Chapter V

Reduced classical phase-space densities and their evolution

The description of a classical N-body systems relies on the N-particle phase space Γ: the evolution of the system is represented by a trajectory $(\{\mathfrak{q}^a(t)\}, \{\mathfrak{p}_a(t)\})$ solution of the Hamilton equations (II.1)—corresponding to the sequence of microstates occupied by the system at successive instants—, while observables are functions $O_N\big(\{q^a\}, \{p_a\}\big)$ on Γ. If, as is generally the case for macroscopic systems, the system state is only known on a statistical basis, one also needs the probability density $\rho_N\big(t, \{q^a\}, \{p_a\}\big)$ on Γ, whose time evolution is governed by the Liouville equation (II.10b), see Sec. II.2.

In the large majority of cases, the macroscopic quantities of interest are a measure for the expectation value of microscopic observables that only involve few particles, often only one or two. For instance, the temperature is related to the average kinetic energy of the particles in the system, which involves a single-particle observable. To compute the expectation values of such observables, it is worthwhile to introduce *reduced phase-space densities*, which integrate out the irrelevant degrees of freedom (Sec. V.1). From the Liouville equation for the Γ-space probability density ρ_N, one can then derive the equations of motion governing the dynamics of the reduced densities (Sec. V.2).

In this Chapter and the following one, the positions and momenta of the N particles will be denoted by $\vec{r}_i$ and $\vec{p}_i$ respectively, where $i = 1, \ldots, N$ labels the particle. Accordingly, the argument of a function on the Γ-space of the N particles will be written $\{\vec{r}_i\}, \{\vec{p}_i\}$ or $\vec{r}_1, \vec{p}_1, \ldots, \vec{r}_N, \vec{p}_N$ instead of $\{q^a\}, \{p_a\}$.

V.1 Reduced phase-space densities

Consider a system of N particles (without internal degrees of freedom), which for simplicity are first assumed to be identical. Starting from the N-particle phase-space density $\rho_N(t, \vec{r}_1, \vec{p}_1, \ldots, \vec{r}_N, \vec{p}_N)$ and integrating out the position and momentum coordinates of $N-1$ particles, one defines the *single-particle phase-space density*

$$f_1(t, \vec{r}, \vec{p}) \equiv \alpha_{N,1} \int \rho_N(t, \vec{r}, \vec{p}, \vec{r}_2, \vec{p}_2, \ldots, \vec{r}_N, \vec{p}_N)\, \mathrm{d}^{6(N-1)}\mathcal{V} \tag{V.1a}$$

where $\mathrm{d}^{6(N-1)}\mathcal{V}$ is the infinitesimal volume element in the subspace spanned by the variables $\vec{r}_2, \vec{p}_2, \ldots, \vec{r}_N, \vec{p}_N$. The remaining single-particle phase space is often referred to as μ-space, to distinguish it from the Γ-space.

Similarly, one introduces the *two-particle phase-space density*

$$f_2(t, \vec{r}, \vec{p}, \vec{r}\,', \vec{p}\,') \equiv \alpha_{N,2} \int \rho_N(t, \vec{r}, \vec{p}, \vec{r}\,', \vec{p}\,', \vec{r}_3, \vec{p}_3, \ldots, \vec{r}_N, \vec{p}_N)\, \mathrm{d}^{6(N-2)}\mathcal{V}. \tag{V.1b}$$

More generally, integrating out the positions and momenta of $N-k$ particles in the Γ-space density ρ_N leads to a k-particle phase-space density f_k.

Remark: For a system of identical—i.e. quantum-mechanically indistinguishable—particles, the density ρ_N should be symmetric under the exchange of any two particles, i.e. of the variables $\vec{r}_i$, $\vec{p}_i$ and $\vec{r}_j$, $\vec{p}_j$ for any i, j. Accordingly, which $N-k$ positions and momenta are being integrated out in the definition of the reduced k-particle density f_k is actually unimportant, and any choice leads to the same reduced density.

