Chapter 2

The kinetic theory of gases

So far, we have argued that statistical ensembles should be relevant to describe complex systems. But can we do better? Can we actually find systems that are complex enough that they are endowed with the kind of 'mixing dynamics' that we have said would guarantee the applicability of statistical mechanics and yet are simple enough that we can characterize them analytically? The answer is yes, and is largely due to the work of Boltzmann. In this chapter, we consider a dilute gas of interacting particles and construct explicitly its large-scale dynamics. We will:

- Show that it relaxes to equilibrium, in a way that we will make more precise later
- Characterize this relaxation to extract transport coefficients, such as viscosity, thermal conductivity, etc.

Explicitly, the model we consider comprises N classical particles in three space dimensions, interacting via a pair potential V and experiencing an external potential U. Its Hamiltonian is given by[1]:

$$H = \sum_{i=1}^{N} \frac{\vec{p}_i^{\,2}}{2m} + U(\vec{q}_i) + \frac{1}{2}\sum_{i\neq j} V(\vec{q}_i - \vec{q}_j)\ . \tag{2.1}$$

In the Hamiltonian (2.1),

$$H_1 \equiv \sum_{i=1}^{N} \frac{\vec{p}_i^{\,2}}{2m} + U(\vec{q}_i) \tag{2.2}$$

describes the evolution of the N particles in the absence of interactions, which we will refer to as the free evolution. On the contrary, the blue term in Eq. (2.1) describes the pairwise interactions between the particles.

Our goal is to start from Eq. (2.1) and to demonstrate and characterize the relaxation to equilibrium, as illustrated in Fig. 2.1. The natural starting point to tackle this challenge is given by Hamilton's equations of motion but, clearly, the joint knowledge of the position and velocities of all particles is way too much information and we would like to construct a coarse-grained description of the system that contains only the information which is relevant at the macroscopic scale. Doing so will require identifying the right level of description, i.e. the right coarse-grained variables and to construct their dynamics.

The outline of the chapter is as follows. In Section 2.1, we will attempt to build coarse-grained variables and derive their dynamics starting from Liouville's equation. This path will fail, but it will deliver the right tools to make progress. In Section 2.2, we construct the Boltzmann equation, and in Section 2.3 we show it accounts for the evolution depicted in Fig 2.1. Finally, we characterize in Section 2.5 the relaxation to equilibrium.

[1] Note that the factor 1/2 is included to avoid double counting. Consider the dynamics of particle k, $\dot{\vec{p}}_k = -\frac{\partial U(\vec{q}_k)}{\partial \vec{q}_k} - \frac{1}{2}\sum_{i\neq j}\frac{\partial V(\vec{q}_i-\vec{q}_j)}{\partial \vec{q}_k}$. (Note that there are $N(N-1)$ terms in the last sum: i goes from 1 to N, and so does j but with $j \neq i$.) The terms in the last sum are non-vanishing whenever either i or j equals k so that $\dot{\vec{p}}_k = -\frac{\partial U(\vec{q}_k)}{\partial \vec{q}_k} - \frac{1}{2}\sum_{i\neq j}\left[\frac{\partial V(\vec{q}_k-\vec{q}_j)}{\partial \vec{q}_k}\delta_{i,k} + \frac{\partial V(\vec{q}_i-\vec{q}_k)}{\partial \vec{q}_k}\delta_{j,k}\right] = -\frac{\partial U(\vec{q}_k)}{\partial \vec{q}_k} - \sum_{j\neq k}\frac{\partial V(\vec{q}_k-\vec{q}_j)}{\partial \vec{q}_k}$, where we have relabelled the dummy variable i into j and used that V is even to obtain the last equality. Note that, this time, there are only $N-1$ terms in the last sum since k is fixed.

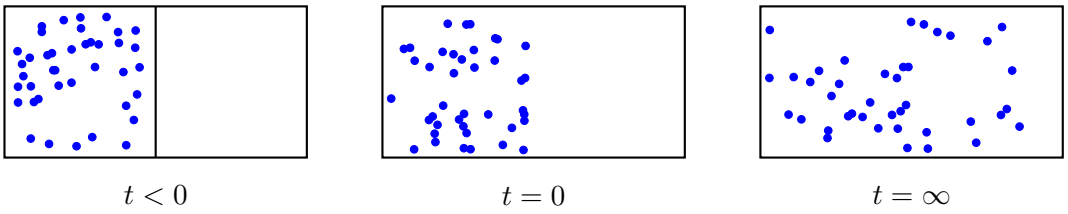


Figure 2.1: *A gas of particles is initially confined in the left half of the system. At $t = 0$, it is released and start exploring the accessible volume. At large time, it has relaxed and no macroscopic evolution can be observed.*

2.1 From Liouville's equation to the BBGKY hierarchy

2.1.1 Liouville's equation for an interacting gas

Using the Hamiltonian (2.1), Liouville's equation take the form

$$\partial_t \rho(\{\vec{q}_i, \vec{p}_i\}, t) = -\{\rho, H\} = -\sum_{i=1}^{N} \frac{\partial \rho}{\partial \vec{q}_i} \cdot \frac{\partial H}{\partial \vec{p}_i} - \frac{\partial \rho}{\partial \vec{p}_i} \cdot \frac{\partial H}{\partial \vec{q}_i} \tag{2.3}$$

$$= -\sum_{i=1}^{N} \Big[\frac{\partial \rho}{\partial \vec{q}_i} \cdot \frac{\partial H_1}{\partial \vec{p}_i} - \frac{\partial \rho}{\partial \vec{p}_i} \cdot \frac{\partial H_1}{\partial \vec{q}_i} \Big] - \sum_{i=1}^{N} \Big[\frac{\partial \rho}{\partial \vec{p}_i} \cdot \sum_{j \neq i} \frac{\partial V(\vec{q}_i - \vec{q}_j)}{\partial \vec{q}_i} \Big] . \tag{2.4}$$

We can thus rewrite the evolution of the probability density ρ as

$$\partial_t \rho(\{\vec{q}_i, \vec{p}_i\}, t) + \{\rho, H_1\} = \sum_{i=1}^{N} \Big[\frac{\partial \rho}{\partial \vec{p}_i} \cdot \sum_{j \neq i} \frac{\partial V(\vec{q}_i - \vec{q}_j)}{\partial \vec{q}_i} \Big] . \tag{2.5}$$

In this expression, the left-hand-side tells us how the particles would evolve if they were not interacting. We refer to this evolution—and thus to $\{\rho, H_1\}$—as the free evolution. On the contrary, the right-hand side gives the contribution of interactions between particles to the evolution of ρ.

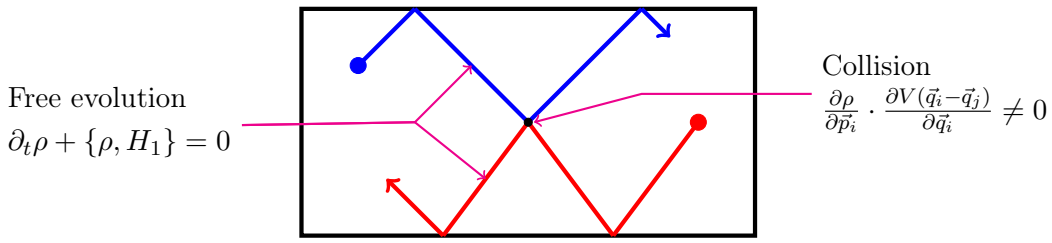


Figure 2.2: *Schematic illustration of the free evolution of two particles, interrupted by sudden collisions.*

2.1.2 Coarse-grained description

To build a coarse-grained description of the system, we need to identify a set of observables that are sufficient to describe the system at large scales and to construct a closed set of evolution equations for these observables. This is very difficult in general, but you may have already encountered examples of such descriptions, like the Navier-Stokes equations that predict the joint evolution of the density and

velocity fields of a fluid:

$$\partial_t \rho(\vec{r},t) = -\nabla\cdot[\rho(\vec{r},t)\vec{u}(\vec{r},t)], \qquad \rho(\vec{r},t)[\partial_t\vec{u}(\vec{r},t)+\vec{u}(\vec{r},t)\cdot\nabla\vec{u}(\vec{r},t)] = -\nabla p(\vec{r},t)+\mu\Delta\vec{u}(\vec{r},t)\ . \quad (2.6)$$

To use this equation, one needs to know the value of the dynamic viscosity μ and how the pressure field should be related to ρ and $\vec{u}$. For an incompressible fluid, the density field is a constant and the pressure is set by enforcing that $\nabla\cdot\vec{u}=0$, in which case Eq. (2.6) becomes a closed equation for $\vec{u}$. The viscosity can be experimentally measured and the Navier-Stokes can then be used to make predictions. However, since we have started from a macroscopic description of the fluid, it is not possible anymore to relate μ to microscopic properties of the system. We also have little control on when Eq. (2.6) is a valid description of a fluid. Statistical physics aims at fixing these problems by starting from the microscopic description of systems to build their coarse-grained description, hence yielding microscopic insight into macroscopic transport parameters.

Another example of a coarse-grained description is offered by the description of a set of particles doing a Brownian random walk in water. The random motion of the particles leads to a large-scale motion described by the diffusion equation:

$$\partial_t n(\vec{r},t) = D\Delta n(\vec{r},t)\ . \quad (2.7)$$

Here, the knowledge of D suffices to make predictions on the evolution of the number density field $n(\vec{r},t)$. Again, it can be measured experimentally but Eq. (2.7) has nothing to say on its microscopic origin.

For our interacting gas, we would like to derive an analog of Eq. (2.6) or Eq. (2.7). This means identifying what are the relevant fields that we need to characterize and to compute all relevant transport parameters. At this stage, many questions are open. How do we know if the density field will be sufficient, as in Eq. (2.7), or whether we will also need a velocity field as in Eq. (2.6)? Or some other fields? And can we even be sure that such closed, self-consistent descriptions exist?

In general, these are very difficult questions and there are many systems for which we do not know how to address them. However, there are also a number of important concepts and principles that help us construct such 'hydrodynamic' descriptions [2].

Scale separation

In principle, it is not obvious at all why the dynamics of a system at some macroscopic scale should decouple from what happens at shorter scales. The reason why we end up being able to construct such close self-contained macroscopic descriptions is that many systems have well-defined and well-separated scales that only interact with each other through the form of transport coefficients like μ and D in Eqs. (2.6) and (2.7).

Consider the case of the diffusion equation. Our small particles are moving around randomly and they travel a distance d equal to their size in a typical time τ_m, which is independent of the size of the system. Now, consider instead their density field $n(\vec{r},t)$. We can study its dynamics starting from an initial profile

[2] Because, in spirit, we are trying to achieve a description akin to what Navier and Stokes did for a fluid, we often refer to deterministic coarse-grained descriptions as 'hydrodynamic' descriptions, despite the lack of any 'water' in the system under study.

at density n_0, perturbed by a small fluctuation $\delta n(\vec{r}, t=0)$. We can then decompose the density field at all times as

$$n(\vec{r},t) = n_0 + \delta n(\vec{r},t) = n_0 + \sum_{\vec{q}} \delta n_{\vec{q}}(t) e^{-i\vec{q}\cdot\vec{r}} \,. \tag{2.8}$$

Injecting Eq. (2.8) into Eq. (2.7) shows that the Fourier modes of the perturbation relax as

$$\delta n_{\vec{q}}(t) = \delta n_{\vec{q}}(0) e^{-t/\tau_q} \quad \text{with} \quad \tau_q = \frac{1}{Dq^2} \,. \tag{2.9}$$

The relaxation time of a mode of size $\ell = \frac{2\pi}{q}$ is thus $\tau_\ell = \ell^2/(4D\pi^2)$. A perturbation of the density field at the scale of the system thus relaxes in a time $\mathcal{O}(L^2)$ that diverges with the system size. We see that the macroscopic relaxation of the density field and the microscopic motion of the particle over a distance of the order of its size take place on time scales that are well separated. We may thus hope to be able to average out what happens at the microscopic scale to create a closed description of what happens at much larger scales. This type of scale separation will be at the root of our computations for the interacting gas.

Slow fields/hydrodynamics fields

Even if we know that there is a scale separation in our system and we hope to be able to describe its macroscopic scale 'independently' of the microscopic one, how can we identify the relevant observables that one needs to characterize? Again, this is a complex question whose generic answer we do not know. But a lot of progress has been made towards identifying the guiding principles.

Conserved fields are slow. Some fields are associated with conserved quantities. Take the example above of the diffusion equation. Because particles are not created or annihilated, the dynamics of the density field has to take the form of a local conservation law, even at the microscopic scale: $\partial_t n(\vec{r},t) = -\nabla\cdot\vec{j}(\vec{r},t)$, where $\vec{j}(\vec{r},t)$ is the average particle current. At the macroscopic scale, Fick's law states that $\vec{j} = -D\nabla n$, but $\vec{j}$ can be a much more complicated quantity at the microscopic scale. Fields like $n(\vec{r},t)$, which measure the local amount of a conserved quantity, are called conserved fields. These fields are necessarily slow because relaxing a fluctuation on the scale of the system size L requires transporting the conserved observable over the same scale. If the transport is ballistic, it will take a time $\tau \sim L$. If it is diffusive, it will take a time $\tau \sim L^2$. To characterize this, one typically defines a dynamic exponent z such that

$$\tau \sim L^z \quad \text{with} \quad z > 0 \,. \tag{2.10}$$

Conserved quantities thus typically lead to hydrodynamic fields that enter the large-scale description of the system.

Spontaneous breaking of symmetry. Consider a system invariant under some symmetry group. For instance, the atomic spins $\vec{S}_i$ in a metallic alloy. At very high temperature, the interactions between the spins are irrelevant and they explore their configuration space isotropically. They thus respect the symmetry of their system and $\langle \vec{S}_i \rangle = 0$. In a ferromagnetic system, as temperature is decreased, the exchange interaction between the spins tend to align them and, at low enough temperature, they order: below a temperature T_c, called the Curie temperature, $\langle \vec{S}_i \rangle \neq 0$. The system is thus not invariant anymore

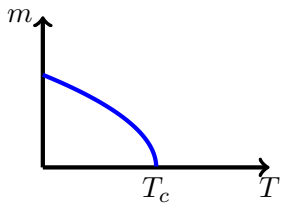


Figure 2.3: *As T is lowered below T_c, the system acquires a spontaneous magnetization. The relaxation time diverges at the transition point and a slow mode associated to the order-parameter field appears in the system.*

under the symmetry group and the symmetry is said to be 'broken'. More precisely, one can define an order parameter

$$m(T) = \left| \frac{1}{N} \sum_{i=1}^{N} \langle \vec{S}_i \rangle \right| , \tag{2.11}$$

such that, in the high temperature phase, $m = 0$, whereas m acquires a non-zero value below $T = T_c$, as shown in Fig. 2.3.

Imagine that you locally order the system in the high temperature phase by aligning all the spins in a given region of space. Each of the spins fluctuates rapidly and, in a finite time, the magnetization will vanish. One thus expects that a fluctuation $\delta m(t)$ relaxes as $\delta m(t) = \delta m(0) e^{-t/\tau}$, where τ is a finite relaxation time. As the system approaches T_c, aligned spins are less likely to fluctuate, since the interactions with their neighbors are about to make them order globally. The relaxation will thus be much slower and $\tau \to \infty$ as $T \to T_c$. At the critical point, the system relaxes infinitely slowly: it can choose any direction in space to order equivalently, due to the invariance by rotation, and this state of bewilderment prevents any form of rapid ordering or relaxation. This fate is common to all spontaneous breaking of symmetries leading to a continuous transition. In such systems, we can associate a hydrodynamic mode to the order parameter field. While we do not discuss the dynamics of phase transitions in this class, we refer the interested reader to Prof. Kardar's class 8.334, offered in the Spring term.

Let us now try to identify the fields that are relevant for our interacting gas and construct their dynamics starting from Liouville's equation.

2.1.3 One-body functions

In our interacting gas, particle number, momentum, and energy are conserved quantities and we thus expect that hydrodynamic modes should be associated with these quantities. At this stage, we know how to predict the evolution of the particle positions and momenta, $\{\vec{q}_i, \vec{p}_i\}$, using Hamilton's equations of motion, as well as the evolution of the phase-space joint probability density $\rho(\{\vec{q}_i, \vec{p}_i\}, t)$.

Density field. Let us first try to build a density field out of these microscopic quantities. A density field $n(\vec{r}, t)$ should measure the local number of particles in any volume of space V:

$$\int_V n(\vec{r}, t) d^3\vec{r} = \text{average number of particles in V} \tag{2.12}$$

A natural object to count whether particle i is in a given volume is the Dirac distribution. Indeed, $\int_V \delta(\vec{r} - \vec{q}_i(t)) = 1$ when particle i is in V at time t, and vanishes otherwise. We can thus compute the

average number of particles in V as:

$$\int_V n(\vec{r},t)d^3\vec{r} = \Big\langle \int_V \sum_{i=1}^{N} \delta(\vec{q}_i(t)-\vec{r})d^3\vec{r} \Big\rangle \tag{2.13}$$

By definition of the probability density, the average of an observable $\langle O(\{\vec{q}_i(t),\vec{p}_i(t)\})\rangle$ is given by

$$\langle O(\{\vec{q}_i(t),\vec{p}_i(t)\})\rangle = \int \prod_k d^3\vec{q}_k d^3\vec{p}_k \, O\big(\{\vec{q}_i,\vec{p}_i\}\big)\, \rho\big(\{\vec{q}_i,\vec{p}_i\},t\big) \tag{2.14}$$

$$= \int \prod_k \mathrm{d}\Gamma_k \, O\big(\{\vec{q}_i,\vec{p}_i\}\big)\, \rho\big(\{\vec{q}_i,\vec{p}_i\},t\big)\ . \tag{2.15}$$

where $\mathrm{d}\Gamma_k \equiv \mathrm{d}^3\vec{q}_k \mathrm{d}^3\vec{p}_k$, as before. Applying the definition (2.14) to Eq. (2.13) then leads to

$$\int_V n(\vec{r},t)d^3\vec{r} = \int \prod_k \mathrm{d}\Gamma_k \Big[\int_V \sum_{i=1}^{N} \delta(\vec{q}_i-\vec{r})d^3\vec{r}\Big]\rho(\{\vec{q}_i,\vec{p}_i\},t) \tag{2.16}$$

$$= \int_V \Big[\int \prod_k \mathrm{d}\Gamma_k \sum_{i=1}^{N} \delta(\vec{q}_i-\vec{r})\rho(\{\vec{q}_i,\vec{p}_i\},t)\Big]d^3\vec{r}\,, \tag{2.17}$$

where we have commuted the order of the integrals to go from the first to the second line. Identifying the blue terms in Eq. (2.16) and (2.17) then leads to

$$n(\vec{r},t) = \int \prod_k \mathrm{d}\Gamma_k \sum_{i=1}^{N} \delta(\vec{q}_i-\vec{r})\rho(\{\vec{q}_i,\vec{p}_i\},t) = \Big\langle \sum_{i=1}^{N} \delta(\vec{q}_i(t)-\vec{r})\Big\rangle\ . \tag{2.18}$$

We note that Eq. (2.18) could have been obtained directly from Eq. (2.13) by commuting average and integrals. Whenever I will write in the following "by linearity, we can commute A and B", I will be referring to the type of computation done above, which I will thus skip from now on[3].

An appealing feature of Eq. (2.18) is that it relates directly the field $n(\vec{r},t)$ to the trajectories $\{\vec{q}_i(t),\vec{p}_i(t)\}$. Note also how, on the left-hand side of Eq. (2.14), $\{\vec{q}_i(t),\vec{p}_i(t)\}$ refer to trajectories of the system while on the right-hand side, $\{\vec{q}_i,\vec{p}_i\}$ are simply vectors that are being integrated over, with the time dependence now entering through $\rho(\{\vec{q}_i,\vec{p}_i\},t)$.

One-body functions. Let us now show how the expression (2.18) for the density field suggests a way to coarse-grain the system. Inverting the sum and integrals indeed leads to

$$n(\vec{r},t) = \sum_{i=1}^{N} \int \mathrm{d}\Gamma_i \delta(\vec{q}_i-\vec{r}) \int \prod_{k\neq i} \mathrm{d}\Gamma_k \rho(\{\vec{q}_j,\vec{p}_j\},t) \tag{2.19}$$

$$= \sum_{i=1}^{N} \int \mathrm{d}\Gamma_i \delta(\vec{q}_i-\vec{r})\rho_1^i(\vec{q}_i,\vec{p}_i,t)\ , \tag{2.20}$$

where we have introduced the one-body phase-space density

$$\rho_1^i(\vec{q}_i,\vec{p}_i,t) \equiv \int \prod_{k\neq i} \mathrm{d}\Gamma_k \rho(\{\vec{q}_j,\vec{p}_j\},t)\ . \tag{2.21}$$

[3]This will be the case for $\partial_t\langle O\rangle$ and $\langle\partial_t O\rangle$, for instance.

