CHAPTER 8

Microscopic Approach: From Liouville to Boltzmann

In the previous chapters, we derived the Navier-Stokes equations using a macroscopic (continuum) approach to fluid dynamics, based on the concept of fluid elements. We now rederive the same set of equations, but using a far more rigorous, microscopic, particle-based approach. Throughout we consider a 3-dimensional <u>configuration space</u>, which means that the position vector of an individual particle has three components. Note, though, that everything that follows is trivially generalized to a higher or lower dimensional configuration space.

Degree of freedom: an independent physical parameter in the formal description of the <u>state</u> of the physical system. In what follows we use n or n_{dof} to indicate the number of degrees of freedom.

Phase-Space: The phase-space of a dynamical system is a space in which all possible states of a system are represented, with each possible state corresponding to one unique point in that phase-space. The dimensionality of phase-space is n_{dof} .

Caution: I will use 'phase-space' to refer to <u>both</u> this n_{dof} -dimensional space, as well as to the 6-dimensional space (\vec{x}, \vec{v}) in which each individual particle is associated with a point in that space. Some textbooks (e.g., Binney & Tremaine) refer to the n_{dof} -dimensional phase-space as Γ -space).

Canonical Coordinates: in classical mechanics, canonical coordinates are coordinates q_i and p_i in phase-space that are used in the Hamiltonian formalism and that satisfy the <u>canonical commutation relations</u>:

 $\{q_i, q_j\} = 0, \qquad \{p_i, p_j\} = 0, \qquad \{q_i, p_j\} = \delta_{ij}$

Often q_i are Cartesian coordinates in configuration space and p_i is the corresponding <u>linear momentum</u>. However, when using curvi-linear coordinates and q_i is an angle, then the corresponding p_i is an angular momentum. Hence,

 p_i is therefore not always equal to $m\dot{q}_i!!!$ To avoid confusion, p_i is called the conjugate momentum.

Poison Brackets Given two functions $A(q_i, p_i)$ and $B(q_i, p_i)$ of the phasespace coordinates q_i and p_i , the Poison bracket of A and B is defined as

$$\{A, B\} = \sum_{i=1}^{3N} \left(\frac{\partial A}{\partial q_i} \frac{\partial B}{\partial p_i} - \frac{\partial A}{\partial p_i} \frac{\partial B}{\partial q_i} \right)$$

In vector notation,

$$\{A,B\} = \sum_{i=1}^{N} \left(\frac{\partial A}{\partial \vec{q_i}} \cdot \frac{\partial B}{\partial \vec{p_i}} - \frac{\partial A}{\partial \vec{p_i}} \cdot \frac{\partial B}{\partial \vec{q_i}} \right)$$

where $\vec{q_i} = (q_{i1}, q_{i2}, q_{i3})$ and $\vec{p_i} = (p_{i1}, p_{i2}, p_{i3})$ and *i* now indicates a particular particle (i = 1, 2, ..., N).

Let N be the number of constituent particles in our fluid. In all cases of interests, N will be a huge number; $N \gg 10^{20}$. How do you (classically) describe such a system? To completely describe a fluid of N particles, you need to specify for each particle the following quantities:

position
$$\vec{q} = (x_1, x_2, x_3)$$

conjugate momenta $\vec{p} = (v_1, v_2, v_3)$
internal degrees of freedom $\vec{s} = (s_1, s_2, ..., s_K)$

Examples of internal degrees of freedom are electrical charge (in case of a plasma), or the rotation or vibrational modes for molecules, etc. The number of degrees of freedom in the above example is $n_{dof} = N(6 + K)$. In what follows we will only consider particles with zero internal dof (i.e., K = 0 so that $n_{dof} = 6N$). Such particles are sometimes called <u>monoatoms</u>, and can be treated as point particles. The <u>microstate</u> of a system composed of N monoatoms is completely described by

$$\vec{\Gamma} = (\vec{q}_1, \vec{q}_2, ..., \vec{q}_N, \vec{p}_1, \vec{p}_2, ..., \vec{p}_N)$$

which corresponds to a single point in our 6N-dimensional phase-space.

The dynamics of our fluid of N monoatoms is described by its <u>Hamiltonian</u>

$$\mathcal{H}(\vec{q}_i, \vec{p}_i, t) \equiv \mathcal{H}(\vec{q}_1, \vec{q}_2, ..., \vec{q}_N, \vec{p}_1, \vec{p}_2, ..., \vec{p}_N, t) = \sum_{i=1}^N \vec{p}_i \cdot \dot{\vec{q}}_i - \mathcal{L}(\vec{q}_i, \dot{\vec{q}}_i, t)$$

where $\mathcal{L}(\vec{q_i}, \dot{\vec{q_i}}, t)$ is the system's Lagrangian, and $\dot{\vec{q_i}} = \mathrm{d}\vec{q_i}/\mathrm{d}t$.