The definitions (V.1a) and (V.1b) involve constants $\alpha_{N,1}$, $\alpha_{N,2}$. These are often chosen so that the single- and two-particle phase-space densities are respectively normalized to

$$\int f_1(t,\vec{r},\vec{p})\,\mathrm{d}^3\vec{r}\;\mathrm{d}^3\vec{p} = N, \tag{V.2a}$$

i.e. the total number of particles, and

$$\int f_2(t,\vec{r},\vec{p},\vec{r}\,',\vec{p}\,')\,\mathrm{d}^3\vec{r}\;\mathrm{d}^3\vec{p}\;\mathrm{d}^3\vec{r}\,'\,\mathrm{d}^3\vec{p}\,' = N(N-1), \tag{V.2b}$$

that is, the total number of ordered pairs. More generally, one requires that the integral of f_k be equal to the total number of ordered k-tuples. This requirement dictates for identical particles the choice $\alpha_{N,k} = 1/(2\pi\hbar)^{3k}$, independent of N. With these normalizations, $f_1(t,\vec{r},\vec{p})\,\mathrm{d}^3\vec{r}\,\mathrm{d}^3\vec{p}$ is the average number of particles in the infinitesimal volume element $\mathrm{d}^3\vec{r}\;\mathrm{d}^3\vec{p}$ around the μ-space point $(\vec{r},\vec{p})$ at time t, while $f_2(t,\vec{r},\vec{p},\vec{r}\,',\vec{p}\,')\,\mathrm{d}^3\vec{r}\;\mathrm{d}^3\vec{p}\;\mathrm{d}^3\vec{r}\,'\,\mathrm{d}^3\vec{p}\,'$ is the average number of ordered pairs with one particle in the volume element $\mathrm{d}^3\vec{r}\;\mathrm{d}^3\vec{p}$ around $(\vec{r},\vec{p})$ and the other in $\mathrm{d}^3\vec{r}\,'\,\mathrm{d}^3\vec{p}\,'$ around $(\vec{r}\,',\vec{p}\,')$. The various f_k are thus number densities in the respective phase spaces, rather than probability densities.

Integrating the single-particle phase-space density (V.1a) normalized according to Eq. (V.2a) over momentum, one recovers the usual *particle number density* (in position space)

$$n(t,\vec{r}) \equiv \int f_1(t,\vec{r},\vec{p})\,\mathrm{d}^3\vec{p}. \tag{V.3a}$$

Remarks:

∗ Up to the normalization $[N!/(N-k)!$ instead of $1]$, the reduced phase-space densities f_k are marginal distributions (see Appendix B.4.1) of the Γ-space density ρ_N.

∗ Given the normalization adopted here, the densities f_k are dimensionful quantities. It is sometimes preferable to work with dimensionless densities, namely $\mathsf{f}_k \equiv (2\pi\hbar)^{3k} f_k$, which correspond to the simpler normalization constant $\alpha_{N,k} = 1$ for all k. Integrating f_1 over a spatial volume on which the system is homogeneous then yields the so-called *phase-space occupancy*—where "phase space" actually means momentum space.

> The various results of this chapter, as e.g. the BBGKY hierarchy (V.14), still hold when replacing the reduced densities f_k by the dimensionless f_k, provided every momentum-space volume element $\mathrm{d}^3\vec{p}$ appearing in an integral is replaced by $\mathrm{d}^3\vec{p}/(2\pi\hbar)^3$. For instance,
>
> $$n(t,\vec{r}) \equiv \int \mathsf{f}_1(t,\vec{r},\vec{p})\,\frac{\mathrm{d}^3\vec{p}}{(2\pi\hbar)^3}. \tag{V.3b}$$

∗ The reduced densities f_k depend on the underlying statistical ensemble. Here, since the number of particles N is fixed, we are implicitly considering the canonical ensemble, yet this is just for the sake of simplicity.