Since we have integrated over all the $\vec{q}_k$ and $\vec{p}_k$, $\rho_1^i(\vec{q}_i, \vec{p}_i, t)$ tells us the probability density of finding particle i at $\vec{q}_i, \vec{p}_i$ at time t, irrespective of the positions and momenta of all other particles.

At this stage, it is important to realize that, since all the gas particles are indistinguishable, their labeling is irrelevant. Relabeling all of them with different numbers should not change anything in the physics of the system. When we pick the initial condition for the probability distribution, it is thus important to choose it so that it respects the invariance by relabelling of the system. In other words, for any permutation σ, we require that $\rho(\{\vec{q}_i, \vec{p}_i\}, 0) = \rho(\{\vec{q}_{\sigma(i)}, \vec{p}_{\sigma(i)}\}, 0)$. This property is then preserved by the dynamics. As a consequence, particle i and particle $j \neq i$ have exactly the same probability to be at $\vec{q}_i, \vec{p}_i$ at time t and

$$\rho_1^i(\vec{q}_i, \vec{p}_i, t) = \rho_1^j(\vec{q}_i, \vec{p}_i, t) \equiv \rho_1(\vec{q}_i, \vec{p}_i, t) \, . \tag{2.22}$$

The function ρ_1 is called the one-body phase-space probability density function. By definition it is normalized to 1:

$$\int d^3\vec{q} d^3\vec{p} \rho_1(\vec{q}, \vec{p}) = 1 \, . \tag{2.23}$$

At this stage, we note that the variables $\vec{q}_i, \vec{p}_i$ are dummy variables in Eq. (2.20). We can relabel them $\vec{q}, \vec{p}$ and integrate over $\vec{q}$ to find:

$$n(\vec{r}, t) = \sum_{i=1}^{N} \int d^3\vec{p} \rho_1(\vec{r}, \vec{p}, t) = N \int d^3\vec{p} \rho_1(\vec{r}, \vec{p}, t) \equiv \int d^3\vec{p} f_1(\vec{r}, \vec{p}, t) \, , \tag{2.24}$$

where we have introduced the phase-space number density

$$f_1(\vec{q}, \vec{p}, t) \equiv N \rho_1(\vec{q}, \vec{p}, t) = \left\langle \sum_{i=1}^{N} \delta[\vec{q} - \vec{q}_i(t)] \delta[\vec{p} - \vec{p}_i(t)] \right\rangle \, . \tag{2.25}$$

By definition, f_1 is such that $f_1(\vec{q}, \vec{p}, t) \mathrm{d}^3\vec{q} \mathrm{d}^3\vec{p}$ represents the average number of particles with position and momenta in the (phase-space) volume element $\mathrm{d}^3\vec{q} \mathrm{d}^3\vec{p}$ near $(\vec{q}, \vec{p})$ at time t.

Starting from the joint phase-space probability density describing the N particles, $\rho(\{\vec{q}_i, \vec{p}_i\}, t)$, we have thus introduced much lower dimensional fields, $\rho_1(\vec{q}, \vec{p}, t)$ and $f_1(\vec{q}, \vec{p}, t)$ that allow us to compute and characterize the number density $n(\vec{r}, t)$ through Eqs. (2.20) or (2.24). Thanks to Eq. (2.21), we can directly relate these objects through

$$\rho_1(\vec{q}, \vec{p}, t) = \int \prod_{k>1} \mathrm{d}\Gamma_k \rho(\vec{q}, \vec{p}, \vec{q}_2, \vec{p}_2, \ldots, \vec{q}_N, \vec{p}_N) \, . \tag{2.26}$$

Since we know how ρ evolves in time, thanks to Liouville's equation, Eq. (2.26) will allow us to construct the evolution equation of ρ_1.

Comment: Mathematically, the "dimensional" reduction of the problem can be seen by comparing the functional spaces in which ρ and ρ_1 live. ρ maps $\{\vec{p}_i, \vec{q}_i\}$ and t onto a real number, $\rho(\{\vec{p}_i, \vec{q}_i\}, t)$. Since there are N particles, ρ is a function from $\mathbb{R}^{6N} \times \mathbb{R} \to \mathbb{R}$. ρ_1 maps $\vec{p}, \vec{q}$ and t onto a real number, $\rho(\vec{p}, \vec{q}, t)$ and is thus a function from $\mathbb{R}^6 \times \mathbb{R} \to \mathbb{R}$. If you wanted to sample ρ at a given value of t for a system with $N = 10$ particles, and you wanted at least 10 values for each coordinates—which is a low-quality grid!—, you would need a grid with
$(10^6)^{10} = 10^{60} = 1\,000\,000\,000\,000\,000\,000\,000\,000\,000\,000\,000\,000\,000\,000\,000\,000\,000\,000\,000\,000$ points.

Using C doubles, this requires $8 \times 10^{60}/(600 \times 10^{15}) \simeq 10^{43}$ times more data than the 600 petabytes produced by LHC run 3... If you want to do the same with ρ_1, you need 1 000 000 points, which means 8Mb of storage space.

2.1.4 The BBGKY hierarchy

The dynamics of f_1.

Let us recall that the Hamiltonian describing the system is

$$H = \sum_{i=1}^{N} \Big[\frac{\vec{p}_i^{\,2}}{2m} + U(q_i) \Big] + \frac{1}{2} \sum_{i=1}^{N} \sum_{\ell \neq i} V(\vec{q}_i - \vec{q}_\ell) = H_1 + \frac{1}{2} \sum_{i=1}^{N} \sum_{\ell \neq i} V(\vec{q}_i - \vec{q}_\ell) \, , \tag{2.27}$$

where we have singled out the "free" noninteracting part H_1. The time-evolution of the probability density to find the system at a position $\rho(\{\vec{q}_i, \vec{p}_i\}, t)$ is then given by Eq. (2.5)

$$\partial_t \rho + \{\rho, H_1\} = \sum_{i=1}^{N} \Big[\frac{\partial \rho}{\partial \vec{p}_i} \cdot \sum_{\ell \neq i} \frac{\partial V(\vec{q}_i - \vec{q}_\ell)}{\partial \vec{q}_i} \Big] \, . \tag{2.28}$$

In Eq. (2.28), the term in magenta tells us how the free evolution makes ρ relax while the term in blue tells us how interactions make ρ relax. We now want to integrate Eq. (2.28) over $\{\vec{q}_i, \vec{p}_i\}_{i \geq 2}$ to deduce the evolution of $\rho_1(\vec{q}_1, \vec{p}_1, t)$ from that of $\rho(\{\vec{q}_i, \vec{p}_i\}, t)$.

Left-hand side of Eq. (2.28). Since the left hand side ignores the presence of interactions, the dynamics of particles $2, \dots, N$ cannot impact those of particle 1, and we should thus expect that

$$\int \prod_{k>1} \mathrm{d}\Gamma_k (\partial_t \rho + \{\rho, H_1\}) = \partial_t \rho_1 + \{\rho_1, H_1\} \, . \tag{2.29}$$

Let us show that this is indeed the case. By linearity, and since the domain of integration is time independent,

$$\int_{\mathbb{R}^{6N-6}} \prod_{k>1} \mathrm{d}\Gamma_k \partial_t \rho(\{\vec{q}_i, \vec{p}_i\}, t) = \partial_t \Big[\int_{\mathbb{R}^{6N-6}} \prod_{k>1} \mathrm{d}\Gamma_k \rho(\{\vec{q}_i, \vec{p}_i\}, t) \Big] = \partial_t \rho_1(\vec{q}_1, \vec{p}_1, t) \, . \tag{2.30}$$

Let us now turn to the Poisson bracket between ρ and H_1:

$$\int \prod_{k>1} \mathrm{d}\Gamma_k \{\rho, H_1\} = \int \prod_{k>1} \mathrm{d}\Gamma_k \Big[\frac{\partial \rho}{\partial \vec{q}_1} \cdot \frac{\partial H_1}{\partial \vec{p}_1} - \frac{\partial \rho}{\partial \vec{p}_1} \cdot \frac{\partial H_1}{\partial \vec{q}_1} \Big] + \sum_{i \geq 2} \int \prod_{k>1} \mathrm{d}\Gamma_k \Big[\frac{\partial \rho}{\partial \vec{q}_i} \cdot \frac{\partial H_1}{\partial \vec{p}_i} - \frac{\partial \rho}{\partial \vec{p}_i} \cdot \frac{\partial H_1}{\partial \vec{q}_i} \Big] \, . \tag{2.31}$$

Let us first consider the term in blue. Since $\frac{\partial H_1}{\partial \vec{p}_i} = \frac{\vec{p}_i}{m}$ does not depend on $\vec{q}_i$ and $\frac{\partial H_1}{\partial \vec{q}_i} = \frac{\partial U(\vec{q}_i)}{\partial \vec{q}_i}$ does not depend on $\vec{p}_i$, it can be rewritten as:

$$\sum_{i \geq 2} \int \prod_{k>1} \mathrm{d}\Gamma_k \Big[\frac{\partial}{\partial \vec{q}_i} \cdot \Big(\rho \frac{\partial H_1}{\partial \vec{p}_i} \Big) - \frac{\partial}{\partial \vec{p}_i} \cdot \Big(\rho \frac{\partial H_1}{\partial \vec{q}_i} \Big) \Big] \, , \tag{2.32}$$

where the operators $\frac{\partial}{\partial \vec{q}_i}$ and $\frac{\partial}{\partial \vec{p}_i}$ apply to the parenthesis on their rights. We then note that $i \geq 2$ so that $\vec{q}_i$ and $\vec{p}_i$ are always integrated over. Since the integrand are total derivatives, the results of the

integrals will involve $\rho\frac{\partial H_1}{\partial \vec{q}_i}$ and $\rho\frac{\partial H_1}{\partial \vec{p}_i}$ evaluated as $|\vec{p}_i| \to \infty$ and $|\vec{q}_i| \to \infty$, respectively. Since ρ has to be normalizable, it must vanish in these limits and these boundary terms do not contribute: the overall integral vanishes[4]. This result is not surprising: The blue term tells us about how particles 2 to N make ρ evolve due to their free dynamics. While this impacts ρ, it does not impact particle 1 and should thus not impact the time evolution of ρ_1.

Consider next the term in magenta. Since $\frac{\partial H_1}{\partial \vec{p}_1} = \frac{\vec{p}_1}{m}$ and $\frac{\partial H_1}{\partial \vec{q}_1} = \frac{\partial U(\vec{q}_1)}{\partial \vec{q}_1}$ do not depend on $\{\vec{q}_k, \vec{p}_k\}$, they can be taken out of the integral. The same hold for the operators $\frac{\partial}{\partial \vec{q}_1}$ and $\frac{\partial}{\partial \vec{p}_1}$ so that one finds

$$\int \prod_{k>1} \mathrm{d}\Gamma_k \Big[\frac{\partial \rho}{\partial \vec{q}_1}\cdot\frac{\partial H_1}{\partial \vec{p}_1} - \frac{\partial \rho}{\partial \vec{p}_1}\cdot\frac{\partial H_1}{\partial \vec{q}_1}\Big] = \frac{\partial H_1}{\partial \vec{p}_1}\cdot\frac{\partial}{\partial \vec{q}_1}\int \prod_{k>1} \mathrm{d}\Gamma_k \rho - \frac{\partial H_1}{\partial \vec{q}_1}\cdot\frac{\partial}{\partial \vec{p}_1}\int \prod_{k>1} \mathrm{d}\Gamma_k \rho \tag{2.33}$$

$$= \frac{\partial H_1}{\partial \vec{p}_1}\cdot\frac{\partial}{\partial \vec{q}_1}\rho_1(\vec{q}_1,\vec{p}_1,t) - \frac{\partial H_1}{\partial \vec{q}_1}\cdot\frac{\partial}{\partial \vec{p}_1}\rho_1(\vec{q}_1,\vec{p}_1,t) \tag{2.34}$$

$$= \{\rho_1, H_1\} \tag{2.35}$$

All in all, we thus get Eq. (2.29) as anticipated.

Right-hand side of Eq. (2.28). We are interested in the evolution of the probability density of observing particle 1 at a given position in phase space. For the same reason as above, the interactions between particles $i \neq 1$ and $j \neq 1$ should not impact $\partial_t \rho_1(\vec{q}_1, \vec{p}_1)$. This suggests splitting the interaction term as

$$\int \prod_{k>1} \mathrm{d}\Gamma_k \sum_{i=1}^{N} \frac{\partial \rho}{\partial \vec{p}_i}\cdot\sum_{\ell\neq i}\frac{\partial V(\vec{q}_i - \vec{q}_\ell)}{\partial \vec{q}_i} = \int \prod_{k>1} \mathrm{d}\Gamma_k \frac{\partial \rho}{\partial \vec{p}_1}\cdot\sum_{\ell>1}\frac{\partial V(\vec{q}_1 - \vec{q}_\ell)}{\partial \vec{q}_1} + \sum_{i\geq 2}\int \prod_{k>1} \mathrm{d}\Gamma_k \frac{\partial \rho}{\partial \vec{p}_i}\cdot\sum_{\ell\neq i}\frac{\partial V(\vec{q}_i - \vec{q}_\ell)}{\partial \vec{q}_i}\,. \tag{2.36}$$

We first note that the term in orange always contains an integration over $\vec{p}_i$. Integrating by parts over $\vec{p}_i$ thus shows this term to vanish since $\frac{\partial V(\vec{q}_i - \vec{q}_\ell)}{\partial \vec{q}_i}$ does not depend on $\vec{p}_i$.The interaction term can then be rewritten as

$$\int \prod_{k>1} \mathrm{d}\Gamma_k \sum_{i=1}^{N} \frac{\partial \rho}{\partial \vec{p}_i}\cdot\sum_{\ell\neq i}\frac{\partial V(\vec{q}_i - \vec{q}_\ell)}{\partial \vec{q}_i} = \sum_{\ell>1}\int \mathrm{d}\Gamma_\ell \frac{\partial V(\vec{q}_1 - \vec{q}_\ell)}{\partial \vec{q}_1}\cdot\int \prod_{k\neq 1,\ell} \mathrm{d}\Gamma_k \frac{\partial \rho}{\partial \vec{p}_1}, \tag{2.37}$$

$$= (N-1)\int \mathrm{d}\Gamma_2 \frac{\partial V(\vec{q}_1 - \vec{q}_2)}{\partial \vec{q}_1}\cdot\frac{\partial}{\partial \vec{p}_1}\int \prod_{k>2} \mathrm{d}\Gamma_k\ \rho. \tag{2.38}$$

The term in blue in Eq. (2.37) is obtained from Eq. (2.36) by noticing that $\frac{\partial V(\vec{q}_i - \vec{q}_\ell)}{\partial \vec{q}_i}$ does not depend on $q_{k\neq 1,\ell}$. Equation (2.38) then stems from the fact that particles $2, \ldots, N$ are indistinguishable and that the last integral does not include an integral over $\vec{p}_1$. Finally, we introduce the two-body probability density

$$\rho_2(\vec{q}_1, \vec{p}_1, \vec{q}_2, \vec{p}_2) = \int \prod_{k>2} \mathrm{d}\Gamma_k \rho(\{\vec{q}_i, \vec{p}_i\})\,, \tag{2.39}$$

which is the joint probability density that particle 1 is at $\vec{q}_1, \vec{p}_1$ and particle 2 is at $\vec{q}_2, \vec{p}_2$. This allows rewriting the interaction term in a relatively compact form:

$$\int \prod_{k>1} \mathrm{d}\Gamma_k \sum_{i=1}^{N} \frac{\partial \rho}{\partial \vec{p}_i}\cdot\sum_{\ell\neq i}\frac{\partial V(\vec{q}_i - \vec{q}_\ell)}{\partial \vec{q}_i} = (N-1)\int \mathrm{d}\Gamma_2 \frac{\partial V(\vec{q}_1 - \vec{q}_2)}{\partial \vec{q}_1}\cdot\frac{\partial \rho_2(\vec{q}_1, \vec{p}_1, \vec{q}_2, \vec{p}_2)}{\partial \vec{p}_1}\,. \tag{2.40}$$

[4]Note that the same result can be obtained by integrating by parts $\frac{\partial \rho}{\partial \vec{q}_i}$ and $\frac{\partial \rho}{\partial \vec{p}_i}$, using similar arguments.

All in all, the dynamics for ρ_1 read

$$\partial_t \rho_1(\vec{q}_1,\vec{p}_1) + \{\rho_1, H_1\} = (N-1)\int \mathrm{d}\Gamma_2 \frac{\partial V(\vec{q}_1-\vec{q}_2)}{\partial \vec{q}_1}\cdot\frac{\partial \rho_2(\vec{q}_1,\vec{p}_1,\vec{q}_2,\vec{p}_2)}{\partial \vec{p}_1}\ . \tag{2.41}$$

Introducing $f_2 = N(N-1)\rho_2$ and multiplying Eq. (2.41) by N then gives the time evolution of the phase-space number density:

$$\partial_t f_1 + \{f_1, H_1\} = \int \mathrm{d}\Gamma_2 \frac{\partial V(\vec{q}_1-\vec{q}_2)}{\partial \vec{q}_1}\cdot\frac{\partial f_2(\vec{q}_1,\vec{p}_1,\vec{q}_2,\vec{p}_2)}{\partial \vec{p}_1}\ . \tag{2.42}$$

Again, f_2 does not contain more physics than ρ_2, and it simply allows absorbing the factor $N-1$ to lighten a little bit the notations.

Comments.

At this stage, we have accomplished what we wanted: we have projected the dynamics of ρ onto that of ρ_1 and f_1, hence obtaining the time evolution of a lower dimensional object. From there, we simply have to integrate its dynamics over $\vec{p}_1$ to obtain the dynamics of the average density field. However, there are several problems with Eq. (2.42).

1. While the 'low'-dimensional nature of Eq. (2.42) almost allows us to put it in a computer to predict the evolution of f_1, we cannot do that since we do not know f_2. To solve that problem, we could derive the evolution equation for f_2: we would start from Liouville's equation and integrate it over $\{\vec{q}_k,\vec{p}_k\}_{k\geq 3}$. However, the evolution of the joint probability density of particle 1 and 2 will depend on their encounters with other particles and the interaction term will require introducing a function f_3 that couple particles 1 and 2 to particle $k\geq 3$. Proceeding further, we would build a dynamics for all f_k that involves f_{k+1} until we arrive at a closed dynamics for $f_N=\rho$, which is simply Liouville's equation. This hierarchy of equations can indeed be derived exactly, and it is called the BBGKY hierarchy. Note that it is not very surprising that we did not end up with a problem simpler than the one we started from since everything we did so far is exact: eliminating 'useless' information will require assumptions that will need to be motivated on physical grounds.

2. A second problem of the BBGKY hierarchy is that it inherits the time-reversibility of Hamilton's equations of motion. Let us review the time-reversibility of classical mechanics.