The corresponding equations of motion are:

$$\dot{\vec{q}_i} = \frac{\partial \mathcal{H}}{\partial \vec{p}_i}; \qquad \dot{\vec{p}_i} = -\frac{\partial \mathcal{H}}{\partial \vec{q}_i}$$

Thus, given $\vec{q_i}$ and $\vec{p_i}$ at any given time t, one can compute the Hamiltonian and solve for the equations of motion to obtain $\vec{q_i}(t)$ and $\vec{p_i}(t)$. They specify a unique trajectory $\vec{\Gamma}(t)$ in this phase-space. Note that no two tracjectories $\vec{\Gamma}_1(t)$ and $\vec{\Gamma}_2(t)$ are allowed to cross each other. If that were the case, it would be a violation of the <u>deterministic character</u> of classical physics. The Hamiltonian formalism described above basically is a <u>complete treatment</u> of fluid dynamics. In practice, though, it is utterly useless, simply because Nis HUGE, making it impossible to specify the complete set of initial conditions. We neither have (nor want) the detailed information that is required to specify a <u>microstate</u>. We are only concerned with (interested in) the average behavior of the <u>macroscopic</u> properties of the system, such as density, temperature, pressure, etc. With each such <u>macrostate</u> corresponds a huge number of microstates, called a <u>statistical ensemble</u>.

The ensemble is described statistically by the N-body distribution function

$$f^{(N)}(\vec{q}_i, \vec{p}_i) \equiv f^{(N)}(\vec{q}_1, \vec{q}_2, ..., \vec{q}_N, \vec{p}_1, \vec{p}_2, ..., \vec{p}_N)$$

which expresses the ensemble's probability distribution, i.e., $f^{(N)}(\vec{q}_i, \vec{p}_i) dV$ is the probability that the actual microstate is given by $\vec{\Gamma}(\vec{q}_i, \vec{p}_i)$, where $dV = \prod_{i=1}^{N} d^3 \vec{q}_i d^3 \vec{p}_i$. This implies the following <u>normalizion condition</u>

$$\int \mathrm{d}V f^{(N)}(\vec{q_i}, \vec{p_i}) = 1$$

In our statistical approach, we seek to describe the evolution of the *N*body distribution function, $f^{(N)}(\vec{q_i}, \vec{p_i}, t)$, rather than that of a particular microstate, which instead is given by $\vec{\Gamma}(\vec{q_i}, \vec{p_i}, t)$. Since probability is locally conserved, it must obey a <u>continuity equation</u>; any change of probability in one part of phase-space must be compensated by a flow of probability into or out of neighboring regions. As we have seen in Chapter 5, the continuity equation of a (continuum) density field, $\rho(\vec{x})$, is given by

$$\frac{\partial \rho}{\partial t} + \nabla(\rho \, \vec{v}) = 0$$

which expresses that the local change in the mass enclosed in some volume is balanced by the divergence of the flow out of that volume. In the case of our probability distribution $f^{(N)}$ we have that ∇ is in 6*N*-dimensional phase-space, and includes $\partial/\partial \vec{q_i}$ and $\partial/\partial \vec{p_i}$ while the 'velocity vector' is given by $(\dot{\vec{q_i}}, \dot{\vec{p_i}})$. Hence, the continuity equation for $f^{(N)}$, which is known as the **Liouville equation**, can be written in any of the following three forms:

$$\frac{\partial f^{(N)}}{\partial t} + \sum_{i=1}^{N} \left(\dot{\vec{q}}_{i} \cdot \frac{\partial f^{(N)}}{\partial \vec{q}_{i}} + \dot{\vec{p}}_{i} \cdot \frac{\partial f^{(N)}}{\partial \vec{p}_{i}} \right) = 0$$
$$\frac{\partial f^{(N)}}{\partial t} + \{f^{(N)}, \mathcal{H}\} = 0$$
$$\frac{\mathrm{d} f^{(N)}}{\mathrm{d} t} = 0$$

The Liouville equation (which is actually due to Gibbs) expresses the Liouville Theorem that the flow of Γ -points through phase-space is incompressible. If you follow some region of phase-space under Hamiltonian evolution, then its shape can change, but not its volume.