> In the "grand-canonical" case of a fluctuating particle number, integrating the phase-space density ρ defined in § II.2.5 over the irrelevant degrees of freedom yields the reduced k-particle density
>
> $$f_k = \sum_{N=k}^{\infty} \pi_N f_{k|N-k}$$

where $f_{k|N-k}$ is the ("canonical") reduced k-particle distribution under the condition that there are exactly N particles in the system while π_N is the probability that this is the case. Accordingly, f_1 is then normalized to $\langle N\rangle$, f_2 to $\langle N(N-1)\rangle$, and so on.
The reader can check that for a classical ideal gas, $f_2(t,\vec{r},\vec{p},\vec{r}\,',\vec{p}\,') = f_1(t,\vec{r},\vec{p})f_1(t,\vec{r}\,',\vec{p}\,')$ in the grand-canonical case—which can be interpreted as signaling the absence of correlations between particles—, while the identity does not hold when the total particle number is fixed.

With the help of the μ-space density f_1, the expectation value of a single-particle observable $O_1(\vec{r},\vec{p})$ reads

$$\big\langle O_1(t)\big\rangle_t = \frac{\displaystyle\int O_1(\vec{r},\vec{p})\, f_1(t,\vec{r},\vec{p})\,\mathrm{d}^3\vec{r}\;\mathrm{d}^3\vec{p}}{\displaystyle\int f_1(t,\vec{r},\vec{p})\,\mathrm{d}^3\vec{r}\;\mathrm{d}^3\vec{p}}. \tag{V.4}$$

The expectation value of a two-particle observable can similarly be expressed as an average weighted by the two-particle density f_2.

V.2 Time evolution of the reduced phase-space densities

We now deduce from the Liouville equation (V.5) in Γ-space the equations of motion for the reduced phase-space densities, first for a system of particles in the absence of vector potential (§ V.2.2), then for charged particles in a external vector potential (§ V.2.3).

V.2.1 Description of the system

Consider identical pointlike particles of mass m, without internal degrees of freedom, whose positions and canonical momenta will be denoted by $\vec{r}_i$ and $\vec{p}_i$. For a system of N such particles, the Liouville equation (II.10b) can be recast as

$$\frac{\partial\rho_N\big(t,\{\vec{r}_j\},\{\vec{p}_j\}\big)}{\partial t} + \sum_{i=1}^{N}\dot{\vec{r}}_i\cdot\vec{\nabla}_{\vec{r}_i}\rho_N\big(t,\{\vec{r}_j\},\{\vec{p}_j\}\big) + \sum_{i=1}^{N}\dot{\vec{p}}_i\cdot\vec{\nabla}_{\vec{p}_i}\rho_N\big(t,\{\vec{r}_j\},\{\vec{p}_j\}\big) = 0, \tag{V.5a}$$

where $\vec{\nabla}_{\vec{r}_i}$, $\vec{\nabla}_{\vec{p}_i}$ stand for the three-dimensional gradients whose coordinates are the derivatives with respect to the canonical variables $\vec{r}_i$, $\vec{p}_i$. In turn, $\dot{\vec{r}}_i$—i.e. the velocity $\vec{v}_i$ of particle i—and $\dot{\vec{p}}_i$ denote the time derivatives of the canonical variables. Invoking the Hamilton equations of motion (II.1) and dropping the variables for brevity, the Liouville equation becomes

$$\frac{\partial\rho_N}{\partial t} + \sum_{i=1}^{N}\vec{\nabla}_{\vec{p}_i}H_N\cdot\vec{\nabla}_{\vec{r}_i}\rho_N - \sum_{i=1}^{N}\vec{\nabla}_{\vec{r}_i}H_N\cdot\vec{\nabla}_{\vec{p}_i}\rho_N = 0 \tag{V.5b}$$

with H_N the Hamilton function of the system, which will be discussed later in this section.