   Time-reversal symmetry of Hamilton's equations of motion. If $\{\vec{q}_i(t),\vec{p}_i(t)\}$ are solutions of Hamilton's equations of motion, then so are $\{\vec{q}_i^{\,r}(t)\equiv\vec{q}_i(t_f-t),\vec{p}_i^{\,r}(t)\equiv-\vec{p}_i(t_f-t)\}$. Indeed, if

   $$\dot{\vec{q}}_i(t) = \frac{\partial H}{\partial \vec{p}_i} \qquad \text{and} \qquad \dot{\vec{p}}_i(t) = -\frac{\partial H}{\partial \vec{q}_i}\ , \tag{2.43}$$

   then the chain rule guarantees that

   $$\dot{\vec{q}}_i^{\,R}(t) = \frac{\mathrm{d}}{\mathrm{d}t}\vec{q}_i(t_f-t) = -\dot{\vec{q}}_i|_{t_f-t} = -\left.\frac{\partial H}{\partial \vec{p}_i}\right|_{t_f-t} = \frac{\partial H}{\partial \vec{p}_i^{\,R}} \quad \text{and} \quad \frac{\mathrm{d}}{\mathrm{d}t}\vec{p}_i^{\,R}(t) = \dot{\vec{p}}_i|_{t_f-t} = -\left.\frac{\partial H}{\partial \vec{q}_i}\right|_{t_f-t} = -\frac{\partial H}{\partial \vec{q}_i^{\,R}}\ .$$

   Time-reversal symmetry of Liouville's equation. Similarly, let us show that, if $\rho(\{\vec{q}_i,\vec{p}_i\},t)$ is a solution of Liouville's equation, then so is

   $$\rho^r(\{\vec{q}_i,\vec{p}_i\},t) \equiv \rho(\{\vec{q}_i,-\vec{p}_i\},t_f-t) = \rho(\{\vec{q}_i^{\,r},\vec{p}_i^{\,r}\},t^r)\ , \tag{2.44}$$

where we have introduced $t^r(t) \equiv t_f - t$. Using the chain rule, we find that

$$\partial_t \rho^r(\{\vec{q}_i, \vec{p}_i\}, t) = \partial_{t^r} \rho(\{\vec{q}_i^{\,r}, \vec{p}_i^{\,r}\}, t^r) \partial_t t^r \tag{2.45}$$

$$= \sum_i \frac{\partial}{\partial q_i^r} \rho(\{\vec{q}_i^{\,r}, \vec{p}_i^{\,r}\}, t^r) \cdot \frac{\partial H}{\partial p_i^r} - \frac{\partial}{\partial p_i^r} \rho(\{\vec{q}_i^{\,r}, \vec{p}_i^{\,r}\}, t^r) \cdot \frac{\partial H}{\partial q_i^r} \,, \tag{2.46}$$

where the second equality comes from applying Liouville's equation to $\rho(\{\vec{q}_i^{\,r}, \vec{p}_i^{\,r}\}, t^r)$. One then need to go back to the original variables $\vec{q}_i, \vec{p}_i, t$. To do so, we note that

$$\partial_{q_{i,\alpha}^r} \rho(\{\vec{q}_i^{\,r}, \vec{p}_i^{\,r}\}, t^r) = \partial_{q_{i,\alpha}^r} \rho^r(\{\vec{q}_i, \vec{p}_i\}, t) = \partial_{q_{i,\alpha}} \rho^r(\{\vec{q}_i, \vec{p}_i\}, t) \frac{\partial q_{i,\alpha}}{\partial q_{i,\alpha}^r} = \partial_{q_{i,\alpha}} \rho^r(\{\vec{q}_i, \vec{p}_i\}, t) \tag{2.47}$$

$$\partial_{p_{i,\alpha}^r} \rho(\{\vec{q}_i^{\,r}, \vec{p}_i^{\,r}\}, t^r) = \partial_{p_{i,\alpha}^r} \rho^r(\{\vec{q}_i, \vec{p}_i\}, t) = \partial_{p_{i,\alpha}} \rho^r(\{\vec{q}_i, \vec{p}_i\}, t) \frac{\partial p_{i,\alpha}}{\partial p_{i,\alpha}^r} = -\partial_{p_{i,\alpha}} \rho^r(\{\vec{q}_i, \vec{p}_i\}, t) \tag{2.48}$$

$$\tag{2.49}$$

Then, since $H(\{\vec{q}_i, \vec{p}_i\}) = H(\{\vec{q}_i^{\,r}, \vec{p}_i^{\,r}\})$, one finds

$$\frac{\partial H(\{\vec{q}_i^{\,r}, \vec{p}_i^{\,r}\})}{\partial_{q_{i,\alpha}^r}} = \frac{\partial H(\{\vec{q}_i, \vec{p}_i\})}{\partial_{q_{i,\alpha}^r}} = \frac{\partial H(\{\vec{q}_i, \vec{p}_i\})}{\partial_{q_{i,\alpha}}} \tag{2.50}$$

$$\frac{\partial H(\{\vec{q}_i^{\,r}, \vec{p}_i^{\,r}\})}{\partial_{p_{i,\alpha}^r}} = \frac{\partial H(\{\vec{q}_i, \vec{p}_i\})}{\partial_{p_{i,\alpha}^r}} = -\frac{\partial H(\{\vec{q}_i, \vec{p}_i\})}{\partial_{p_{i,\alpha}}} \,. \tag{2.51}$$

Together, these equations turn Eq. (2.52) into

$$\partial_t \rho^r(\{\vec{q}_i, \vec{p}_i\}, t) = -\sum_i \frac{\partial}{\partial q_i} \rho^r(\{\vec{q}_i, \vec{p}_i\}, t) \cdot \frac{\partial H}{\partial p_i} - \frac{\partial}{\partial p_i} \rho^r(\{\vec{q}_i, \vec{p}_i\}, t) \cdot \frac{\partial H}{\partial q_i} \,, \tag{2.52}$$

which shows that $\rho^r(\{\vec{q}_i, \vec{p}_i\}, t) = \rho(\{\vec{q}_i, -\vec{p}_i\}, t_f - t)$ is also a solution of the Liouville equation. The Liouville equation can thus predict the evolution from the second panel of Fig. 2.1 to the third panel as well as the reverse dynamics.

Time-reversal symmetry of BBGKY hierarchy.

Since Liouville's equation and the BBGKY hierarchy contains the same information, the same symmetry holds and if $f_k(\{\vec{q}_i, \vec{p}_i\}_{i \le k}, t)$ is a set of solutions of the hierarchy, so is $f_k^r(\{\vec{q}_i, \vec{p}_i\}_{i \le k}, t) \equiv f_k(\{\vec{q}_i, -\vec{p}_i\}_{i \le k}, t_f - t)$. Explicitly, for the one-body density, we find:

$$\partial_t f_1^r + \{f_1^r, H_1\}_{\vec{q}_i, \vec{p}_i} = -\partial_t f_1 + \{f_1, H_1\}_{\vec{q}_i^{\,r}, \vec{p}_i^{\,r}} = -\int d\vec{q}_2 d\vec{p}_2 \frac{\partial V(\vec{q}_1^{\,r} - \vec{q}_2)}{\partial q_1^r} \cdot \frac{\partial f_2(\vec{q}_1^{\,r}, \vec{p}_1^{\,r}, \vec{q}_2, \vec{p}_2, t^r)}{\partial \vec{p}_1^{\,r}} \tag{2.53}$$

where the first equality comes from the same chain rule as in the Liouville equation above and the second equality comes from the fact that $f_1(\vec{q}_1^{\,r}, \vec{p}_1^{\,r}, t_r)$ is solution to Eq. (2.42). Finally, changing variable $\vec{p}_2 \to -\vec{p}_2$, using that $\vec{q}_1^{\,r} = \vec{q}_1$, $f_2(\vec{q}_1^{\,r}, \vec{p}_1^{\,r}, \vec{q}_2, -\vec{p}_2) = f_2{}^r(\vec{q}_1, \vec{p}_1, \vec{q}_2, \vec{p}_2, t)$, and $\partial_{p_{1,\alpha}} p_{1,\alpha}^r = -1$, we get

$$\partial_t f_1^r + \{f_1^r, H_1\}_{\vec{q}_i, \vec{p}_i} = \int d\vec{q}_2 d\vec{p}_2 \frac{\partial V(\vec{q}_1 - \vec{q}_2)}{\partial q_1} \cdot \frac{\partial f_2^r(\vec{q}_1, \vec{p}_1, \vec{q}_2, \vec{p}_2, t)}{\partial \vec{p}_1} \tag{2.54}$$

Mathematically, this reversibility is due to the fact that all terms in the hierarchy include either one time derivative or one derivative with respect to a momentum variable, as can be checked in Eq. (2.42). As a result, to any solution of the BBGKY hierarchy that would describe the evolution shown in Fig. 2.1 corresponds the exact time reversed solution, and it's not clear how we can prove convergence to equilibrium—which is a time-irreversible process—in this context.

It turns out that we will solve both problems in the next section by coarse-graining our description of the system to build the Boltzmann equation. Since I will not be using higher order equation of the BBGKY hierarchy, they are not included in these notes, but an alternative route can be found in [1].

2.2 The Boltzmann Equation

2.2.1 The relevant time scales

The free evolution

We first note that, when the interaction potential vanishes, Eq. (2.42) reads

$$\partial_t f_1 + \{f_1, H_1\} = 0 \, . \tag{2.55}$$

This is a closed equation for f_1 that describes the exact evolution of the one-particle density induced by the external potential, through $\dot{\vec{p}}_i = -\partial_{\vec{q}_i} V'(\vec{q}_i)$, and by the free transport of particles, through $\dot{\vec{q}}_i = \vec{p}_i$. As shown in Fig. 1.1, this evolution plays an important role on a scale that is extrinsic to the gas: the size of the box in which the system is confined, the typical scale of the external potential that is applied to the system, etc.

Time-scales. If we consider a gas confined in a box as in Fig. 2.1, the discussion on conserved modes presented in Sec. 2.1.2 suggests that the typical relaxation time of f_1 induced by free transport will diverge with system size, $\tau_{\rm F} \sim L^z$, where z is the dynamics exponent. We can try to estimate $\tau_{\rm F}$ as follows. In the absence of interactions between the particles, we expect $z = 1$ due to the ballistic nature of particle motion: Figure 2.1 shows that the evolution of f_1 is induced by collisions between the particles and the sides of the box. For a box of linear size L, if we denote by $\bar{v}$ the typical speed the particles, we thus expect that $\tau_{\rm F}$ scales as $L/\bar{v}$.

Let us consider the case of nitrogen, whose atomic mass is $14\,\mathrm{g.Mol}^{-1}$. The weigth of a nitrogen molecule is thus $m_{N_2} = 28 \times 10^{-3}/\mathcal{N}_A \simeq 4.6 \times 10^{-26}$ kg, where $\mathcal{N}_A$ is Avogadro's number. Since each degree of freedom of our gas is expected to have a kinetic energy equal to $k_B T/2$, we find

$$\bar{v} = \sqrt{\frac{3k_B T}{m_{N_2}}} \simeq 5 \times 10^2 \mathrm{m}.s^{-1} \qquad \text{leading to} \qquad \tau_{\rm F} \sim 2 \times 10^{-3}\,\mathrm{s} \tag{2.56}$$

for a box of linear size $L = 1m$. Let us now compare this time scale with the time scales that are relevant for the interactions between particles when $V \neq 0$.

Collisions

In a dilute gas, interactions between particles are rare and sudden. As suggested by these two adjectives, there are two corresponding time scales: the duration of a collision and the time between two successive collisions.

Duration of a collision. If we denote by d the diameter of a particle, then the typical duration of a collision is of the order of

$$\tau_{\rm col} = \frac{d}{\bar{v}} \simeq 5 \times 10^{-13} s \,, \tag{2.57}$$

where we have used the tabulated value $d \simeq 0.3\,\text{nm}$ for the diameter of a nitrogen molecule[5]. While there is a spectacular scale separation between the duration of a collision and the time it takes for an atom to cross the box, $\tau_{\rm col}$ is not the *largest microscopic time scale* associated with collisions. Indeed, most of the time, there are no collisions! Another important time scale is thus the typical time one has to wait to observe a collision.

Let us consider a particle moving at speed $\bar{v}$. In a time t, it will collide with any particle that would be located in a volume $\mathcal{V}(t) = \pi d^2 \bar{v} t$. If the density of the gas is n, the typical time between collisions, called the mean-free time, is such that $n\mathcal{V}(t) \simeq 1$, so that[6]

$$\tau_{\rm mft} = \frac{1}{n\pi d^2 \bar{v}} \,. \tag{2.58}$$

For the air in a classroom, $n = P/(k_B T)$, where $P = 10^5\,\text{N.m}^{-2}$ is the atmospheric pressure and $T = 300\,\text{K}$, so that $n \simeq 2.4 \times 10^{25}\,\text{m}^{-3}$, leading to

$$\tau_{\rm mft} = \frac{k_B T}{P \pi d^2 \bar{v}} \simeq 3.10^{-10}\ \text{s} \,. \tag{2.59}$$

There are thus three well separated time scales in the problem:

$$\tau_{\rm col} \simeq 10^{-13}\,\text{s} \ll \tau_{\rm mft} \simeq 10^{-10}\,\text{s} \ll \tau_{\rm F} \simeq 10^{-3}\,\text{s} \tag{2.60}$$

that correspond to three distinct length scales

$$d \simeq 10^{-10}\,\text{m} \ll \ell_{\rm mfp} \simeq 100\,\text{nm} \ll L \sim 1\,\text{m} \,, \tag{2.61}$$

where $\ell_{\rm mfp}$ is call the mean-free path and corresponds to the average distance traveled by a particle between two collisions.

The idea of the Boltzmann equation, that we will construct in the next section, is to describe the evolution of the system over a time scale τ and a length-scale ℓ intermediate between the collision scale and the mean-free path: $\tau_{\rm col} \ll \tau \ll \tau_{\rm mft}$ and $d \ll \ell \ll \ell_{\rm mfp}$. At such scales, collisions look instantaneous since $\tau \gg d$, and they remain very rare since $\tau \ll \tau_{\rm mft}$, so that they appear as random instantaneous events that lead to very small variations of the average density f_1.

[5] We are quoting here the kinetic diameter of the nitrogen molecule, based on the likelihood of collisions between two such molecules. It differs from the estimate based on the atomic diameter, which is estimates the distance between nuclei and electrons, and is typically much smaller.

[6] Another way of estimating $\tau_{\rm mft}$ can be obtained as follows. Every $\tau_{\rm col}$, a particle explore a new volume d^3. The average number $\bar{n}$ of particles in this volume is $\bar{n} = nd^3 \ll 1$ and its distribution is Poissonian: $p(k) = \bar{n}^k e^{-\bar{n}}/(k!)$. The probability that there is a particle in this volume is $\sum_{k\geq 1} p(k) = 1 - p(0) = 1 - e^{-\bar{n}} \simeq \bar{n}$. The probability that the first collision is after n steps is then $P(n) = (1-\bar{n})^n \bar{n} \simeq \bar{n} e^{-n\bar{n}}$ so that $\langle n \rangle = 1/\bar{n}$. The time until this collision is then $\tau_{\rm col}/\bar{n} = k_B T/(d^2 P \bar{v})$—where P is now the pressure—which is consistent with Eq. (2.58) up to the geometric factor π.

2.2.2 The coarse-graining

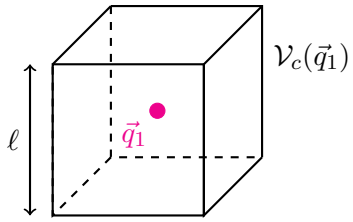
We now want to start from the time evolution of f_1 given in Eq. (2.42):

$$\partial_t f_1 + \{f_1, H_1\} = \int \mathrm{d}\Gamma_2 \frac{\partial V(\vec{q}_1 - \vec{q}_2)}{\partial \vec{q}_1} \cdot \frac{\partial f_2(\vec{q}_1, \vec{p}_1, \vec{q}_2, \vec{p}_2)}{\partial \vec{p}_1} \,, \tag{2.62}$$

and to coarse-grain it over a time $\tau_{\rm col} \ll \tau \ll \tau_{\rm mft}$ and a length $d \ll \ell \ll \ell_{\rm mfp}$.

2.2.2.1 The spatial coarse-graining

To build our coarse-grained description of the dynamics, we introduced $\tilde{f}_1(\vec{q}_1, \vec{p}_1, t)$, the average number density of particles with momentum $\vec{p}_1$ whose positions lie within a volume $\mathcal{V}_c(\vec{q}_1)$ around $\vec{q}_1$:



$$\tilde{f}_1(\vec{q}_1, \vec{p}_1, t) \equiv \frac{1}{|\mathcal{V}_c|} \int_{\mathcal{V}_c(\vec{q}_1)} \mathrm{d}^3\vec{q}_1{}' \; f_1(\vec{q}_1{}', \vec{p}_1, t) \,, \tag{2.63}$$

where $|\mathcal{V}_c| = \ell^3$ is the volume enclosed in $\mathcal{V}_c(\vec{q}_1)$. In Eq. (2.25), $f_1(\vec{q}_1, \vec{p}_1, t)$ is defined as the statistical average of a distribution that localizes particles exactly at $\vec{q}_1, \vec{p}_1$. Instead, $\tilde{f}_1$ measures the average density of particles around $\vec{q}_1$ over a scale ℓ much larger than the particle size d. Let us now show how to construct the time evolution of $\tilde{f}_1$ starting from Eq. (2.62).

Comment: Equation (2.63) can be seen as applying a top-hat filter to f_1. Defining $K(\vec{u}) = \frac{1}{|\mathcal{V}_c|}$ if $\vec{u}$ is in a box centered at $\vec{0}$ of volume $\mathcal{V}_c$ and $K(\vec{u}) = 0$ otherwise, we see that $\tilde{f}_1(\vec{q}_1, \vec{p}_1, t) = f * K(\vec{q}_1, \vec{p}_1, t)$, where $f * g(\vec{r}) = \int \mathrm{d}^3\vec{r}\,' f(\vec{r}\,') g(\vec{r} - \vec{r}\,')$ is the convolution between f and g. The signal contained in f_1 can be very noisy since it measures with infinite precision the positions of the particles. Instead, $\tilde{f}_1$ will have smoother variations.

Time evolution of $\tilde{f}_1$: Integrating Eq. (2.62) over $\vec{q}_1$ and dividing by $|\mathcal{V}_c|$, we get

$$\begin{aligned} \frac{1}{|\mathcal{V}_c|} \int_{\mathcal{V}_c(\vec{q}_1)} \mathrm{d}^3\vec{q}_1{}' \partial_t f_1(\vec{q}_1{}', \vec{p}_1, t) = & -\frac{1}{|\mathcal{V}_c|} \int_{\mathcal{V}_c(\vec{q}_1)} \mathrm{d}^3\vec{q}_1{}' \{f_1, H_1\} \\ & + \frac{1}{|\mathcal{V}_c|} \int_{\mathcal{V}_c(\vec{q}_1)} \mathrm{d}^3\vec{q}_1{}' \int \mathrm{d}\Gamma_2 \frac{\partial V(\vec{q}_1{}' - \vec{q}_2)}{\partial \vec{q}_1} \cdot \frac{\partial}{\partial \vec{p}_1} f_2(\vec{q}_1{}', \vec{p}_1, \vec{q}_2, \vec{p}_2, t) \end{aligned} \tag{2.64}$$

We first note that the volume $\mathcal{V}_c(\vec{q}_1)$ does not evolve in time so that

$$\frac{1}{|\mathcal{V}_c|} \int_{\mathcal{V}_c(\vec{q}_1)} \mathrm{d}^3\vec{q}_1{}' \partial_t f_1(\vec{q}_1{}', \vec{p}_1, t) = \partial_t \Big[\frac{1}{|\mathcal{V}_c|} \int_{\mathcal{V}_c(\vec{q}_1)} \mathrm{d}^3\vec{q}_1{}' f_1(\vec{q}_1{}', \vec{p}_1, t) \Big] = \partial_t \hat{f}_1(\vec{q}_1{}', \vec{p}_1, t) \,. \tag{2.65}$$

We now turn to analyze separately the impact of the free evolution, corresponding to the ochre term in Eq. (2.64) and the evolution induced by collisions, which corresponds to the magenta term in Eq. (2.64).

The free evolution. Since H_1 does not induce any notable evolution of the scale ℓ, we expect that $\tilde{f}_1$ has the same free evolution as f_1 so Eq. (2.64) should lead to

$$\partial_t \hat{f}_1 + \{\hat{f}_1, H_1\} = [\text{collision term}] \equiv \left. \frac{\partial \hat{f}_1}{\partial t} \right|_{\rm col} \,, \tag{2.66}$$

where we have introduced the notation $\left.\frac{\partial \hat{f}_1}{\partial t}\right|_{\rm col}$ to refer to the time-evolution of $\hat{f}_1$ that is solely due to collisions. Let us show that the ochre term in Eq. (2.64) indeed leads to the left-hand side of Eq. (2.66).

