = \mathbf{v} - \mathbf{u}$. \mathbf{J}^q and P_{ij} are the currents associated with the energy density and the momentum density, respectively.

Our goal here is to compute the gas' Prandtl number, defined by

$$\text{Pr} = \frac{\eta c_p}{\kappa}, \quad (8)$$

where η denotes the shear viscosity, κ is the thermal conductivity, and c_p is the specific heat capacity per unit mass at constant pressure. Throughout this section we will limit ourselves to seeking a perturbative solution to the general problem Eq. (4) under the form $f = f_0 + f_1$, where the first-order correction f_1 is of order 1 in τ .

2.1 (preliminaries, unessential for the following) Using dimensional arguments (without calculation), indicate the dependence of η and κ with respect to the parameters of the problem (τ , kT , the density n , the mass m). What conclusion can you draw regarding the Prandtl number?

2.2 We first aim to compute the thermal conductivity κ . To that effect, we assume that the gas is at rest (implying a constant pressure $P_{ij} = nT\delta_{ij}$) and subjected to a stationary temperature gradient along the x -axis. Compute f_1 , and deduce from it the heat flux \mathbf{J}^q . Show that

$$\kappa = \frac{1}{6} m \tau \frac{\partial}{\partial T} \left(\int v^4 f_0 d\mathbf{v} \right). \quad (9)$$

Compute κ .

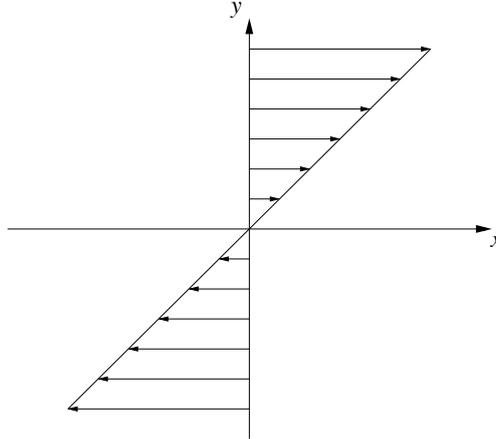


Figure 1: Geometry considered for a uniform stationary laminar shear flow with a density $n = \text{constant}$. Arrows picture the velocity field \mathbf{u} , which is such that $u_x = ay$. The temperature is assumed uniform with respect to the position \mathbf{r} .

2.3 To compute the viscosity, we place ourselves under isothermal conditions, and consider a laminar, stationary shear flow with a flow velocity profile $\mathbf{u} = ay\hat{\mathbf{x}}$ (see Fig. 1). For this uniform shear flow, use the results of Sec. 1 to show that the viscous force per unit surface (that is, the xy component of the pressure tensor) reads

$$P_{xy} = -\eta \frac{\partial u_x}{\partial y} = -\eta a. \quad (10)$$

Compute the correction f_1 , then P_{xy} , and deduce the viscosity from this.

2.4 Recall the value of the specific heat c_p in the frame of our approximations (we assume that the gas is monoatomic), then give the expression of the Prandtl number. Most dilute gases have $\text{Pr} \simeq 2/3$. What can you conclude from this?