In both this Chapter and the following we shall implicitly work in the "thermodynamic limit" of infinitely many particles occupying an infinitely large volume, thereby allowing for an infinitely large total energy of the system. As a result, the Cartesian components of both spatial and momentum variables can take values spanning the whole real axis from $-\infty$ to $+\infty$. Now, to ensure its normalizability [Eq. (II.3)], the probability density ρ_N must vanish when any of the phase-space variables goes to infinity: the partial differential equation (V.5a) is thus to be complemented with the boundary conditions

$$\lim_{|\vec{r}_i|\to\infty}\rho_N\big(t,\{\vec{r}_j\},\{\vec{p}_j\}\big) = 0 \quad\text{and}\quad \lim_{|\vec{p}_i|\to\infty}\rho_N\big(t,\{\vec{r}_j\},\{\vec{p}_j\}\big) = 0 \qquad \forall i\in\{1,\dots,N\}. \tag{V.6}$$

Accordingly, integrals of the type

$$\int \vec{\nabla}_{\vec{r}_i} \rho_N\big(t, \{\vec{r}_j\}, \{\vec{p}_j\}\big)\, \mathrm{d}^3\vec{r}_i \quad \text{resp.} \quad \int \vec{\nabla}_{\vec{p}_i} \rho_N\big(t, \{\vec{r}_j\}, \{\vec{p}_j\}\big)\, \mathrm{d}^3\vec{p}_i \tag{V.7}$$

over the whole allowed range for $\vec{r}_i$ resp. $\vec{p}_i$ identically vanish.

> For the sake of completeness, let us briefly mention some of the necessary changes taking place if the spatial volume $\mathcal{V}$ occupied by the system is not infinite—as is e.g. the case of a gas enclosed in a fixed box. In short, the treatment becomes slightly more tedious.
>
> First, the total number N of particles is then finite, and so is the total energy of the system. As a result, the (kinetic) energy of an individual particle cannot be infinitely large, which means that the range of allowed momentum values is finite: the behavior of ρ_N at the edges of the momentum range is no longer obvious, although it is natural to assume that ρ_N vanishes.
>
> Since the spatial volume is finite, the variables $\vec{r}_i$ are also restricted to a finite range. It is then necessary to specify the boundary conditions at these spatial edges ("walls"). A useful choice is to assume that the boundaries behave like perfect mirrors for the particles, which are thus reflected elastically according to the Snell[(bq)]–Descartes[(br)] law of reflection: this has the advantage of ensuring the conservation of kinetic energy; however such a particle-wall collision does not conserve (linear) momentum, which is unsatisfactory. The "proper" approach is then to resort to a microscopic description of the walls themselves, which become part of the system under study.

Let us now specify the Hamilton function H_N of the system. For the sake of simplicity, we shall assume that the particles can only interact with each other pairwise, i.e. we discard possible genuine three-, four-, ..., many-body interaction terms. These two-body interactions can be described in terms of an interaction potential W,[(75)] which will be assumed to depend on the inter-particle distance only.

We also allow for the possible presence of external potentials acting on the particles. Here one has to distinguish between two possibilities. Thus, a scalar potential $V(t, \vec{r})$—e.g. electrostatic, (Newtonian) gravitational, or a potential well enclosing particles in a specified volume—only constitutes a minor modification, since it does not affect the canonical momentum $\vec{p}_i$ conjugate to position. In contrast, any vector potential $\vec{A}(t, \vec{r})$ directly enters the canonical momentum, so that we shall have to discuss the gauge invariance of the evolution equations for the reduced phase-space densities.

In the absence of vector potential, the Hamilton function of the system is thus of the type

$$H_N = \sum_{i=1}^{N} \frac{\vec{p}_i^{\,2}}{2m} + \sum_{i=1}^{N} V(t, \vec{r}_i) + \sum_{1 \leq i < j \leq N} W\big(|\vec{r}_i - \vec{r}_j|\big). \tag{V.8}$$

For a system of electrically charged particles with charge q in an external electromagnetic field described by scalar and vector potentials $(\phi, \vec{A})$, the Hamiltonian reads

$$H_N = \sum_{i=1}^{N} \frac{\big[\vec{p}_i - q\vec{A}(t, \vec{r}_i)\big]^2}{2m} + \sum_{i=1}^{N} q\phi(t, \vec{r}_i) + \sum_{1 \leq i < j \leq N} W\big(|\vec{r}_i - \vec{r}_j|\big), \tag{V.9}$$

where the energy corresponding to the scalar potential has been denoted by $q\phi$ instead of V.