First, we note that $H_1(\vec{q_1}', \vec{p}_1)$ barely varies in $\mathcal{V}_c(\vec{q}_1)$ so that $H_1(\vec{q_1}', \vec{p}_1) \simeq H_1(\vec{q}_1, \vec{p}_1)$. Consequently,

$$\frac{1}{|\mathcal{V}_c|}\int_{\mathcal{V}_c(\vec{q}_1)} \mathrm{d}^3\vec{q_1}' \frac{\partial H_1(\vec{q_1}', \vec{p}_1)}{\partial \vec{q}_1}\cdot\frac{\partial}{\partial \vec{p}_1} f_1(\vec{q_1}', \vec{p}_1, t) \simeq \frac{\partial H_1(\vec{q}_1, \vec{p}_1)}{\partial \vec{q}_1}\cdot\frac{\partial}{\partial \vec{p}_1}\frac{1}{|\mathcal{V}_c|}\int_{\mathcal{V}_c(\vec{q}_1)} \mathrm{d}^3\vec{q_1}' f_1(\vec{q_1}', \vec{p}_1, t) = \frac{\partial H_1(\vec{q}_1, \vec{p}_1)}{\partial \vec{q}_1}\cdot\frac{\partial \hat{f}_1}{\partial \vec{p}_1}\,, \tag{2.67}$$

where $\frac{\partial H_1(\vec{q_1}', \vec{p}_1)}{\partial \vec{q}_1}$ is a shorter notation for $\left.\frac{\partial H_1(\vec{q}, \vec{p})}{\partial \vec{q}}\right|_{\vec{q_1}', \vec{p}_1}$. Similarly, we can write

$$\frac{1}{|\mathcal{V}_c|}\int_{\mathcal{V}_c(\vec{q}_1)} \mathrm{d}^3\vec{q_1}' \frac{\partial H_1(\vec{q_1}', \vec{p}_1)}{\partial \vec{p}_1}\cdot\frac{\partial}{\partial \vec{q}_1} f_1(\vec{q_1}', \vec{p}_1, t) = \frac{\partial H_1(\vec{q}_1, \vec{p}_1)}{\partial \vec{p}_1}\cdot\frac{1}{|\mathcal{V}_c|}\int_{\mathcal{V}_c(\vec{q}_1)} \mathrm{d}^3\vec{q_1}' \frac{\partial}{\partial \vec{q}_1} f_1(\vec{q_1}', \vec{p}_1, t) \tag{2.68}$$

$$= \frac{\partial H_1(\vec{q}_1, \vec{p}_1)}{\partial \vec{p}_1}\cdot\frac{\partial}{\partial \vec{q}_1}\hat{f}_1(\vec{q}_1, \vec{p}_1, t)\,, \tag{2.69}$$

where the last equality comes from the fact that, by linearity, the average of the gradient is the gradient of the average.

[Proof: To verify this last statement, consider a function $F(\vec{r}) = \frac{1}{|V|}\int_{V(\vec{r})} \mathrm{d}^3\vec{r}' f(\vec{r}')$. For any infinitesimal vector $\mathrm{d}\vec{\ell}$, $F(\vec{r}+\mathrm{d}\vec{\ell}) - F(\vec{r}) = \mathrm{d}\vec{\ell}\cdot\nabla F(\vec{r})$. Using the explicit definition of F, this also reads

$$F(\vec{r}+\mathrm{d}\vec{\ell}) - F(\vec{r}) = \frac{1}{|V|}\int_{V(\vec{r}+\mathrm{d}\vec{\ell})} \mathrm{d}^3\vec{r}' f(\vec{r}') - \frac{1}{|V|}\int_{V(\vec{r})} \mathrm{d}^3\vec{r}' f(\vec{r}') \tag{2.70}$$

$$= \frac{1}{|V|}\int_{V(\vec{r})} \mathrm{d}^3\vec{r}' [f(\vec{r}'+\mathrm{d}\vec{\ell}) - f(\vec{r}')]\,, \tag{2.71}$$

where we have changed variable $\vec{r}' \to \vec{r}' + \mathrm{d}\vec{\ell}$ in the first integral to go from the first line to the second line. Using the definition of the gradient, $f(\vec{r}'+\mathrm{d}\vec{\ell}) - f(\vec{r}') = \mathrm{d}\vec{\ell}\cdot\nabla f(\vec{r}')$, and we thus get

$$F(\vec{r}+\mathrm{d}\vec{\ell}) - F(\vec{r}) = \frac{1}{|V|}\int_{V(\vec{r})} \mathrm{d}^3\vec{r}' [\mathrm{d}\vec{\ell}\cdot\nabla f(\vec{r}')] = \mathrm{d}\vec{\ell}\cdot\frac{1}{|V|}\int_{V(\vec{r})} \mathrm{d}^3\vec{r}' [\nabla f(\vec{r}')]\,. \tag{2.72}$$

We thus get that

$$\nabla F(\vec{r}) = \frac{1}{|V|}\int_{V(\vec{r})} \mathrm{d}^3\vec{r}' [\nabla f(\vec{r}')]\,, \tag{2.73}$$

which we what we used to go from Eq. (2.68) to (2.69).]

All in all, Eqs (2.67) and (2.69) thus show that

$$\partial_t f_1 + \{f_1, H_1\} \xrightarrow{\frac{1}{|\mathcal{V}_c|}\int_{\mathcal{V}_c(\vec{q}_1)}} \partial_t \tilde{f}_1 + \{\tilde{f}_1, H_1\}\,. \tag{2.74}$$

Let us now turn to the collision term.

The collision term. We now want to derive a closed expression for the collision term

$$\left.\frac{\partial \hat{f}_1}{\partial t}\right|_{\rm col} \equiv \frac{1}{|\mathcal{V}_c|}\int_{\mathcal{V}_c(\vec{q}_1)} \mathrm{d}^3\vec{q_1}' \int \mathrm{d}\Gamma_2 \frac{\partial V(\vec{q_1}' - \vec{q}_2)}{\partial \vec{q}_1}\cdot\frac{\partial}{\partial \vec{p}_1} f_2(\vec{q_1}', \vec{p}_1, \vec{q}_2, \vec{p}_2, t)\,. \tag{2.75}$$

This rather complex expression measures the rate of change of the phase-space density, averaged over the volume $\mathcal{V}_c(\vec{q}_1)$, due to collisions between particles. At this stage, it is not clear why this should be simple! Let us now show that coarse-graining over time will help.

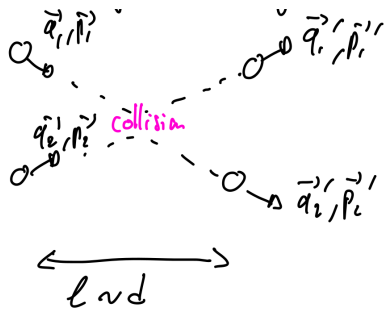


Figure 2.4: *Collisions happen over a scale $\sim d$ and last a time $\sim \tau_{\rm col}$. They lead to significant momentum changes $(\vec{p}_1, \vec{p}_2) \to (\vec{p}_1{}', \vec{p}_2{}')$. They are, however, quite rare for times $t \sim \tau_{\rm col}$ and they only induce significant changes in the average number of particles in $\mathcal{V}_c$ with momenta $\vec{p}_1$ over times $t \sim \tau_{\rm mft}$, when many collisions happen.*

2.2.2.2 The temporal coarse-graining

Before we proceed, let us analyze how $\hat{f}_1$ evolves on the different time scales that are relevant to the problem.

- As depicted in Fig. 2.4, the particle momenta change significantly during a collision, leading to an important evolution of the probability of finding a particle with a given momentum. One could thus think that $\tau_{\rm col}$ is the natural time scale of evolution for $\hat{f}_1$. However, collisions are extremely rare on this time scale so that the evolution of the *average* number of particles with a given momentum is completely negligible for $t \sim \tau_{\rm col}$. We also note that taking into account the impact of a collision on $\hat{f}_1$ on this time scale would be quite difficult since it requires resolving the evolution of momenta *during* a collision. The way to do so depend on all the detail of the interaction potential V and leads to a system-dependent description that will be difficult to generalize. This is thus not the scale at which we should try to analyze Eq. (2.75).

- On times $t \sim \tau_{\rm mft}$, there is a significant number of collisions, which collectively induce an $\mathcal{O}(1)$ evolution of $\hat{f}_1$. This suggest a scaling form

$$\hat{f}_1(\vec{q}_1, \vec{p}_1, t) = g(\vec{q}_1, \vec{p}_1, \tilde{t} = t/\tau_{\rm mft}) \qquad \text{with} \qquad \partial_{\tilde{t}}^n g(\vec{q}_1, \vec{p}_1, \tilde{t}) \simeq \mathcal{O}(1) \; . \tag{2.76}$$

  This is a mathematical scaling form which encodes the fact that the typical time scale over which $\hat{f}_1$ varies is $\tau_{\rm mft}$. However, having to handle multiple collisions makes it hard to model the time evolution of $\hat{f}_1$ directly on a time scale $t \sim \tau_{\rm mft}$.

- We will thus try to construct the time evolution of $\hat{f}_1$ on time τ such that $\tau_{\rm col} \ll \tau \ll \tau_{\rm mft}$. On such a time scale, collisions are rare so they induce small changes to $\hat{f}_1$ and they are sudden so that we can simply compare incoming and outgoing momenta to assess the changes in $\hat{f}_1$ induced by a collision, without having to resolve the collision itself.

Let us thus integrate the dynamics of $\hat{f}_1$ between t and $t + \tau$.

Free transport.

- Since H_1 is time-independent,

$$\int_t^{t+\tau} ds\{H_1, \hat{f}_1\} = \{H_1, \int_t^{t+\tau} ds\hat{f}_1(s)\} \,, \tag{2.77}$$

where we omit the dependency of $\hat{f}_1$ on $\vec{q}$ and $\vec{p}$ for clarity. Then, since $\hat{f}_1$ barely evolves over a time τ, $\int_t^{t+\tau} ds\hat{f}_1(s) \sim \tau\hat{f}_1(t)$.
Proof:

$$\hat{f}_1(\vec{q},\vec{p},s) = g(\vec{q},\vec{p},s/\tau_{\rm mft}) \simeq g(\vec{q},\vec{p},t/\tau_{\rm mft}) + \frac{s-t}{\tau_{\rm mft}}\partial_{\tilde{t}}g(\vec{q},\vec{p},t/\tau_{\rm mft}) + \frac{(s-t)^2}{2\tau_{\rm mft}^2}\partial_{\tilde{t}}^2 g(\vec{q},\vec{p},t/\tau_{\rm mft}) \,. \tag{2.78}$$

Integrating over s then leads to

$$\int_t^{t+\tau} ds\hat{f}_1 = \tau g + \frac{\tau^2}{2\tau_{\rm mft}}\partial_{\tilde{t}}g \simeq \tau\hat{f}_1[1+\mathcal{O}(\tau/\tau_{\rm mft})] \,. \tag{2.79}$$

Free transport thus integrates as:

$$\int_t^{t+\tau} ds\{H_1, \hat{f}_1(s)\} \simeq \tau\{H_1, \hat{f}_1(t)\} \,. \tag{2.80}$$

- Similarly, since $\hat{f}_1$ barely evolves during τ, so does $\partial_t\hat{f}_1$ and

$$\int_t^{t+\tau} ds\partial_s\hat{f}_1(s) = \hat{f}_1(t+\tau) - \hat{f}_1(\tau) \simeq \tau\partial_t\hat{f}_1(t) \,. \tag{2.81}$$

Proof: taking the derivative of Eq. (2.78) with respect to s and integrating over s, one gets

$$\int_t^{t+\tau} ds\partial_s\hat{f}_1(\vec{q},\vec{p},s) = \int_t^{t+\tau}\Big[\frac{1}{\tau_{\rm mft}}\partial_{\tilde{t}}g(\vec{q},\vec{p},t/\tau_{\rm mft}) + \frac{(s-t)}{\tau_{\rm mft}^2}\partial_{\tilde{t}}^2 g(\vec{q},\vec{p},t/\tau_{\rm mft})\Big]ds \,. \tag{2.82}$$

$$= \frac{\tau}{\tau_{\rm mft}}\partial_{\tilde{t}}g(\vec{q},\vec{p},t/\tau_{\rm mft}) + \frac{\tau^2}{2\tau_{\rm mft}^2}\partial_{\tilde{t}}^2 g(\vec{q},\vec{p},t/\tau_{\rm mft}) \tag{2.83}$$

$$= \tau\partial_t\hat{f}_1(\vec{q},\vec{p},t)[1+\mathcal{O}(\tau/\tau_{\rm mft})] \,, \tag{2.84}$$

where we used the chaine rule to get $\partial_t\hat{f}_1(\vec{q},\vec{p},t) = \frac{1}{\tau_{\rm mft}}\partial_{\tilde{t}}g(\vec{q},\vec{p},t/\tau_{\rm mft})$.

So far, we have thus shown that integrating the free evolution over a space $\mathcal{V}_c$ and a time τ coarse-grains transparently according to:

$$\partial_t f_1 + \{f_1, H_1\} \xrightarrow[H_1 \text{ constant over } \mathcal{V}_c]{\frac{1}{|\mathcal{V}_c|}\int d\vec{q}} \partial_t\hat{f}_1 + \{\hat{f}_1, H_1\} \xrightarrow[\hat{f}_1 \text{ constant over } \tau]{\int_t^{t+\tau}} \tau[\partial_t\hat{f}_1 + \{\hat{f}_1, H_1\}]$$

We now need to do this coarse-graining for the collision term. Because reasoning with densities is always more cumbersome than counting numbers, let us introduce the phase-space volume

$$d\Gamma(\vec{q},\vec{p}) = \mathcal{V}_c(\vec{q}) \quad \times \prod_{\alpha=x,y,z}[p_\alpha, p_\alpha + dp_\alpha] \,, \tag{2.85}$$

so that the average number of particles in $d\Gamma(\vec{q},\vec{p})$ at time t is $N(\vec{q},\vec{p},t)=\hat{f}_1(\vec{q},\vec{p},t)d\Gamma(\vec{q},\vec{p})$. Our coarse-graining has established that $N(\vec{q}_1,\vec{p}_1)$ varies between t and $t+\tau$ by an amount:

$$\delta N(\vec{q}_1,\vec{p}_1,t,t+\tau) = [\hat{f}_1(\vec{q}_1,\vec{p}_1,t+\tau)-\hat{f}_1(\vec{q}_1,\vec{p}_1,\tau)]d\Gamma(\vec{q}_1,\vec{p}_1) \tag{2.86}$$

$$\simeq \tau\partial_t\hat{f}_1(\vec{q}_1,\vec{p}_1,t)d\Gamma(\vec{q}_1,\vec{p}_1) \tag{2.87}$$

$$= \tau\{\hat{f}_1,H_1\}d\Gamma(\vec{q}_1,\vec{p}_1) + \underbrace{\int_t^{t+\tau}\left.\frac{\partial\hat{f}_1}{\partial s}\right|_{\rm col} d\Gamma(\vec{q}_1,\vec{p}_1)}_{\delta N(\vec{q}_1,\vec{p}_1,t,t+\tau)|_{\rm col}}, \tag{2.88}$$

where the collision term is given by Eq. (2.75). While the final term in Eq. (2.88) has a complex mathematical form, it has a simple physical interpretation: it measure the average change $\delta N|_{\rm col}$ in the number of particles in the phase-space volume $d\Gamma(\vec{q}_1,\vec{p}_1)$ during a time τ due to the rare collisions that happen in that time window. This variation occurs because, on average, N^+ particles in $d\Gamma$ see their momenta evolve from $\vec{p}_1{}'$ to $\vec{p}_1$ due to collisions, while N^- particles see their momenta evolve from $\vec{p}_1$ to $\vec{p}_1{}'$, leading to:

$$\delta N(\vec{p}_1,\vec{q}_1,t,t+\tau)|_{\rm col} = N^+(\vec{p}_1,\vec{q}_1,t,t+\tau) - N^-(\vec{p}_1,\vec{q}_1,t,t+\tau)\,. \tag{2.89}$$

Let us now try to compute $N^+(\vec{p}_1,\vec{q}_1,t,t+\tau)$ and $N^-(\vec{p}_1,\vec{q}_1,t+\tau)$.

Loss and gain terms.

Dilute gas. We first note that we are working in the dilute gas limit, where $d^3n\ll 1$. In this limit, the number of collisions involving 3 particles scale as $(d^3n)^3$ which is much smaller than the number of binary collisions, which scales as $(d^3n)^2$. We can thus safely neglect the influence of collisions involving more than 2 particles when determining the leading-order impact of collisions on $\hat{f}_1$.

Locality. Since $\ell\gg d$, most collisions happen in the bulk of the volume $\mathcal{V}_c$ and two particles collide only if both were in the same volume $\mathcal{V}_c$. N^+ and N^- can then be determined as follow:

- $N^+(\vec{q}_1,\vec{p}_1,t,t+\tau)$ is the average number of collisions between two particles in $\mathcal{V}_c(\vec{q}_1)$ whose momenta evolve from $\vec{p}_1{}'$ and $\vec{p}_2{}'$ to $\vec{p}_1$ and $\vec{p}_2$. This is a *gain* term that leads to an increase in $\hat{f}_1$.
- $N^-(\vec{q}_1,\vec{p}_1,t,t+\tau)$ is the average number of collisions between two particles in $\mathcal{V}_c(\vec{q}_1)$ whose momenta evolve from $\vec{p}_1$ and $\vec{p}_2$ to $\vec{p}_1{}'$ and $\vec{p}_2{}'$. This is a *loss* term that leads to a decrease in $\hat{f}_1$.

The collisions $\vec{p}_1,\vec{p}_2\to\vec{p}_1{}',\vec{p}_2{}'$ are often refered to as scattering events.

Determination of $N^-(\vec{p}_1,\vec{q}_1,t,t+\tau)$.

To compute N^-, we need to determine the average number of binary collisions that lead to particle transitioning from $\vec{p}_1$ to $\vec{p}_1{}'$. For this to happen, we need a second particle in $\mathcal{V}_c(\vec{q}_1)$ with (any) momentum $\vec{p}_2$ to collide with the first one such that $\vec{p}_1,\vec{p}_2\to\vec{p}_1{}',\vec{p}_2{}'$. The average number density of such pairs of particles is [7] $\hat{f}_2(\vec{q}_1,\vec{p}_1,\vec{q}_1,\vec{p}_2)$, where

$$\hat{f}_2(\vec{q}_1,\vec{p}_1,\vec{q}_2,\vec{p}_2) = \frac{1}{\mathcal{V}_c^2}\int_{\mathcal{V}_c(\vec{q}_1)} d\vec{q}_1{}'\int_{\mathcal{V}_c(\vec{q}_2)} d\vec{q}_2{}' f_2(\vec{q}_1{}',\vec{p}_1,\vec{q}_2{}',\vec{p}_2)\,. \tag{2.90}$$

[7] We note that we are studying the fate of particle 1, so that the two particles play a very different role in our derivation. The total integral of f_2 over the full phase space is $N(N-1)$, and not $N(N_1)/2$, as one would expect if the two particles were indistinguishable in our derivation and we were simply counting the number of pairs.

Molecular chaos approximation. To make progress, we note that two particles that are present in the same volume $\mathcal{V}_c$ and are about to collide are very unlikely to have collided recently, so that we can assume that they are statistically independent, leading to:

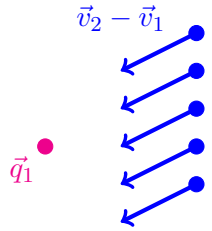
$$\hat{f}_2(\vec{q}_1,\vec{p}_1,\vec{q}_1,\vec{p}_2) = \hat{f}_1(\vec{q}_1,\vec{p}_1)\hat{f}_1(\vec{q}_1,\vec{p}_2)\ . \tag{2.91}$$

We can thus consider separately the number of particles with momentum $\vec{p}_1$, given by $\hat{f}_1(\vec{q}_1,\vec{p}_1,t)\mathrm{d}\Gamma(\vec{q}_1,\vec{p}_1)$, and the number of particles with momentum $\vec{p}_2$ which are going to collision with them during a time τ.

We first note that the total number of collisions can be written as

$$N^-(\vec{p}_1,\vec{q}_1,t,t+\tau) = \underbrace{\hat{f}_1(\vec{q}_1,\vec{p}_1,t)\,\mathcal{V}_c\,d^3\vec{p}_1}_{\text{Numb. of part. with momentum } \vec{p}_1} \times\tau\times R^-(\vec{p}_1)\ , \tag{2.92}$$

where $R^-(\vec{p}_1)$ is the rate of collision[8] for a particle with momentum $\vec{p}_1$. Then, in the frame of reference of particle 1, we note that particles 2 are incoming at speed $|\vec{v}_2-\vec{v}_1|$. Particle 1 is thus facing an incoming flux of particles $I(\vec{p}_2)=|\vec{v}_2-\vec{v}_1|\hat{f}_1(\vec{q}_1,\vec{p}_2,t)$, leading to



$$R^-(\vec{p}_1) = \int d^2\vec{p}_2|\vec{v}_2-\vec{v}_1|\hat{f}_2(\vec{q}_1,\vec{p}_2,t)[\dots]\ . \tag{2.93}$$

and we are left with characterising the bracket $[\dots]$.