Although we have moved away from trying to describe the evolution of single microstates, $\vec{\Gamma}(t)$, by considering instead the evolution of the *N*-body DF $f^{(N)}(\vec{q_i}, \vec{p_i})$, this hasn't really made life any easier. After all, $f^{(N)}$ is still a function of 6*N* variables, which is utterly unmanageable. In order to proceed, we first simplify notation by defining

$$\vec{w_i} \equiv (\vec{q_i}, \vec{p_i})$$

Next we define the <u>reduced</u> or <u>K-body DF</u>, which is obtained by integrating the N-body DF, $f^{(N)}$, over N - K six-vectors $\vec{w_i}$. Since $f^{(N)}$ is symmetric in $\vec{w_i}$, without loss of generality we may choose the integration variables to be $\vec{w_{K+1}}, \vec{w_{K+2}}, ..., \vec{w_N}$:

$$f^{(K)}(\vec{w}_1, \vec{w}_2, ..., \vec{w}_K, t) \equiv \frac{N!}{(N-K)!} \int \prod_{i=K+1}^N \mathrm{d}^6 \vec{w}_i f^{(N)}(\vec{w}_1, \vec{w}_2, ..., \vec{w}_N, t)$$

where the choice of the prefactor will become clear in what follows.

In particular, the 1-particle distribution function is

$$f^{(1)}(\vec{w}_1, t) \equiv N \int \prod_{i=2}^N \mathrm{d}^6 \vec{w}_i f^{(N)}(\vec{w}_1, \vec{w}_2, ..., \vec{w}_N, t)$$

Because of the prefactor, we now have that

$$\int d^6 \vec{w} f^{(1)}(\vec{w}, t) = \int d^3 \vec{q} \int d^3 \vec{p} f^{(1)}(\vec{q}, \vec{p}, t) = N$$

Hence, $f^{(1)}(\vec{q}, \vec{p}, t) = dN/d^3\vec{q} d^3\vec{p}$ is the number of particles in the phase-space volume $d^3\vec{q} d^3\vec{p}$ centered on (\vec{q}, \vec{p}) .

That $f^{(1)}(\vec{w},t)$ is an important, relevant DF is evident from the following. Consider an <u>observable</u> $Q(\vec{w})$ that involves only quantities that depend additively on the phase-space coordinates of <u>single</u>, individual particles. Examples are velocity, kinetic energy, or any other velocity moment v^k . The expectation value, $\langle Q \rangle$, can be written as

$$\langle Q \rangle = \int d^6 \vec{w}_1 \dots d^6 \vec{w}_N f^{(N)}(\vec{w}_1, \vec{w}_2, \dots, \vec{w}_N) \sum_{i=1}^N Q_i$$

Since all particles are statistically identical, $f^{(N)}$ is a symmetric function of $\vec{w_i}$, which implies that

$$f^{(N)}(...,\vec{w_i},...,\vec{w_j},...) = f^{(N)}(...,\vec{w_j},...,\vec{w_i},...) \qquad \forall (i,j)$$

In words; if you flip the indices of any two particles, nothing changes. This allows us to write that

$$\langle Q \rangle = \int d^6 \vec{w_1} Q(\vec{w_1}) f^{(1)}(\vec{w_1})$$

Hence, computing the expectation value for any observable $Q(\vec{w})$ only requires knowledge of the one-particle DF.

For the time evolution of each reduced DF we can write

$$\frac{\partial f^{(K)}}{\partial t} = \frac{N!}{(N-K)!} \int \prod_{i=K+1}^{N} \mathrm{d}^{6} \vec{w_{i}} \frac{\partial f^{(N)}}{\partial t} (\vec{w_{1}}, \vec{w_{2}}, ..., \vec{w_{N}})$$
$$= \frac{N!}{(N-K)!} \int \prod_{i=K+1}^{N} \mathrm{d}^{6} \vec{w_{i}} \{\mathcal{H}, f^{(N)}\}$$

Now we substitute the Hamiltonian. To do so, we adopt that $\vec{w_i} = (\vec{r_i}, \vec{p_i})$, with $\vec{r_i}$ the Cartesian position vector of particle *i*, and $\vec{p_i} = m \vec{v_i}$ the corresponding linear momentum. This allows us to write

$$\begin{aligned} \mathcal{H}(\vec{r}_i, \vec{p}_i, t) &= \mathcal{H}(\vec{r}_1, \vec{r}_2, ..., \vec{r}_N, \vec{p}_1, \vec{p}_2, ..., \vec{p}_N) \\ &= \sum_{i=1}^N \frac{\vec{p}_i^2}{2m} + \sum_{i=1}^N V(\vec{r}_i) + \sum_{i < j} U(\vec{r}_i - \vec{r}_j) \end{aligned}$$