Cross section. Dimensional analysis tells us that $[\mathrm{R}]=\mathrm{T}^{-1}$ while $[d^2\vec{p}_2|\vec{v}_2-\vec{v}_1|\hat{f}_2(\vec{q}_1,\vec{p}_2,t)]=\mathrm{L}^{-2}\mathrm{T}^{-1}$. The magenta term in bracket in Eq. (2.93) is thus an area that tells us, given an incoming flux of particles, what fraction will actually collide with particle 1. This term is called the cross section. All in all, we get

$$N^-(\vec{p}_1,\vec{q}_1,t,t+\tau) = \hat{f}_1(\vec{q}_1,\vec{p}_1,t)\,\mathcal{V}_c\,d^3\vec{p}_1\tau\int d^2\vec{p}_2|\vec{v}_2-\vec{v}_1|\hat{f}_1(\vec{q}_1,\vec{p}_2,t)\sigma(\vec{p}_1,\vec{p}_2)\ . \tag{2.94}$$

Note that, at this stage, σ is system dependent: its value depends on the particular choice of the interaction potential $V(\vec{q})$. If particles are hard spheres of diameter d, simple geometric considerations illustrated in Fig. 2.5 tell us that $\sigma=\pi d^2$, which is independent of $\vec{p}_1$ and $\vec{p}_2$. In the presence of attractive interactions, $\sigma(\vec{p}_1,\vec{p}_2)>\pi d^2$ since a larger fraction of the beam will collide with particle 1.

As we shall see below, we do not need to compute explicitly the value of σ to establish the relaxation to equilibrium, but we will need to analyze its symmetry properties. To do so, we first note that all the particles with momentum $\vec{p}_2$ in Fig. 2.5 that collide with particles 1 do not lead to the same pairs of momenta $\vec{p}_1{}',\vec{p}_2{}'$ after the collisions. To elucidate the properties of σ, we need to characterize the possible values $\vec{p}_1{}',\vec{p}_2{}'$ of the outgoing momenta and to study particle collisions in more detail.

Particle collisions: Momentum conservation requires that the total momentum of particles 1 and 2 before and after collisions are equal, so that the momentum of the center of mass, p_{cm}, is a collisional invariant:

$$\vec{p}_1+\vec{p}_2\equiv 2\vec{p}_{\mathrm{cm}}=\vec{p}_1{}'+\vec{p}_2{}'\equiv 2\vec{p}_{\mathrm{cm}}{}'\ . \tag{2.95}$$

[8] i.e. the number of collisions per unit of time

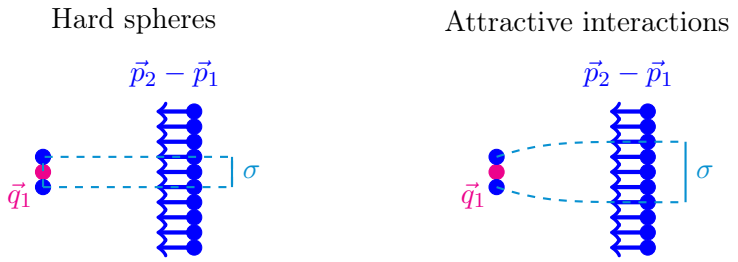


Figure 2.5: *Sketch of the cross section for a deterministic, classical dynamics. For hard spheres, whose sole interactions are an infinite repulsion at contact, collisions happen as long the shortest distance between the particles is smaller than their diameter d, leading to $\sigma = \pi d^2$. Attractive interactions will make a larger fraction of the incoming flux of particles collide with particle 1, so that $\sigma > \pi d^2$.*

Another important conservation law is that of energy: during a collision, part of the kinetic energy of the incoming particles is transformed into potential interaction energy, stored in $V(\vec{q}_1 - \vec{q}_2)$, but, after the collision, this energy is back in the form of kinetic energy, so that the sum of the particle energies are also a collisional invariant. (Since the external potential do not vary over the scale ℓ, the corresponding energy remains constant throughout the collision.) Conservation of energy thus leads to

$$K \equiv \frac{\vec{p}_1{}^2}{2m} + \frac{\vec{p}_2{}^2}{2m} = \frac{1}{4m}[(\vec{p}_1 + \vec{p}_2)^2 + (\vec{p}_1 - \vec{p}_2)^2] = \frac{1}{m}(\vec{p}_{\rm cm}{}^2 + \vec{p}_{\rm d}{}^2) \quad \text{with} \quad \vec{p}_{\rm d} \equiv \frac{1}{2}(\vec{p}_1 - \vec{p}_2)\ . \tag{2.96}$$

Since K and $\vec{p}_{\rm cm}$ are conserved by the collision, so is $\vec{p}_{\rm d}{}^2$ and we thus have $|\vec{p}_{\rm d}| = |\vec{p}_{\rm d}{}'|$. The collision thus amounts to a rotation of $\vec{p}_{\rm d}$ into $\vec{p}_{\rm d}{}' = {\rm Rot}(\theta,\varphi)\cdot p_{\rm d}$, where ${\rm Rot}(\theta,\varphi)$ is a rotation matrix that is uniquely characterized by two Euler angle θ, φ. The outgoing vectors $\vec{p}_1{}', \vec{p}_2{}'$ are thus also characterized by the values of θ and φ. The total cross section can thus be decomposed as

$$\sigma(\vec{p}_1, \vec{p}_2) = \int {\rm d}\Omega \frac{{\rm d}\sigma(\vec{p}_1, \vec{p}_2, \theta, \varphi)}{{\rm d}\Omega}\ , \tag{2.97}$$

where $\frac{{\rm d}\sigma}{{\rm d}\Omega}$ is called the differential cross section, which measures the fraction of the incoming flux of particles that result in $\vec{p}_{\rm d}$ being scattered into $\vec{p}_{\rm d}{}'(\theta,\varphi)$. For clarity, we often write

$${\rm d}\Omega \frac{{\rm d}\sigma(\vec{p}_1, \vec{p}_2, \theta, \varphi)}{{\rm d}\Omega} \equiv {\rm d}^2\sigma(\vec{p}_1, \vec{p}_2 \to \vec{p}_1{}', \vec{p}_2{}')\ , \tag{2.98}$$

which will allow us to identify more easily the symmetries of the scattering process.

All in all, N^- can thus be written as

$$N^-(\vec{p}_1, \vec{q}_1, t, t+\tau) = \tau \mathcal{V}_c\, d^3\vec{p}_1 \int d^2\vec{p}_2 d^2\sigma(\vec{p}_1, \vec{p}_2 \to \vec{p}_1{}', \vec{p}_2{}')|\vec{v}_2 - \vec{v}_1| \hat{f}_1(\vec{q}_1, \vec{p}_1, t)\hat{f}_1(\vec{q}_1, \vec{p}_2, t)\ . \tag{2.99}$$

Note that another way to understand Eq. (2.99) is to think at $\mathcal{V}_c {\rm d}^3\vec{p}_1 f_1$ as the number of target particles with momentum $\vec{p}_1$ and at ${\rm d}^3\vec{p}_2 {\rm d}^2\sigma|\vec{v}_2 - \vec{v}_1|\tau f_2$ at the number of particles that collide with them. ${\rm d}^2\sigma|\vec{v}_2 - \vec{v}_1|\tau$ can indeed be thought at the volume occupied by the particles that collide with particle 1 during a time τ.

Determination of $N^+(\vec{p}_1, \vec{q}_1, t, t+\tau)$. Let us now show how the computation of N^- detailed above allows us to infer the expression of $N^+(\vec{p}_1, \vec{q}_1, t, t+\tau)$ using symmetry considerations. First, we note that

$N^-(\vec{p}_1,\vec{q}_1) = \int dN(\vec{p}_1,\vec{p}_2 \to \vec{p}_1{}',\vec{p}_2{}')$, where

$$dN(\vec{p}_1,\vec{p}_2 \to \vec{p}_1{}',\vec{p}_2{}') = \mathcal{V}_c d^3\vec{p}_1 d^3\vec{p}_2 \tau d^2\sigma(\vec{p}_1,\vec{p}_2 \to \vec{p}_1{}',\vec{p}_2{}')|\vec{v}_2 - \vec{v}_1|\hat{f}_1(\vec{q}_1,\vec{p}_1,t)\hat{f}_1(\vec{q}_1,\vec{p}_2,t) \tag{2.100}$$

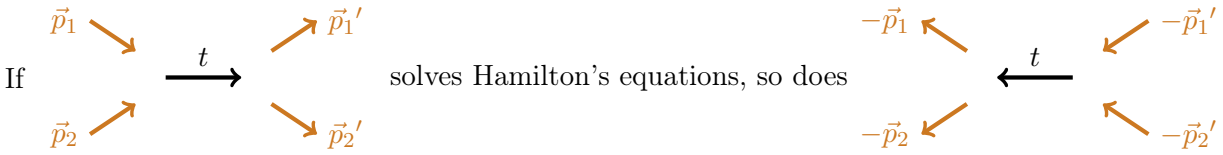
is the number of collisions that take $\vec{p}_1,\vec{p}_2$ to $\vec{p}_1{}',\vec{p}_2{}'$. Similarly, we can define

$$dN^+ = dN(\vec{p}_1{}',\vec{p}_2{}' \to \vec{p}_1,\vec{p}_2) \tag{2.101}$$

$$= \mathcal{V}_c d^3\vec{p}_1{}' d^3\vec{p}_2{}' \tau d^2\sigma(\vec{p}_1{}',\vec{p}_2{}' \to \vec{p}_1,\vec{p}_2)|\vec{v}_2{}' - \vec{v}_1{}'|\hat{f}_1(\vec{q}_1,\vec{p}_1{}',t)\hat{f}_1(\vec{q}_1,\vec{p}_2{}',t)\ . \tag{2.102}$$

Let us now show that this expression can be brought to a form much closer to that of N^-.

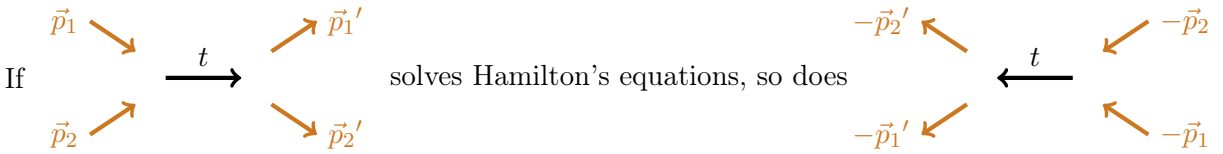
Let us start by analyzing the cross section entering Eq. (2.102). Classical mechanics satisfies time-reversal symmetry, so that:



Consequently, the cross sections of these two scattering events are the same:

$$\sigma(\vec{p}_1,\vec{p}_2 \to \vec{p}_1{}',\vec{p}_2{}') = \sigma(-\vec{p}_1{}',-\vec{p}_2{}' \to -\vec{p}_1,-\vec{p}_2)\ . \tag{2.103}$$

Furthermore, the system is isotropic and thus satisfies parity symmetry. Rotating everything by an angle π in the plane $\vec{p}_1{}',\vec{p}_2{}'$ shows that:



Consequently, the cross sections also satisfies:

$$\sigma(\vec{p}_1,\vec{p}_2 \to \vec{p}_1{}',\vec{p}_2{}') = \sigma(-\vec{p}_1,-\vec{p}_2 \to -\vec{p}_1{}',-\vec{p}_2{}')\ . \tag{2.104}$$

Using Eqs. (2.104) and then (2.103) leads to

$$\sigma(\vec{p}_1,\vec{p}_2 \to \vec{p}_1{}',\vec{p}_2{}') = \sigma(-\vec{p}_1,-\vec{p}_2 \to -\vec{p}_1{}',-\vec{p}_2{}') = \sigma(\vec{p}_1{}',\vec{p}_2{}' \to \vec{p}_1,\vec{p}_2)\ . \tag{2.105}$$

Backward and forward scattering thus have the same cross sections.

Since collisions are rotations of $\vec{p}_\mathrm{d}$, we also have that

$$|\vec{v}_1 - \vec{v}_2| = |\vec{v}_1{}' - \vec{v}_2{}'|\ . \tag{2.106}$$

Furthermore, using that $\vec{p}_1 = \vec{p}_\mathrm{cm} + \vec{p}_\mathrm{d}$ and $\vec{p}_2 = \vec{p}_\mathrm{cm} - \vec{p}_\mathrm{d}$ leads to[9]

$$\mathrm{d}\vec{p}_1\mathrm{d}\vec{p}_2 = K\mathrm{d}\vec{p}_\mathrm{cm}\mathrm{d}\vec{p}_\mathrm{d} = K\mathrm{d}\vec{p}_\mathrm{cm}{}'\mathrm{d}\vec{p}_\mathrm{d}{}' = \mathrm{d}\vec{p}_1{}'\mathrm{d}\vec{p}_2{}'\ , \tag{2.107}$$

[9] $K = \begin{vmatrix} \frac{\mathrm{d}\vec{p}_1}{\mathrm{d}\vec{p}_\mathrm{cm}} & \frac{\mathrm{d}\vec{p}_1}{\mathrm{d}\vec{p}_\mathrm{d}} \\ \frac{\mathrm{d}\vec{p}_2}{\mathrm{d}\vec{p}_\mathrm{cm}} & \frac{\mathrm{d}\vec{p}_2}{\mathrm{d}\vec{p}_\mathrm{d}} \end{vmatrix} = \begin{vmatrix} \mathbb{I} & \mathbb{I} \\ \mathbb{I} & -\mathbb{I} \end{vmatrix} = 8$. Alternatively, one can directly write $\vec{p}_1{}' = \frac{1}{2}(\vec{p}_1+\vec{p}_2) + \frac{1}{2}\Omega\cdot(\vec{p}_1-\vec{p}_2)$, where $\vec{p}_\mathrm{d}{}' = \Omega\cdot\vec{p}_\mathrm{d}$, and $\vec{p}_2{}' = \frac{1}{2}(\vec{p}_1+\vec{p}_2) - \frac{1}{2}\Omega\cdot(\vec{p}_1-\vec{p}_2)$. The Jacobian of the total transformation satisfies $J = \begin{vmatrix} \frac{\mathrm{d}\vec{p}_1{}'}{\mathrm{d}\vec{p}_1} & \frac{\mathrm{d}\vec{p}_1{}'}{\mathrm{d}\vec{p}_2} \\ \frac{\mathrm{d}\vec{p}_2{}'}{\mathrm{d}\vec{p}_1} & \frac{\mathrm{d}\vec{p}_2{}'}{\mathrm{d}\vec{p}_2} \end{vmatrix} = 2^{-6}\begin{vmatrix} \mathbb{I}+\Omega & \mathbb{I}-\Omega \\ \mathbb{I}-\Omega & \mathbb{I}+\Omega \end{vmatrix} = 2^{-6}\begin{vmatrix} \mathbb{I}+\Omega & 2\mathbb{I} \\ \mathbb{I}-\Omega & 2\mathbb{I} \end{vmatrix} = 2^{-6}\begin{vmatrix} 2\Omega & 0 \\ \mathbb{I}-\Omega & 2\mathbb{I} \end{vmatrix} = 1$, where the third equality comes from adding the first column to the second, and the fourth from subtracting the second row from the first one.

where the second equality comes from $\vec{p}_{\rm cm} = \vec{p}_{\rm cm}{}'$ and that the determinant of the rotation that maps $\vec{p}_{\rm d}$ onto $\vec{p}_{\rm d}{}'$ is 1.

All in all, using Eqs. (2.105), (2.106), and (2.107) in Eq. (2.102), we rewrite dN^+ as

$$dN^+ = \mathcal{V}_c d^3\vec{p}_1 d^3\vec{p}_2 \tau d^2\sigma(\vec{p}_1,\vec{p}_2 \to \vec{p}_1{}',\vec{p}_2{}')|\vec{v}_2 - \vec{v}_1|\hat{f}_1(\vec{q}_1,\vec{p}_1{}',t)\hat{f}_1(\vec{q}_1,\vec{p}_2{}',t) \; . \tag{2.108}$$

so that

$$N^+(\vec{q}_1,\vec{p}_1,\tau) = d^3\vec{p}_1 \tau \mathcal{V}_c \int d^3\vec{p}_2 d^2\sigma(\vec{p}_1,\vec{p}_2 \to \vec{p}_1{}',\vec{p}_2{}')|\vec{v}_2 - \vec{v}_1|\hat{f}_1(\vec{q}_1,\vec{p}_1{}',t)\hat{f}_1(\vec{q}_1,\vec{p}_2{}',t) \; . \tag{2.109}$$

Using Eqs. (2.89), (2.99), and (2.109) to evaluate the collision term in Eq. (2.88), and dividing by dΓ, we find

$$\int_t^{t+\tau} \frac{\partial \hat{f}_1}{\partial t}\bigg|_{\rm col} = \tau \int d^3\vec{p}_2 d^2\sigma(\vec{p}_1,\vec{p}_2 \to \vec{p}_1{}',\vec{p}_2{}')|\vec{v}_2 - \vec{v}_1|[\hat{f}_1(\vec{q}_1,\vec{p}_1{}',t)\hat{f}_1(\vec{q}_1,\vec{p}_2{}',t) - \hat{f}_1(\vec{q}_1,\vec{p}_1,t)\hat{f}_1(\vec{q}_1,\vec{p}_2,t)] \tag{2.110}$$

Taking into account both collisions and transport, Eqs. (2.87) and (2.110) then lead to the celebrated Boltzman equation:

$$\boxed{\partial_t \hat{f}_1 + \{\hat{f}_1, H_1\} = \int d^3\vec{p}_2 d^2\sigma(\vec{p}_1,\vec{p}_2 \to \vec{p}_1{}',\vec{p}_2{}')|\vec{v}_2 - \vec{v}_1|[\hat{f}_1(\vec{q}_1,\vec{p}_1{}')\hat{f}_1(\vec{q}_1,\vec{p}_2{}') - \hat{f}_1(\vec{q}_1,\vec{p}_1)\hat{f}_1(\vec{q}_1,\vec{p}_2)] \; ,} \tag{2.111}$$

where we have dropped the time dependency for clarity.

To lighten the notation, from now on, we drop the 'hat' notation and simply remember that f has been coarse-grained:

$$\hat{f}_1(\vec{q}_1,\vec{p}_1,t) \longrightarrow f_1(\vec{q}_1,\vec{p}_1,t) \; . \tag{2.112}$$

We also drop the subscript "1" and remember that we are dealing with one-body function:

$$f_1(\vec{q}_1,\vec{p}_1,t) \longrightarrow f(\vec{q}_1,\vec{p}_1,t) \; . \tag{2.113}$$

We also write $f(\vec{p}_i)$ for a proxy to $f(\vec{q}_i,\vec{p}_i)$. Finally, we use subscripts and primes to indicate the argument of f:

$$f(\vec{p}_1),\; f(\vec{p}_2),\; f(\vec{p}_1{}'),\; f(\vec{p}_2{}'), \longrightarrow f_1,\; f_2,\; f_1',\; f_2' \; , \tag{2.114}$$

so that the Boltzmann equation can be more concisely written as:

$$\boxed{\partial_t f + \{f, H_1\} = \int d^3\vec{p}_2 d^2\sigma(\vec{p}_1,\vec{p}_2 \to \vec{p}_1{}',\vec{p}_2{}')|\vec{v}_2 - \vec{v}_1|(f_1' f_2' - f_1 f_2) \; ,} \tag{2.115}$$

A final simplification comes from introducing the collision operator

$$\boxed{C(f,f) = \int \mathrm{d}^3\vec{p}_2 \mathrm{d}^2\sigma|\vec{v}_1 - \vec{v}_2|(f_1' f_2' - f_1 f_2) \; .} \tag{2.116}$$

which leads to

$$\boxed{\partial_t \hat{f} + \{\hat{f}, H_1\} = C(f,f) \; .} \tag{2.117}$$

By deriving Eq. (2.111), we have achieved one of our first goals: we have constructed a closed equation for the time evolution of $\hat{f}_1$. There are still two pending questions that we have not addressed:

1. Liouville's equation is reversible, so that predicting that the typical dynamics is that described in Fig. 2.1 and not its time-reversed counterpart is hard to do at this level. Upon deriving the Boltzmann equation (2.115), we have coarse-grained the level of description of the system, hence losing some information. A first goal below will be to show that the resulting Boltzmann equation is irreversible, and thus more likely to help us prove convergence to equilibrium.

2. $\hat{f}_1$ is not one of the conserved hydrodynamic modes that we have argued should suffice to describe the large-scale long-time dynamics of the system. A second goal below will be to derive the dynamics of such conserved modes and to use them to show convergence towards an equilibrium state.

2.3 The H theorem and the irreversibility of Boltzmann equation

Now that we have established the Boltzmann equation, we would like to show that, if f solves the Boltzmann equation, then it relaxes towards $f^{\rm eq} = \frac{N}{Z} e^{-\beta H_1}$.

2.3.1 How coarse-graining induces irreversibility

A first question is why this is even possible. Indeed, since the Liouville equation is reversible, one of its solution for the one-body function that goes from $f_1^i(\vec{q},\vec{p}) = f_1(\vec{q},\vec{p},0)$ to $f_1^f(\vec{q},\vec{p}) = f_1(\vec{q},\vec{p},t)$ is as likely as the evolution that goes from $f_1^f(\vec{q},-\vec{p})$ to $f_1^i(\vec{q},-\vec{p})$, suggesting a lack of convergence of classical mechanics towards a given steady-state measure. The paradox is resolved by noticing that $\hat{f}_1$ is coarse-grained with the same grid at time t as at time 0, as illustrated in Fig. 2.6. Because of the coarse-graining, sampling the coarse-graining of $f_1^f(\vec{q},-\vec{p})$ into $\hat{f}_1$ is not equivalent to sampling $f_1^f(\vec{q},-\vec{p})$. While the Liouville equation is reversible and would lead back to $f_1^i(\vec{q},-\vec{p})$, this is not true for the Boltzmann equation.

Let us now show how we can prove the irreversibility of the Boltzmann equation, using Boltzmann H-theorem.

2.3.2 Boltzmann H-theorem

Let f be a solution of the Boltzmann equation, then

$$H(t) = \int d\vec{p}d\vec{q} f(\vec{q},\vec{p},t) \log f(\vec{q},\vec{p},t) \tag{2.118}$$

is a decreasing function of time.

Proof of H-theorem

Direct algebra shows that

$$\frac{d}{dt}H(t) = \int d\vec{p}\,d\vec{q}\,\partial_t[f\ln f] = \int d\vec{p}\,d\vec{q}\,[\ln f + 1]\partial_t f = \underbrace{\int d\vec{p}\,d\vec{q}\,\ln f \partial_t f}_{\equiv G} + \underbrace{\partial_f \underbrace{\int d\vec{p}\,d\vec{q}\, f}_{=N}}_{=0} \tag{2.119}$$

We thus are left with evaluating the term:

$$G = \int d\vec{p}d\vec{q}\ln(f)\partial_t f\ . \tag{2.120}$$

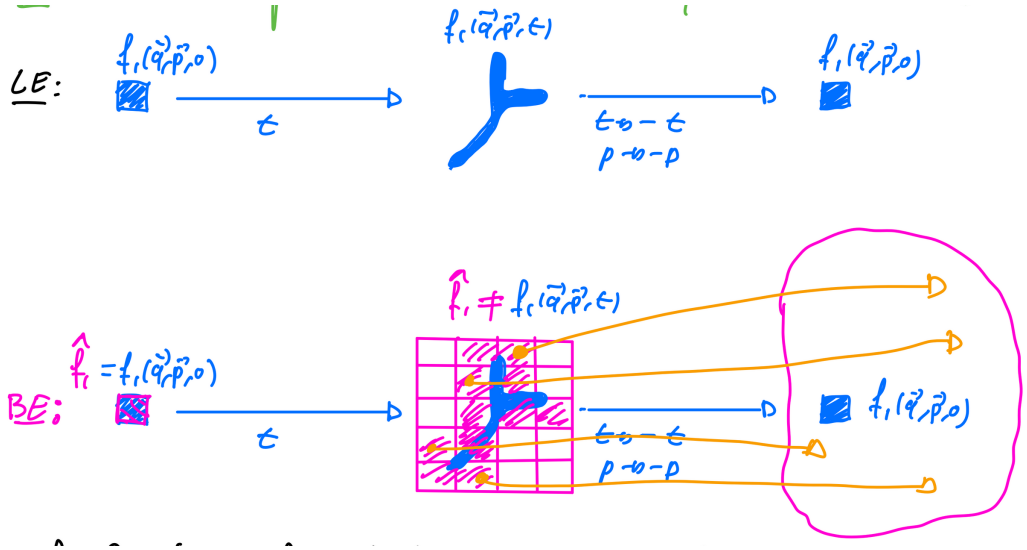


Figure 2.6: *Top row: if f_1 is evolved with the Liouville equation from 0 to t, and then one flips $p \to -p$, a further evolution during a time t sends back f_1 to its original value. Bottom-row. At $t = 0$, we take $\hat{f}_1 = f_1$, but we see that they differ at time t. Any volume element which overlaps with the support of $f_1(\vec{q}, \vec{p}, t)$ has a non-zero value for $\hat{f}_1(\vec{q}, \vec{p}, t)$. Flipping p and imposing a further evolution of time t will map part of the points that are in the support of $\hat{f}_1$ to their initial position, but there also many values, shown in orange, that can be sampled from $\hat{f}_1(\vec{q}, -\vec{p}, t)$ that will lead to new part of phase space, hence leading to the irreversible spreading of the support of $\hat{f}_1$. Coarse-graining, due to the loss of information, induces irreversibility.*

We can now use the Boltzmann equation (2.115) to replace $\partial_t f$ and get

$$G = \underbrace{\int d\vec{p}d\vec{q}\ln(f)\Big[\frac{\partial H_1}{\partial \vec{q}}\cdot\frac{\partial f}{\partial \vec{p}} - \frac{\partial H_1}{\partial \vec{p}}\cdot\frac{\partial f}{\partial \vec{q}}\Big]}_{①} + \underbrace{\int d^3\vec{p}_2\mathrm{d}^3\vec{p}_1 d^3\vec{q}d^2\sigma(\vec{p}_1,\vec{p}_2\to\vec{p}_1{}',\vec{p}_2{}')|\vec{v}_2-\vec{v}_1|[f_1'f_2'-f_1f_2]O(\vec{q},\vec{p},t)}_{②} \ , \tag{2.121}$$

where

$$O(\vec{q},\vec{p},t) = \ln f(\vec{q},\vec{p},t) \tag{2.122}$$

To show that ① vanishes, we integrate by parts:

$$① = \int d\Gamma\Big[-\frac{1}{f}\frac{\partial f}{\partial \vec{p}}\cdot\frac{\partial H_1}{\partial \vec{q}}f + \frac{1}{f}\frac{\partial f}{\partial \vec{q}}\cdot\frac{\partial H_1}{\partial \vec{p}}f\Big] = \int d\Gamma - \frac{\partial}{\partial \vec{p}}\cdot\Big(f\frac{\partial H_1}{\partial \vec{q}}\Big) + \frac{\partial}{\partial \vec{q}}\cdot\Big(f\frac{\partial H_1}{\partial \vec{p}}\Big) = 0\,. \tag{2.123}$$

In the first equality of Eq. (2.123), we have used that the integration by parts leads to vanishing boundary terms because, to be normalizable, f has to vanish as $|\vec{q}| \to \infty$ or $|\vec{p}| \to \infty$. The final equality is due to the same reason: the divergence theorem allows integrating the two terms over $\vec{p}$ or $\vec{q}$ and leads to vanishing boundary terms for normalization reasons.

Let us now turn to the computation of ②. The first thing we note in that, in the integral entering ②, $\vec{p}_1$ and $\vec{p}_2$ are dummy variables so that ② remains unchanged if we swap $\vec{p}_1$ and $\vec{p}_2$, which leads to

$$② = \frac{1}{2}[② + ②(\vec{p}_1 \leftrightarrow \vec{p}_2)] = \frac{1}{2}\int d^3\vec{p}_2\mathrm{d}^3\vec{p}_1 d^3\vec{q}d^2\sigma(\vec{p}_1,\vec{p}_2\to\vec{p}_1{}',\vec{p}_2{}')|\vec{v}_2-\vec{v}_1|[f_1'f_2'-f_1f_2][O(f_1)+O(f_2)]\,. \tag{2.124}$$

Let us now show that we can do essentially the same thing and swap primed and unprimed variables, up to a global sign. As argued previously,

$$\mathrm{d}\vec{p}_1\mathrm{d}\vec{p}_2 = \mathrm{d}\vec{p}\,'_1\mathrm{d}\vec{p}\,'_2\,, \quad \sigma(\vec{p}_1,\vec{p}_2\to\vec{p}\,_1{}',\vec{p}\,_2{}') = \sigma(\vec{p}\,_1{}',\vec{p}\,_2{}'\to\vec{p}_1,\vec{p}_2)\,, \quad \text{and} \quad |\vec{v}_1-\vec{v}_2| = |\vec{v}\,_1{}'-\vec{v}\,_2{}'|\,. \tag{2.125}$$

Injecting this in Eq. (2.124) leads to

$$\textcircled{2} = \frac{1}{2}\int d^3\vec{q}d^3\vec{p}_2{}'\mathrm{d}^3\vec{p}_1{}'d^2\sigma(\vec{p}_1{}',\vec{p}_2{}'\to\vec{p}_1,\vec{p}_2)|\vec{v}_2{}'-\vec{v}_1{}'|[f_1'f_2'-f_1f_2][O(f_1)+O(f_2)]\,. \tag{2.126}$$

But $\sigma(\vec{p}_1{}',\vec{p}_2{}'\to\vec{p}_1,\vec{p}_2)$ tells us that $\vec{p}_1$ and $\vec{p}_2$ are the images of $\vec{p}_1{}'$ and $\vec{p}_2{}'$ after the collision, which is an unfortunate collision of notations. We thus introduce new momenta variables

$$\vec{p}_1{}' = \vec{k}_1, \vec{p}_2{}' = \vec{k}_2 \quad \text{so that} \quad \vec{p}_1 = \vec{k}_1{}', \vec{p}_2 = \vec{k}_2{}'\,, \tag{2.127}$$

which allows rewriting Eq. (2.126) as

$$\textcircled{2} = \frac{1}{2}\int \mathrm{d}^3\vec{q}\mathrm{d}^3\vec{k}_1\mathrm{d}^3\vec{k}_2\mathrm{d}^2\sigma(\vec{k}_1,\vec{k}_2\to\vec{k}_1{}',\vec{k}_2{}')|\vec{k}_1-\vec{k}_2|(f_1f_2-f_1'f_2')(O_1'+O_2')\,, \tag{2.128}$$

where $f_i = f(\vec{q},\vec{k}_i)$ and $f_i' = f(\vec{q},\vec{k}_i{}')$. But we now recognize that, in Eq. (2.128), $\vec{k}_1$ and $\vec{k}_2$ are dummy variables, which we could as well rename $\vec{p}_1$ and $\vec{p}_2$, obtaining an expression very close to (2.124), but with primed and unprimed variables swaped in the last two terms. This time, however, the swap is antisymmetric, replacing $(f_1'f_2'-f_1f_2)$ by $(f_1f_2-f_1'f_2')$. Rewriting $\textcircled{2}$ as the half sum between Eqs. (2.124) and (2.128) thus leads to

$$\textcircled{2} = \frac{1}{4}\int d^3\vec{p}_2\mathrm{d}^3\vec{p}_1d^3\vec{q}d^2\sigma(\vec{p}_1,\vec{p}_2\to\vec{p}_1{}',\vec{p}_2{}')|\vec{v}_2-\vec{v}_1|[f_1'f_2'-f_1f_2][O(f_1)+O(f_2)-O(f_1')-O(f_2')]\,. \tag{2.129}$$

We note that this derivation for $\textcircled{2}$ holds for any function $O(f)$, which we will use to derive hydrodynamic equations later on.

Let us now replace O by $\ln(f)$ to get

$$\frac{d}{dt}H(t) = \frac{1}{4}[\textcircled{2}+\textcircled{2}(\vec{p}_1\leftrightarrow\vec{p}_2)] = \frac{1}{2}\int d^3\vec{p}_2\mathrm{d}^3\vec{p}_1d^3\vec{q}d^2\sigma(\vec{p}_1,\vec{p}_2\to\vec{p}_1{}',\vec{p}_2{}')|\vec{v}_2-\vec{v}_1|[f_1'f_2'-f_1f_2][\ln(f_1f_2)-\ln(f_1'f_2')]\,. \tag{2.130}$$

Since the logarithm is an increasing function, the sign of $\ln(f_1f_2)-\ln(f_1'f_2')$ is the sign of $f_1f_2-f_1'f_2'$. The product of the last two terms in Eq. (2.130) is thus always negative and

$$\frac{\mathrm{d}}{\mathrm{d}t}H(t)\le 0 \quad \text{and} \quad \frac{\mathrm{d}}{\mathrm{d}t}H(t) = 0 \quad \text{iff} \quad f_1f_2 = f_1'f_2'\,. \tag{2.131}$$

$H(t)$ is thus a functional of f_1 that is a decreasing function of time.

2.3.3 Local equilibrium distribution

What we would like to prove is that, ultimately, f evolves to an equilibrium measure. We cannot yet prove this, but we can ask under which condition $H(t)$ stops evolving, i.e. $\frac{\mathrm{d}H}{dt} = 0$. The reasoning above shows that we need to have $f_1f_2 = f_1'f_2'$, which is equivalent to

$$\ln f(\vec{p}_1,\vec{q}) + \ln f(\vec{p}_2,\vec{q}) = \ln f(\vec{p}_1{}',\vec{q}) + \ln f(\vec{p}_2{}',\vec{q})\,. \tag{2.132}$$

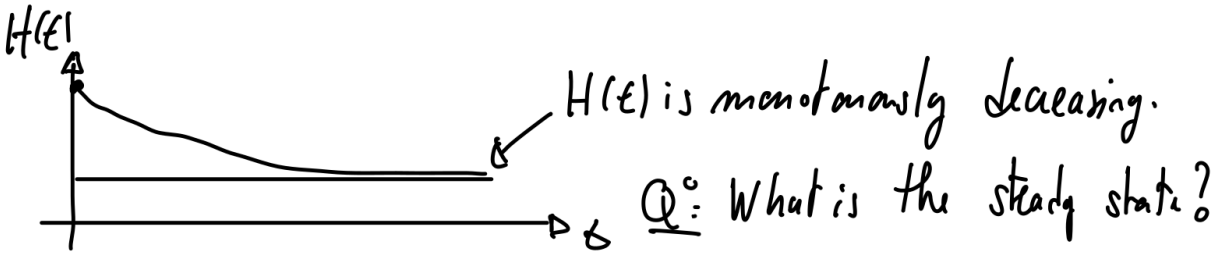


Figure 2.7: *Starting from an initial value H_0, the collision term makes H decrease monotonously. H will stop decreasing only when f has reached a local equilibrium form (2.134).*

.

$\ln f$ is thus a quantity whose sum over colliding particles is conserved by collisions. This is called an additive collisional invariant. From the analysis of the symetry of the system, we know of five such independent quantities:

- The particle number: there are two particles before and after the collision, $1 + 1 = 1 + 1$.
- The components of the momentum: conservation of momentum implies that $p_{1,\alpha}+p_{2,\alpha} = p'_{1,\alpha}+p'_{2,\alpha}$.
- The kinetic energy: the conservation of energy implies that $\vec{p}_1{}^2 + \vec{p}_2{}^2 = (\vec{p}_1{}')^2 + (\vec{p}_2{}')^2$.

As a result, the most general collisional invariant reads:

$$\ln f_1(\vec{p},\vec{q}) = \gamma(\vec{q}) - \alpha(\vec{q})\cdot\vec{p} - \beta(\vec{q})\frac{\vec{p}^2}{2m}\,, \tag{2.133}$$

where γ, α, and β are *a priori* arbitrary functions (as long as $\ln f_1$ is positive and normalizable). We stress that $\vec{q}$ varies over the scale ℓ of the coarse graining. It is thus unaltered during a collision that happens within a volume $\mathcal{V}_c$. Equation (2.133) can thus be seen as solving condition (2.132) independently in each box, hence the dependency on $\vec{q}$.

Rescaling the function γ as $\gamma = \tilde{\gamma}e^{-\beta(\vec{q})U(\vec{q})}$, we can rewrite f_1 as a so-called local-equilibrium density function:

$$f^{\mathrm{LEQ}}(\vec{p},\vec{q}) = \tilde{\gamma}(\vec{q})e^{-\vec{\alpha}(\vec{q})\cdot\vec{p}-\beta(\vec{q})\left[\frac{\vec{p}^2}{2m}+U(\vec{q})\right]}\,. \tag{2.134}$$

We note that f^{LEQ} is such that $\frac{\mathrm{d}H[f^{\mathrm{LEQ}}]}{\mathrm{d}t} = 0$ for all functions $\tilde{\gamma}$, $\vec{\alpha}$, and β. There is thus a five-dimensional manifold in the space of functions f_1 that are such that $\frac{\mathrm{d}H[f^{\mathrm{LEQ}}]}{\mathrm{d}t} = 0$.

2.3.4 The relaxation of H and global equilibrium

The evolution of H is thus a relaxation induced by the collision term, over a characteristic time scale τ_{mft}, as sketched in Fig. 2.7. A natural question is whether the local equilibria given in Eq. (2.134) are all steady-sate solutions of the Boltzmann equation itself. For this to be true, we need

$$-\{f^{\mathrm{LEQ}}, H_1\} + C(f^{\mathrm{LEQ}}, f^{\mathrm{LEQ}}) = 0\,, \tag{2.135}$$

where we have used the collision operator (2.116). We have already established that $C(f^{\mathrm{LEQ}}, f^{\mathrm{LEQ}}) = 0$ but, in general $\{f^{\mathrm{LEQ}}, H_1\} \neq 0$, so that f^{LEQ} is not a steady-state solution of the Boltzmann equation.

Global equilibrium. A particular f^{LEQ} that satisfies Eq. (2.135) is the so-called global equilibrium, such that $\tilde{\gamma}$ is a number, $\vec{\alpha} = 0$, and β is a constant:

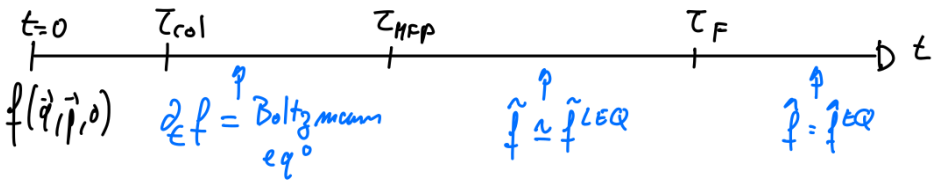
$$f^{\mathrm{EQ}}(\vec{p},\vec{q}) = \tilde{\gamma} e^{-\beta\left[\frac{\vec{p}^2}{2m}+U(\vec{q})\right]} . \tag{2.136}$$

Indeed, $f^{\mathrm{EQ}}(\vec{p},\vec{q}) = g(H_1(\vec{p},\vec{q}))$ so that $\{H_1, f^{\mathrm{EQ}}\} = g'(H_1)\{H_1,H_1\} = 0$.

Overall dynamics. The analysis of the time scale contained in the Boltzmann equation and the discussion above thus suggest the following scenario. In the Boltzmann equation, the collision term makes f relax very close to the set of local equilibria on a time of order τ_{mft}. Then, the transport term makes f relax to the global equilibrium on a time τ_{F}:

$$\partial_t f = \underbrace{-\{f,H_1\}}_{\text{relaxes on time } \sim \tau_{\mathrm{F}}} + \underbrace{C(f,f)}_{\text{relaxes on time } \sim \tau_{\mathrm{mft}}} . \tag{2.137}$$

This suggest the following evolution of f on various time scales:



Canonical distribution. f^{EQ} is proportional to the canonical distribution of a single particle at temperature $T = \beta^{-1}/k_B$. This seems quite surprising since we are describing an isolated system, and we might thus have expected to obtain the microcanonical measure, not the canonical one.