Note that the Hamiltonian contains three terms; a <u>kinetic</u> energy term, a term describing the potential energy due to an <u>external force</u> $\vec{F} = -\nabla V$ that acts equally on all particles, and the potential energy $U(\vec{r_i} - \vec{r_j})$ related to <u>two-body interactions</u> between particles *i* and *j*. Examples of the latter are the VanderWaals force in the case of a liquid, the Coulomb force in the case of a plasma, and the gravitational force in the case of dark matter halo. Without derivation (see any good textbook on kinetic theory), substituting this Hamiltonian into the evolution equation for the one-particle DF yields

$$\frac{\partial f^{(1)}}{\partial t} = N \int \prod_{i=2}^{N} \mathrm{d}^{6} \vec{w_{i}} \left\{ \mathcal{H}, f^{(N)} \right\} = \left\{ \mathcal{H}^{(1)}, f^{(1)} \right\} + \left(\frac{\partial f^{(1)}}{\partial t} \right)_{\mathrm{coll}}$$

where $\mathcal{H}^{(1)} = \vec{p_i}^2/(2m) + V(\vec{r})$ is the one-particle Hamiltonian, and

$$\left(\frac{\partial f^{(1)}}{\partial t}\right)_{\text{coll}} = \int \mathrm{d}^3 \vec{r}_2 \, \mathrm{d}^3 \vec{p}_2 \, \frac{\partial U(\vec{r} - \vec{r}_2)}{\partial \vec{r}} \cdot \frac{\partial f^{(2)}}{\vec{p}}$$

Using the convective derivative, the above can be written in concise form as

$$\frac{\mathrm{d}f^{(1)}}{\mathrm{d}t} = \left(\frac{\partial f^{(1)}}{\partial t}\right)_{\mathrm{coll}}$$

which expresses that the 1-particle DF at the location of any particle only changes in time due to collisions which scatter particles into or out of phasespace. Note that the collision term depends on the two-particle DF, $f^{(2)}$. In fact, you can write a similar equation for $\partial f^{(2)}/\partial t$, but will find that it depends on $f^{(3)}$, etc. The resulting set of N coupled equations is known as the **BBGKY hierarchy** (after Bogoliubov, Born, Green, Kirkwood and Yvon, who discovered the equations independently between 1935 and 1946).

We started with the Liouville equation, governing a complicated function of N variable, and it looks like all we have achieved is to replace it with a set of N coupled equations. However, the BBKGY hierarchy is useful since it allows us to make some simplifying assumptions (which will be sufficiently accurate under certain conditions), that truncates the series. The simplest and most useful of these truncations is the **Boltzmann equation**, which is a closed equation for $f^{(1)}$ alone given by

$$\frac{\mathrm{d}f^{(1)}}{\mathrm{d}t} = \left(\frac{\partial f^{(1)}}{\partial t}\right)_{\mathrm{coll}} = I[f^{(1)}]$$

where $I[f^{(1)}]$ is called the collision integral.

The Boltzmann equation is valid uder the following conditions:

- dilute gas; density is sufficiently low so that only binary collisions need to be considered
- "molecular chaos": velocities of colliding particles are uncorrelated
- spatial dependence of gas properties is sufficiently slow so that DF is constant over the interaction region.
- collisions can be thought of as instantaneous.

The first and fourth assumptions imply that the collision timescale is much shorter than the timescale between collisions. The third and fourth imply that the interaction potential U(r) must be such that $\partial U/\partial r \neq 0$ only over a small region (short-range force). A good example of the latter is the <u>vanderWaals force</u>, for which $F \propto 1/r^6$. For a plasma the collision potential is the Coulomb potential, for which $F \propto 1/r^2$. However, Debye shielding assures that the interaction force remains short-ranged (under certain conditions). In the case of a gravitational system, we again have that $F \propto 1/r^2$, but this times there is no shielding. However, as we will see, in a gravitational N-body system the <u>rate</u> of collisions is typically so low that $(\partial f/\partial t)_{coll} \approx 0$, and the Boltzmann equation becomes the <u>collisionless Boltmann equation</u> (CBE), df/dt = 0.

Finally, a word about **Molecular chaos**. Introduced by Boltzmann (who called it Stosszahlansatz, which translates to collision number hypothesis), molecular chaos implies that

$$f^{(2)}(\vec{r}, \vec{r}, \vec{p}_1, \vec{p}_2) = f^{(1)}(\vec{r}, \vec{p}_1) f^{(1)}(\vec{r}, \vec{p}_2)$$

In words, it assumes that the collision, which occurs at location \vec{r} , is between particles with <u>uncorrelated velocities</u>. However, after the collision, the momenta (let's call them \vec{p}'_1 and \vec{p}'_2) **are** correlated by momentum and energy conservation. So in the limit of many collisions, the ansatz of 'molecular chaos' simply cannot be correct. Most importantly, the ansatz of molecular chaos introduces an element of <u>time-asymmetry</u>, which gives rise to the thermodynamic <u>arrow of time</u> (i.e., the increase of entropy). For comparison, the Liouville equation, which has no underlying assumptions, is perfectly time-reversible!