The 'paradox' is resolved by realizing that f is a single-body quantity, and that the energy of a single particle is not conserved: it exchange energy during collisions with the other particles, that collectively act as a thermostat. We have thus encountered our first physical realization of the canonical ensemble!

A mystery remains: in the canonical ensemble, we expect the probability to the Boltzmann factor $e^{-\beta E}$, where E is the total energy. Instead, we obtained $e^{-\beta H_1}$, which is only the one-body contribution. This can be understood by realizing that we work in the dilute limit, so that

$$H = \sum_{i=1}^{N} \left\{ \underbrace{\frac{\vec{p}_i{}^2}{2m} + U(\vec{q}_i)}_{\sim\mathcal{O}(1)} + \underbrace{\frac{1}{2}\sum_{j\neq i} V(\vec{q}_i - \vec{q}_j)}_{\mathcal{O}(nd^3)\ll 1} \right\} \simeq \sum_{i=1}^{N} \frac{\vec{p}_i{}^2}{2m} + U(\vec{q}_i) . \tag{2.138}$$

The canonical distribution would thus be:

$$P(\{\vec{q}_i,\vec{p}_i\}) \propto \prod_i e^{-\beta\left[\frac{\vec{p}_i{}^2}{2m}+U(\{\vec{q}_i\})\right]} , \tag{2.139}$$

which is nothing but the canonical distribution of an Ideal gas. The latter is thus a gas which is dense enough that collisions make the gas relax to equilibrium, but dilute enough that interactions do not influence the steady-state measure[10].

[10] Note that we have NOT derived Eq. (2.139) for our gas, which is isolated and thus not in the canonical ensemble, but simply the equivalent one-body marginal.

Of the two questions that we had asked at the end of Section 2.2.2.2, we have thus answered the first one: the coarse-graining of f_1 into $\hat{f}_1$ has indeed led to a description of the system that leads to an irreversible evolution, captured by the H theorem. The second challenge, which is the description of this evolution in terms of hydrodynamic modes, remains, and it is the topic of the next section.

2.4 Hydrodynamic equations

In Section 2.1.2, we identified that conserved quantities typically lead to slow modes. In our interacting gas, we have identified particle number, momentum and energy as conserved quantities. Let us now show that we can build hydrodynamic modes associated to these quantities. For simplicity, we work here in the absence of external potential so that $H_1 = \sum_i \vec{p}_i^{\,2}/2m$ and

$$\{f, H_1\} = \vec{v} \cdot \frac{\partial}{\partial \vec{q}} f(\vec{q}, \vec{p}, t) \tag{2.140}$$

2.4.1 Evolution of the density field

The (coarse-grained) density field is simply obtained by integrating $f(\vec{q}, \vec{p})$ over $\vec{p}$:

$$n(\vec{q}, t) = \int \mathrm{d}^3\vec{p} f(\vec{q}, \vec{p}, t) \, . \tag{2.141}$$

We then get $\partial_t n$ by integrating the Boltzmann equation over $\vec{p}$ to get:

$$\partial_t n(\vec{q}, t) = -\int \mathrm{d}^3\vec{p}\, \vec{v} \cdot \frac{\partial}{\partial \vec{q}} f(\vec{q}, \vec{p}, t) + \underbrace{\int \mathrm{d}^3\vec{p}_1 \mathrm{d}^3\vec{p}_2 \mathrm{d}^2\sigma |\vec{v}_1 - \vec{v}_2| (f_1' f_2' - f_1 f_2)}_{I} \, . \tag{2.142}$$

Current and velocity fields. Let us first consider the term in ochre. Since f is the sole function that depends on $\vec{q}$, we can rewrite this term as

$$-\int \mathrm{d}^3\vec{p}\, \vec{v} \cdot \frac{\partial}{\partial \vec{q}} f(\vec{q}, \vec{p}, t) = -\frac{\partial}{\partial \vec{q}} \cdot \vec{j}(\vec{q}, t) \quad \text{with} \quad \vec{j}(\vec{q}, t) \equiv \int \mathrm{d}^3\vec{p}\, \vec{v}\, f(\vec{q}, \vec{p}, t) \, . \tag{2.143}$$

We have here introduced the current field $\vec{j}(\vec{q}, t)$, which measures the local flux of particles at $\vec{q}$. Since $\vec{j}$ is extensive in the local number of particles (through f), we make this explicit by introducing the intensive velocity field $\vec{u}(\vec{q}, t)$ through

$$\vec{j}(\vec{q}, t) = n(\vec{q}, t)\vec{u}(\vec{q}, t) \quad \longleftrightarrow \quad \vec{u}(\vec{q}, t) = \frac{1}{n(\vec{q}, t)} \int \mathrm{d}^3\vec{p}\, \vec{v}\, f(\vec{q}, \vec{p}, t) \equiv \langle \vec{v} \rangle_q \, . \tag{2.144}$$

In Eq. (2.144), we have introduced the notion of average *at fixed* q, denoted $\langle \dots \rangle_q$, defined through

$$\langle O(\vec{q}, \vec{p}) \rangle_q = \int \mathrm{d}^3\vec{p} O(\vec{q}, \vec{p}) \, \frac{f(\vec{q}, \vec{p}, t)}{n(\vec{q}, t)} = \int \mathrm{d}^3\vec{p} O(\vec{q}, \vec{p}) \, \rho_1(\vec{p}|\vec{q}) \, , \tag{2.145}$$

where we have introduced the conditional probability density $\rho_1(\vec{p}|\vec{q})$ that a particle has a momentum $\vec{p}$ given that it is at position $\vec{q}$. To understand where the last equality comes from, note that

$$\frac{f(\vec{q}, \vec{p}, t)}{n(\vec{q}, t)} = \frac{N \rho_1(\vec{q}, \vec{p}, t)}{\int \mathrm{d}\vec{p} N \rho_1(\vec{q}, \vec{p}, t)} = \frac{\rho_1(\vec{q}, \vec{p}, t)}{\rho_1(\vec{q}, t)} \, , \tag{2.146}$$

where $\rho_1(\vec{q})$ is the marginal of $\rho_1(\vec{q},\vec{p})$ over $\vec{p}$. Then, Bayes theorem tells us that $\rho_1(\vec{q},\vec{p}) = \rho_1(\vec{p}|\vec{q})\rho_1(\vec{q})$, which yields Eq. (2.145). The velocity field $\vec{u}(\vec{q},t)$ can thus be understood as the average velocity of the particles "at $\vec{q}$".

Let us now turn to the magenta term in Eq. (2.142), which we rewrite as

$$I = \int \mathrm{d}^3\vec{p}_1\mathrm{d}^3\vec{p}_2\mathrm{d}^2\sigma(\vec{p}_1,\vec{p}_2\to\vec{p}_1{}',\vec{p}_2{}')|\vec{v}_1-\vec{v}_2|(f_1'f_2'-f_1f_2)O_1\ , \tag{2.147}$$

where $O_1 = O(\vec{q},\vec{p}_1) = 1$. We note that, up to an unimportant integral over $\vec{q}$, this term is identical to the term (2) in Eq. (2.121), except that $O(\vec{q},\vec{p}_1) = 1$ here instead of $O(\vec{q},\vec{p}_1) = \ln f(\vec{q},\vec{p}_1)$. Since 1 (the particle number) is a collisional invariant, the result will be identical and $I = 0$. For completeness, we reproduce the proof below.

Proof: We first note that $\vec{p}_1$ and $\vec{p}_2$ are dummy variables in I, and that the integrand is symmetric in $\vec{p}_1 \leftrightarrow \vec{p}_2$, so that

$$I = \frac{1}{2}I + \frac{1}{2}I(\vec{p}_1\leftrightarrow\vec{p}_2) = \frac{1}{2}\int \mathrm{d}^3\vec{p}_1\mathrm{d}^3\vec{p}_2\mathrm{d}^2\sigma(\vec{p}_1,\vec{p}_2\to\vec{p}_1{}',\vec{p}_2{}')|\vec{v}_1-\vec{v}_2|(f_1'f_2'-f_1f_2)(O_1+O_2)\ , \tag{2.148}$$

Let us now show that we can do essentially the same thing and swap primed and unprimed variables, up to a global sign. As argued previously,

$$\mathrm{d}\vec{p}_1\mathrm{d}\vec{p}_2 = \mathrm{d}\vec{p}_1{}'\mathrm{d}\vec{p}_2{}'\ ,\quad \sigma(\vec{p}_1,\vec{p}_2\to\vec{p}_1{}',\vec{p}_2{}') = \sigma(\vec{p}_1{}',\vec{p}_2{}'\to\vec{p}_1,\vec{p}_2)\ ,\quad \text{and}\quad |\vec{v}_1-\vec{v}_2| = |\vec{v}_1{}'-\vec{v}_2{}'|\ . \tag{2.149}$$

Injecting this in I leads to

$$I = \frac{1}{2}\int \mathrm{d}^3\vec{p}_1{}'\mathrm{d}^3\vec{p}_2{}'\mathrm{d}^2\sigma(\vec{p}_1{}',\vec{p}_2{}'\to\vec{p}_1,\vec{p}_2)|\vec{v}_1{}'-\vec{v}_2{}'|(f_1'f_2'-f_1f_2)(O_1+O_2)\ , \tag{2.150}$$

But $\sigma(\vec{p}_1{}',\vec{p}_2{}'\to\vec{p}_1,\vec{p}_2)$ tells us that $\vec{p}_1$ and $\vec{p}_2$ are the images of $\vec{p}_1{}'$ and $\vec{p}_2{}'$ after the collision, which is an unfortunate collision of notations. We thus introduce new momenta variables

$$\vec{p}_1{}' = \vec{k}_1, \vec{p}_2{}' = \vec{k}_2 \quad \text{so that} \quad \vec{p}_1 = \vec{k}_1{}', \vec{p}_2 = \vec{k}_2{}'\ , \tag{2.151}$$

which allows rewriting Eq. (2.150) as

$$I = \frac{1}{2}\int \mathrm{d}^3\vec{k}_1\mathrm{d}^3\vec{k}_2\mathrm{d}^2\sigma(\vec{k}_1,\vec{k}_2\to\vec{k}_1{}',\vec{k}_2{}')|\vec{k}_1-\vec{k}_2|(f_1f_2-f_1'f_2')(O_1'+O_2')\ , \tag{2.152}$$

where $f_i = f(\vec{q},\vec{k}_i)$. But we now recognize that, in Eq. (2.152), $\vec{k}_1$ and $\vec{k}_2$ are dummy variables, which we could as well rename $\vec{p}_1$ and $\vec{p}_2$, obtaining an expression very close to (2.148), but with primed and unprimed variables swaped in the last two terms. This time, however, the swap is antisymmetric, replacing $(f_1'f_2'-f_1f_2)$ by $(f_1f_2-f_1'f_2')$. Rewriting I as the half sum between Eqs. (2.148) and (2.152) thus leads to

$$I = \frac{1}{4}\int \mathrm{d}^3\vec{p}_1\mathrm{d}^3\vec{p}_2\mathrm{d}^2\sigma(\vec{p}_1,\vec{p}_2\to\vec{p}_1{}',\vec{p}_2{}')|\vec{v}_1-\vec{v}_2|(f_1'f_2'-f_1f_2)(O_1+O_2-O_1'-O_2')\ . \tag{2.153}$$

Inspection of Eq. (2.153) shows that replacing O by any collisional invariant leads to $I = 0$, as can be immediately checked using $O = 1$.

The time evolution of the density field thus reduces to

$$\boxed{\partial_t n(\vec{q},t) = -\nabla\cdot[n(\vec{q},t)\vec{u}(\vec{q},t)]\ ,} \tag{2.154}$$

where we have replaced $\frac{\partial}{\partial \vec{q}}$ by the usual gradient symbol. Expanding the gradient, this can be rewritten as

$$\boxed{D_t n(\vec{q},t) = -n(\vec{q},t)\nabla\cdot[\vec{u}(\vec{q},t)]\ ,} \tag{2.155}$$

where we have introduced the material derivatives

$$D_t = \partial_t + \vec{u}(\vec{q},t)\cdot\nabla\ . \tag{2.156}$$

The material derivative mesures the evolution of a quantity in the frame co-moving with the flow $\vec{u}(\vec{q},t)$. To see this, consider the solution of $\dot{\vec{x}} = \vec{u}$. The chain rule immediately tells us that

$$\frac{d}{dt}O(\vec{x}(t),t) = \vec{u}\cdot\nabla O(\vec{x}(t),t) + \partial_t O(\vec{x}(t),t) = D_t O(\vec{x}(t),t)\ . \tag{2.157}$$

Equation (2.155) thus tells us that if the velocity field is divergence free, the density is constant in time *in the frame of the flow*. In this chapter, the material derivative will be a useful shorthand notation, but we will remain in the (Eulerian) frame of the lab and not move to the (Lagrangian) frame of the flow.

2.4.2 Evolution of the velocity field

We now turn to our second conserved quantity: momentum. Since Eq. (2.154) involves the velocity field, which is the momentum field divided by the particle mass, we will derive the time evolution of the velocity field, instead of that of the momentum field. We rewrite Eq. (2.144) component by component as

$$u_\alpha = \frac{1}{n}\int \mathrm{d}\vec{p}\, v_\alpha f \tag{2.158}$$

Taking the time derivative of Eq. (2.158) and using the Boltzmann equation, one finds

$$D_t u_\alpha(\vec{q},t) = -\frac{1}{n(\vec{q},t)}\partial_{q_\beta}\Big[n\langle[v_\alpha - u_\alpha(\vec{q},t)][v_\beta - u_\beta(\vec{q},t)]\rangle\Big]\ . \tag{2.159}$$

From now one, summation over repeated indices—as is the case for β in Eq. (2.159), is assumed. See page 5 of Lecture 10 for the derivation of Eq. (2.159). Equation (2.159) suggests introducing the pressure tensor

$$\boxed{P_{\alpha\beta}(\vec{q},t) = nm\langle\delta v_\alpha(\vec{q},t)\delta v_\beta(\vec{q},t)\rangle\ ,\quad \text{where}\quad \delta\vec{v}\,(\vec{v},\vec{q},t) \equiv \vec{v} - \vec{u}(\vec{q},t)} \tag{2.160}$$

measures the difference between a particle velocity and the average velocity at position $\vec{q}$ and time t. At this stage, it is not clear at all why $P_{\alpha\beta}$ should be call a pressure tensor. This will become clearer later on, when we compute it explicitly. At this stage, we can say that, in the frame co-moving with the average velocity field $\vec{u}$, $P_{\alpha\beta}$ measure the flux of (relative) momentum $m\delta v_a$ in the direction β. The time evolution of the velocity field can thus be written in a compact way:

$$\boxed{mD_t u_\alpha = -\frac{1}{n}\partial_{q_\beta}P_{\alpha\beta} \quad\Leftrightarrow\quad mD_t\vec{u} = \frac{1}{n}\nabla\cdot\mathbf{P}} \tag{2.161}$$

At this stage, we have derived in Eqs. (2.154) and (2.161) the equivalent of the Navier-Stoke equations for our weakly interacting gas. We note, however, that if we do not find a way to predict the value of $\mathbf{P}$, we will not be able to predict the evolution of $\vec{u}$.

2.4.3 Kinetic energy density and temperature field

The last conservation law that we have to consider is that of energy. We first note that, since $\vec{v} = \vec{u} + \delta\vec{v}$, the average kinetic energy can be decomposed as:

$$\langle \frac{1}{2} m \vec{v}^{\,2} \rangle = \frac{1}{2} m \vec{u}^{\,2} + m\vec{u} \cdot \langle \delta\vec{v} \rangle + \frac{1}{2} m \langle \delta\vec{v}^{\,2} \rangle \; . \tag{2.162}$$

Since the evolution of $\vec{u}^{\,2}$ is already given by that of $\vec{u}$ and since $\langle \delta\vec{v} \rangle = 0$ by construction, the new independent field is

$$\varepsilon(\vec{q}, t) = \langle \frac{1}{2} m \delta\vec{v}^{\,2} \rangle = \langle \frac{1}{2} m \vec{v}^{\,2} - \frac{1}{2} m \vec{u}^{\,2} \rangle \; . \tag{2.163}$$

ε measures the kinetic energy of the particles in the co-moving frame and its time evolution can be computed as:

$$\boxed{\partial_t \varepsilon + u_\alpha \partial_{q_\alpha} \varepsilon = -\frac{1}{n} \partial_{q_\alpha} h_\alpha - \frac{1}{n} P_{\alpha\beta} u_{\alpha\beta} \; ,} \tag{2.164}$$

where we have introduced the strain rate tensor

$$\boxed{u_{\alpha\beta} = \frac{1}{2} (\partial_{q_\alpha} u_\beta + \partial_{q_\beta} u_\alpha)} \tag{2.165}$$

and the heat flux

$$\boxed{h_\alpha = \frac{nm}{2} \langle \delta\vec{v}_\alpha \delta\vec{v}_\beta \delta\vec{v}_\beta \rangle \quad \Leftrightarrow \quad \vec{h} = \frac{nm}{2} \langle \delta\vec{v} \, ||\delta\vec{v}||^2 \rangle \; .} \tag{2.166}$$

See pages 6 & 7 of Lecture 10 for a derivation. The kinetic energy of the particle in the co-moving frame can be seen as a measure of thermal agitation, and we thus introduce the temperature field

$$T(\vec{q}, t) = \frac{2}{3 k_B} \varepsilon(\vec{q}, t) \quad \text{such that} \quad \varepsilon = \frac{3}{2} k_B T \; . \tag{2.167}$$

At this stage, nothing guarantees that T is a bona fide measurement of the local temperature, but this will prove later to be a relevant choice. From the dynamics of ε, we derive that of T as

$$\boxed{D_t T = -\frac{2}{3 n k_B} \partial_{q_\alpha} h_\alpha - \frac{2}{3 n k_B} P_{\alpha\beta} u_{\alpha\beta} \; .} \tag{2.168}$$

Closure and hydrodynamic equations. We have now constructed the time evolution of the five fields which, we claimed, were sufficient to describe all the large-scale long-time physics of the system. However, at this stage, these equations are not closed since we do not know the pressure tensor $\mathbf{P}$ and the heat flux $\vec{h}$. Furthermore, it is not clear why these hydrodynamic equations should drive the system to a state of thermal equilibrium. Addressing these two points is the goal of the next section.

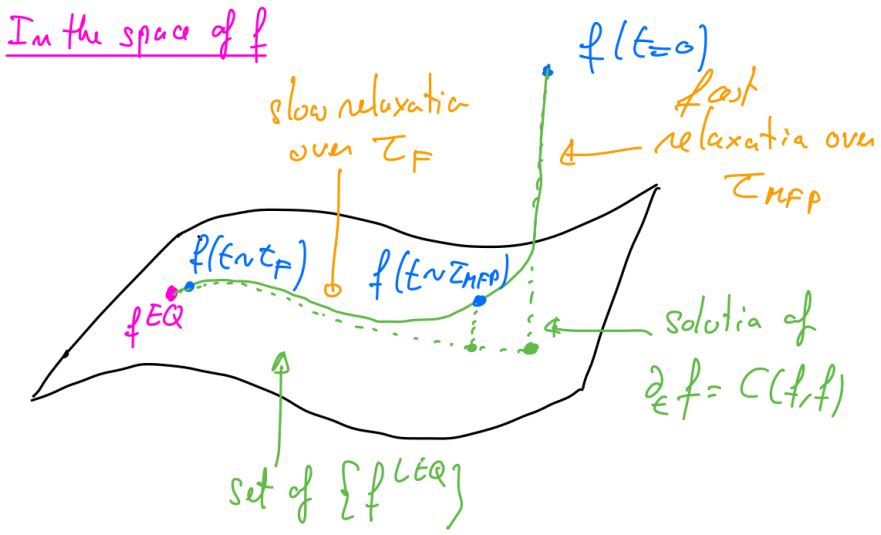


Figure 2.8: *On a time $t \sim \tau_{\rm mft}$, f relaxes very close to the manifold of local equilibria. Then, on a long time scale $t \sim \tau_{\rm F}$, it relaxes to global equilibrium. We want to characterize this evolution in the limit $\tau_{\rm mft}/\tau_{\rm F} \ll 1$, which is relevant for atomic gases at room temperature.*

2.5 Relaxation and transport properties

To close the hydrodynamic equations, we need to estimate

$$P_{\alpha\beta}(\vec{q},t) = \langle \delta v_\alpha \delta v_\beta \rangle = \frac{1}{n}\int \mathrm{d}^3\vec{p}\, \delta v_\alpha \delta v_\beta f(\vec{q},\vec{p},t) \quad \text{and} \quad h_\alpha(\vec{q},t) = \langle \delta v_\alpha \delta v_\beta \delta v_\beta \rangle = \frac{1}{n}\int \mathrm{d}^3\vec{p}\, \delta v_\alpha \delta v_\beta \delta v_\beta f(\vec{q},\vec{p},t)\,. \tag{2.169}$$

Clearly, this requires some knowledge of f.

Relevant time scales. Let us first recap the time evolution of f that we predicted in Section 2.3.4. Starting from the Boltzmann equation

$$\partial_t f = -\frac{\vec{p}}{m}\cdot\frac{\partial f}{\partial \vec{q}} + C(f,f)\,, \tag{2.170}$$

we identified two relevant regimes, recapitulated in Fig. 2.8: a short-time relaxation close to a local equilibrium $f^{\rm LEQ}$, for $t \sim \tau_{\rm mft}$, followed by a slower relaxation on a time $t \sim \tau_{\rm F}$. We now construct a perturbation theory in the limit $\tau_{\rm mft} \ll \tau_{\rm F}$ to characterize this relaxation analytically.

We start by making all time scales explicit in the Boltzmann Eq. (2.170) by introducing

$$L_F f = \tau_{\rm F}\vec{v}\cdot\frac{\partial}{\partial\vec{q}} f \quad \text{and} \quad \hat{C}(f,f) = \tau_{\rm mft} C(f,f)\,, \tag{2.171}$$

so that the Boltzmann equation becomes:

$$\partial_t f = -\frac{1}{\tau_{\rm F}} L_F f + \frac{1}{\tau_{\rm mft}}\hat{C}(f,f)\,. \tag{2.172}$$

To characterize the relaxation of f over time $\tau_{\rm F}$, we now rescale time as $t = \tau_{\rm F}\hat{t}$ so that $\hat{t} \sim \mathcal{O}(1)$ implies $t \sim \mathcal{O}(\tau_{\rm F})$. This turns the Boltzmann Eq. into

$$\partial_{\hat{t}} f = -L_F f + \frac{1}{\varepsilon}\hat{C}(f,f) \quad \text{with} \quad \varepsilon = \frac{\tau_{\rm mft}}{\tau_{\rm F}} \ll 1\,. \tag{2.173}$$

Perturbation theory. We now want to develop a perturbation theory to solve Eq. (2.173). We thus expand f as

$$f(\vec{q},\vec{p},t) = f_0(\vec{q},\vec{p},t) + \varepsilon f_1(\vec{q},\vec{p},t) + \mathcal{O}(\varepsilon^2) \,. \tag{2.174}$$

Injecting this ansatz in Eq. (2.173), and using that $\hat{C}$ is bilinear in f, we get

$$\partial_{\hat{t}} f_0 + \varepsilon \partial_{\hat{t}} f_1 = -L_F f_0 - \varepsilon L_F f_1 + \frac{1}{\varepsilon}\hat{C}(f_0,f_0) + \hat{C}(f_0,f_1) + \hat{C}(f_1,f_0) + \mathcal{O}(\varepsilon^2) \,. \tag{2.175}$$

To leading order in ε, we get

$$\mathcal{O}(\varepsilon^{-1}) : 0 = C(f_0,f_0) \,, \tag{2.176}$$

which tells us that, to leading order $f \simeq f_0 = f^{\mathrm{LEQ}}$. To next order,

$$\mathcal{O}(\varepsilon^0) : \partial_{\hat{t}} f_0 + L_F f_0 = C(f_0,f_1) + C(f_1,f_0) \,. \tag{2.177}$$

Once f_0 is determined, solving Eq. (2.177) for f_1 will provide us, if need be, with the first-order correction to $f \simeq f_0$.

2.5.1 Zeroth-order dynamics

Local equilibrium. To leading order, $f \simeq f_0$, where

$$f_0(\vec{q},\vec{p},t) = f^{\mathrm{LEQ}}(\vec{q},\vec{p},t) = \tilde{\gamma}(\vec{q}) e^{-\vec{\alpha}(\vec{q},t)\cdot\vec{p} - \beta(\vec{q},t)\frac{\vec{p}^2}{2m}} \,, \tag{2.178}$$

which is a Gaussian distribution in $\vec{p}$. We also know that f is related to the hydrodynamic modes through

$$\int f \mathrm{d}^3\vec{p} = n, \quad \int \vec{v} f \mathrm{d}^3\vec{p} = n\vec{u}, \quad \int \frac{m}{2}(v-\vec{u})^2 f \mathrm{d}^3\vec{p} = n\varepsilon = \frac{3}{2} n k_B T \,. \tag{2.179}$$

To zeroth order, f_0 is a Gaussian whose normalization, average and variance are fixed by Eq. (2.179), leading to

$$f_0(\vec{q},\vec{p},t) = \frac{n_0(\vec{q},t)}{[2\pi m k_B T_0(\vec{q},t)]^{3/2}} e^{-\frac{[\vec{p}-m\vec{u}_0(\vec{q},t)]^2}{2mk_BT_0(\vec{q},t)}} = \frac{n_0(\vec{q},t)}{[2\pi m k_B T_0(\vec{q},t)]^{3/2}} e^{-\frac{m\delta\vec{v}^2}{2k_BT_0(\vec{q},t)}} \,, \tag{2.180}$$

where the subscripts "$_0$" on the hydrodynamic fields show that there will be corrections to order ε to the fields when solving Eq.(2.179) perturbatively. Now that we have an ansatz for f_0, we can compute the pressure tensor and heat flux to leading order in ε.

Pressure and heat flux. Direct algebra using Gaussian integrals shows that

$$P^0_{\alpha\beta} = n_0 m \langle \delta v_\alpha \delta v_\beta \rangle_{f_0} = n_0 k_B T_0 \delta_{\alpha\beta} \,. \tag{2.181}$$

The pressure is isotropic and its diagonal entries obey the ideal gas law. This justifies the name of the pressure tensor, but also shows the connection between the thermodynamic pressure and momentum fluxes. To order ε^0, the heat flux vanishes:

$$h^0_\alpha \propto \langle \delta\vec{v}^2 \delta v_\alpha \rangle_{f_0} = 0 \,, \tag{2.182}$$

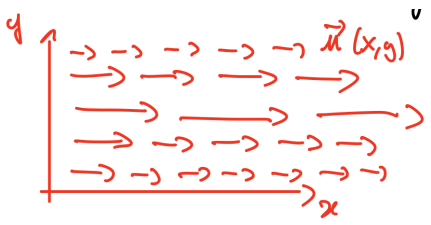


Figure 2.9: *If the gas is initialized in a homogeneous density and temperature state, but with a sheared velocity field, no relaxation of $\vec{u}$ is observed to leading order and the system does not equilibrate.*

since the average involves an odd power of δv and a Gaussian distribution centered on $\delta\vec{v} = 0$. We can now use the values of $\mathbf{P}$ and $\vec{h}$ to close the hydrodynamic equations.

Leading-order hydrodynamics. Direct algebra leads to

$$\partial_t n_0 + \vec{u}_0 \cdot \nabla \vec{u}_0 = -n_0 \nabla \cdot \vec{u}_0 \tag{2.183}$$

$$\partial_t \vec{u}_0 + \vec{u}_0 \cdot \nabla n_0 = -\frac{1}{n_0} \nabla (n_0 k_B T_0) \tag{2.184}$$

$$\partial_t T_0 + \vec{u}_0 \cdot \nabla T_0 = -\frac{2}{3} T_0 \nabla \cdot \vec{u}_0 \tag{2.185}$$

To order ε^0, $f = f_0$ is left invariant by collisions, but the transport occurs due to $\{f, H_1\}$, which in turns induces an evolution of $m_0, \vec{u}_0, T_0$. The natural question is then whether this evolution suffices to equilibrate the system, leading to n_0 and T_0 uniform and making $\vec{u}_0$ vanish.

Shear modes do not relax to 0^{th} order in ε. Let us consider an initial condition where temperature and density are uniform, but where the gas is sheared, so that its velocity field is along $\hat{x}$ and varies along $\hat{y}$, as illustrated in Fig. 2.9: $\vec{u}_0 = u(y)\hat{x}$. Direct inspection then shows that, in the dynamics (2.184) for $\vec{u}_0$,

$$\nabla \cdot (n_0 T_0) = 0 \quad \& \quad \vec{u} \cdot \nabla \vec{u} = u(y) \partial_x u(y) \hat{x} = 0 \,, \tag{2.186}$$

so that $\partial_t \vec{u}_0 = 0$. The velocity field does NOT relax to zero and the system does not equilibrate at this order. Let us thus work out the next order correction to f and check whether it suffices to induce relaxation to steady state.

2.5.2 First-order hydrodynamics

Single time approximation. We know that $C(f, f)$ is a bilinear operator that makes f relax to $f^{\rm LEQ}$ over a time scale $\tau_{\rm mft}$. This relaxation may be quite complex and involve a variety of time scales between $\tau_{\rm col}$ and $\tau_{\rm mft}$.

To solve for f_1 in terms of f_0 using Eq. (2.177) would require inverting this operator, which is difficult. Instead, we assume that the relaxation from f to $f^{\rm LEQ}$ is dominated by a single time scale, so that we approximate C as:

$$C(f, f) = -\frac{1}{\tau_{\rm mft}} (f - f_0) \quad \rightarrow \quad \partial_t f = -\frac{1}{\tau_{\rm F}} L_F f - \frac{1}{\tau_{\rm mft}} (f - f_0) \,. \tag{2.187}$$

This simplifies the $\mathcal{O}(\varepsilon^0)$ equation (2.177) for f_1 into:

$$f_1 = -\partial_{\tilde{t}} f_0 - L_F f_0 \,. \tag{2.188}$$

Since we know f_0, we can now compute f_1.

We run, however, in a slight notational issue. Our perturbation theory was developed in time $\tilde{t}$, which is very nice since it makes the small parameter ε explicit. Our hydrodynamic equations, however, have been derived using the microscopic time t. We thus have two choices: 1/ Rescale the hydrodynamic equations, work out $\partial_{\tilde{t}} f_0$, compute the first-order dynamics, and then restore everything to time t; 2/ Rewrite Eq. (2.188) using time t and stick to this time unit. Option 1/ is mathematically nicer, since factors of ε will appear in front of all the first order corrections. It is also much heavier and we thus chose option 2/ here, at the cost of making the scale of the "small" corrections harder to gauge. If this discussion is not clear at this stage, it will become clearer later on. We thus recast Eq. (2.188) into

$$f_1 = -\tau_F(\partial_t f_0 + \vec{v}\cdot\nabla f_0) \,. \tag{2.189}$$

Since f_0 is Gaussian, it is nicer to take derivative of $\ln f_0$ than of f_0. We thus introduce $g_1 = \varepsilon f_1/f_0$ such that

$$f = f_0(1+g_1) \quad \text{and} \quad g_1 = -\tau_{\rm mft}(\partial_t + \vec{v}\cdot\nabla)\ln f_0 \,. \tag{2.190}$$

Using Eq. (2.180) then directly leads to

$$g_1 = -\frac{m\tau_{\rm mft}}{k_B T_0}\vec{u}^0_{\alpha\beta}(\delta v^0_\alpha \delta v^0_\beta - \frac{\delta\vec{v}_0{}^2}{3}\delta_{\alpha\beta}) - \frac{\tau_{\rm mft}}{T_0}\delta v^0_\alpha(\partial_{q_\alpha}T_0)(\frac{m}{2k_BT_0}\delta\vec{v}_0{}^2 - \frac{5}{2}) \tag{2.191}$$

$$= \Big[-\frac{m\tau_{\rm mft}}{k_B T}\vec{u}_{\alpha\beta}(\delta v_\alpha \delta v_\beta - \frac{\delta\vec{v}^2}{3}\delta_{\alpha\beta}) - \frac{\tau_{\rm mft}}{T}\delta v_\alpha(\partial_{q_\alpha}T)(\frac{m}{2k_BT}\delta\vec{v}^2 - \frac{5}{2})\Big][1+\mathcal{O}(\varepsilon)] \,. \tag{2.192}$$

The derivation of the first equality stems from direct (painful) algebra, which can be found page 6 of Lecture 11. The second stems from realizing that we need only the leader order estimate of g_1, and that replacing the zeroth order hydrodynamic fields by their total value induces only corrections of higher order.

First order pressure and heat flux. We now have our first-order estimate of $f = f_0(1+g_1)$. This form is very convenient since it allows us to rewrite averages as follows:

$$\langle O(\vec{p},\vec{q})\rangle_f = \frac{1}{n}\int \mathrm{d}^3\vec{p}\, O(\vec{p},\vec{q})[1+g_1(\vec{p},\vec{q},t)]f_0(\vec{q},\vec{p},t) = \langle O(1+g_1)\rangle_{f_0} \,, \tag{2.193}$$

which amounts to integrating $O(1+g_1)$ against the Gaussian distribution f_0. For pressure, this yields

$$P_{\alpha\beta} = nm\langle\delta v_\alpha \delta v_\beta\rangle_f \tag{2.194}$$

$$= nm\langle\delta v_\alpha\delta v_\beta\rangle_{f_0} - nm^2\frac{\tau_{\rm mft}}{k_BT}u_{\gamma\delta}[\langle\delta v_\alpha\delta v_\beta\delta v_\gamma\delta v_\delta\rangle_{f_0} - \frac{\delta_{\gamma\delta}}{3}\langle\delta v_\alpha\delta v_\beta\delta v_\mu\delta v_\mu\rangle_{f_0}] + 0 \,, \tag{2.195}$$

where the "0" stems from integrating odd powers of $\delta\vec{v}$ against f_0.

Thanks to Wick theorem, we know that the moments of a Gaussian distribution can be computed by summing all possible pairings of two-point functions involved in such moments. As a result

$$\langle\delta v_\alpha\delta v_\beta\delta v_\gamma\delta v_\delta\rangle_{f_0} = \frac{(k_BT)^2}{m^2}(\delta_{\alpha\beta}\delta_{\gamma\delta} + \delta_{\alpha\gamma}\delta_{\beta\delta} + \delta_{\alpha\delta}\delta_{\gamma\beta}) \,, \tag{2.196}$$

which leads to

$$u_{\gamma\delta}\langle\delta v_\alpha\delta v_\beta\delta v_\gamma\delta v_\delta\rangle_{f_0} = \frac{(k_BT)^2}{m^2}(u_{\gamma\gamma}\delta_{\alpha\beta}+2u_{\alpha\beta}), \quad \text{and} \quad \langle\delta v_\alpha\delta v_\beta\delta v_\mu\delta v_\mu\rangle_{f_0} = \frac{(k_BT)^2}{m^2}5\delta_{\alpha\beta}\ . \tag{2.197}$$

This leads to an estimate of the pressure tensor "to first order in $\tau_{\rm mft}/\tau_{\rm F}$" given by:

$$P_{\alpha\beta} = nk_BT\delta_{\alpha\beta} - nk_BT\tau_{\rm mft}(2u_{\alpha\beta}+u_{\gamma\gamma}\delta_{\alpha\beta}-\frac{5}{3}u_{\gamma\gamma}\delta_{\alpha\beta})\ . \tag{2.198}$$

At this stage, you may rightfully complained and ask where the factor $\tau_{\rm mft}/\tau_{\rm F}$ is in this expression. Working back in unit of $\tilde{t}$ and not t, would shift $\vec{u}\to\vec{u}/\tau_{\rm F}$, which would replace $\tau_{\rm mft}$ by $\varepsilon=\tau_{\rm mft}/\tau_{\rm F}$. This is thus consistent with our perturbation theory, just less obvious than if we had rescaled all the hydrodynamic equations.

Finally, we can rewrite the pressure tensor in a slightly nicer form:

$$P_{\alpha\beta} = mk_BT[\delta_{\alpha\beta}(1+\frac{2}{3}\tau_{\rm mft}u_{\gamma\gamma})-2\tau_m u_{\alpha\beta}]\ . \tag{2.199}$$

While the renormalization of the diagonal term is unlikely to help us with shear modes, let us show how the off-diagonal terms in $u_{\alpha\beta}$ prove crucial in reaching equilibrium.

Relaxation of shear flows. Again, we consider $\vec{u}(\vec{q})=u(y)\hat{x}$, so that

$$u_{\alpha\beta} = \frac{1}{2}(\partial_\alpha u_\beta+\partial_\beta u_\alpha) = \frac{1}{2}(\delta_{\alpha y}\delta_{\beta x}+\delta_{\beta y}\delta_{\alpha x})u'(y)\ , \tag{2.200}$$

which turns the pressure tensor into

$$P_{\alpha\beta} = nk_BT\delta_{\alpha\beta} - nk_BT\tau_{\rm mft}(\delta_{\alpha y}\delta_{\beta x}+\delta_{\beta y}\delta_{\alpha x})u'(y)\ . \tag{2.201}$$

In turn, the time evolution of $\vec{u}$ becomes

$$mD_tu_x = -\frac{1}{n}\partial_{q_\alpha}P_{\alpha x} \quad \leftrightarrow \quad m\partial_t u(y) = -\frac{1}{n}\partial_y[nk_BT\tau_{\rm mft}u'(y)]\ . \tag{2.202}$$

When $n=n_0$ and $T=T_0$, this simplifies into a diffusion equation for $u(y)$:

$$\partial_t u(y,t) = \nu\partial_{yy}u(y,t) \qquad \text{where} \qquad \nu = \frac{\tau_{\rm mft}k_BT}{m} \tag{2.203}$$

is the kinematic viscosity. The steady-state solution of the diffusion equation is $u(y)=0$, and the shear mode vanishes, leading the system to an equilibrium state. Equation (**??**) is also very nice because it gives us a microscopic intuition of where viscosity comes from: it is the collisions between the gas particles that prevent the development of strong velocity gradients.

The relaxation mechanism of the shear mode is thus due to the fact that f relaxes to $f^{\rm LEQ}$ but does not reach it. The small distance to $f^{\rm LEQ}$, given by εf_1, induces a small shift in the pressure which, given enough time ($t\sim\tau_{\rm F}$) suffice to equilibrate the system.

Heat conductivity. Using similar algebra, one finds the heat flux to be given by

$$\vec{h} = -\kappa\nabla T, \qquad \text{where} \qquad \kappa = \frac{5nk_B^2T\tau_{\rm mft}}{m} \tag{2.204}$$

is the heat conductivity. (See derivation page 8 of Lecture 11.)

First order hydrodynamic. All in all, the first order hydrodynamic reads

$$D_t n = -n\partial_{q_\alpha} u_\alpha \tag{2.205}$$

$$mD_t u_\alpha = -\frac{1}{n}\partial_{q_\alpha}(nk_BT + \frac{2}{3}nk_BT\tau_{\rm mft}\partial_{q_\gamma}u_\gamma) + \frac{1}{n}\partial_{q_\beta}(nk_BT\tau_{\rm mft}u_{\alpha\beta}) \tag{2.206}$$

$$D_t T = \frac{5}{3nk_B}\partial_{q_\alpha}[\frac{n\tau_{\rm mft}k_B^2 T}{m}\partial_{q_\alpha}T] - \frac{2T}{3}[\partial_{q_\alpha}u_\alpha - \tau_{\rm mft}u_{\alpha\beta}u_{\alpha\beta} + \frac{2}{3}\tau_{\rm mft}(\partial_{q_\gamma}u_\gamma)^2] \tag{2.207}$$

The relaxation to equilibrium can be established by linearizing the dynamics

$$n(\vec{q},t) = n_0 + \delta n(\vec{q},t), \qquad \vec{u}\,(\vec{q},t) = \delta\vec{u}\,(\vec{q},t), \qquad T(\vec{q},t) = T_0 + \delta T(\vec{q},t)\ . \tag{2.208}$$

Linearizing the dynamics (2.205)-(2.207) then leads to an eigenvalue problem:

$$\partial_t \begin{pmatrix} \delta n \\ \delta\vec{u} \\ \delta T \end{pmatrix} = M \cdot \begin{pmatrix} \delta n \\ \delta\vec{u} \\ \delta T \end{pmatrix}\ . \tag{2.209}$$

The eigenvalues of M have negative real parts, leading to the decay of the perturbation & the convergence to equilibrium.

Bibliography

[1] Mehran Kardar. *Statistical physics of particles.* Cambridge University Press, 2007.