In the remainder of this Chapter, we shall use the shorthand notations $W_{ij} \equiv W\big(|\vec{r}_i - \vec{r}_j|\big)$ for the interaction potential, as well as

$$\vec{F}_i \equiv -\vec{\nabla}_{\vec{r}_i} V(\vec{r}_i) \tag{V.10a}$$

[(75)] More precisely, $W\big(|\vec{r}_i - \vec{r}_j|\big)$ is the interaction potential energy.

[(bq)] W. Snellius, 1580–1626 [(br)] R. Descartes, 1596–1650

and

$$\vec{K}_{ij} \equiv -\vec{\nabla}_{\vec{r}_i} W\big(|\vec{r}_i - \vec{r}_j|\big) \tag{V.10b}$$

for the forces upon particle i due to the external potential V and to particle $j \neq i$, respectively. In accordance with Newton's third law,

$$\vec{K}_{ij} = -\vec{K}_{ji}, \tag{V.10c}$$

which follows from $\vec{\nabla}_{\vec{r}_j} W_{ij} = -\vec{\nabla}_{\vec{r}_i} W_{ij}$ and the relabeling of particles.

Remarks:

∗ The above forms of the Hamilton function implicitly assume that the forces at play in the system are additive, as is always the case in Newtonian physics.

∗ In the absence of interactions, the Hamilton function (V.8) clearly reduces to that of a classical ideal gas.

V.2.2 System of neutral particles

In the absence of external vector potential, the equations of motion (II.1) resulting from the Hamilton function (V.8) read

$$\dot{\vec{r}}_i = \vec{\nabla}_{\vec{p}_i} H_N = \frac{\vec{p}_i}{m}, \qquad \dot{\vec{p}}_i = -\vec{\nabla}_{\vec{r}_i} H_N = \vec{F}_i + \sum_{j\neq i} \vec{K}_{ij} \tag{V.11}$$

for every particle i. The first equation simply states that linear momentum and canonical momentum coincide, from where it follows that the second equation is Newton's second law.

Accordingly, the Liouville equation (V.5) becomes

$$\frac{\partial \rho_N}{\partial t} + \sum_{i=1}^{N} \vec{v}_i \cdot \vec{\nabla}_{\vec{r}_i} \rho_N + \sum_{i=1}^{N} \vec{F}_i \cdot \vec{\nabla}_{\vec{p}_i} \rho_N + \sum_{i=1}^{N} \sum_{\substack{j=1 \\ j\neq i}}^{N} \vec{K}_{ij} \cdot \vec{\nabla}_{\vec{p}_i} \rho_N = 0. \tag{V.12}$$

V.2.2 a BBGKY hierarchy

The reduced k-particle phase density $f_k(t, \vec{r}_1, \vec{p}_1, \ldots, \vec{r}_k, \vec{p}_k)$ follows from the Γ-space probability density ρ_N after integrating out the degrees of freedom of the remaining $N-k$ particles. Similarly, integrating the Liouville equation (V.12) over the positions and momenta $\vec{r}_j$, $\vec{p}_j$ of $N-k$ particles gives the evolution equation obeyed by f_k.

This integration is made simpler by the boundary conditions (V.6): since the velocity $\vec{v}_i$ resp. the force $\vec{F}_i$ is independent of $\vec{r}_i$ resp. $\vec{p}_i$, it can be factored outside of the integral

$$\int \vec{v}_i \cdot \vec{\nabla}_{\vec{r}_i} \rho_N \, \mathrm{d}^3\vec{r}_i \quad \text{resp.} \quad \int \vec{F}_i \cdot \vec{\nabla}_{\vec{p}_i} \rho_N \, \mathrm{d}^3\vec{p}_i, \tag{V.13}$$

leaving an integral of the type (V.7) that vanishes. Additionally, we shall assume that we are allowed to exchange the integration and partial differentiation operations when needed.

Integrating the Liouville equation (V.12) over the positions and momenta of the $N-1$ particles labeled 2, 3, …, N and multiplying with the proper normalization factor $\alpha_{N,1} = 1/(2\pi\hbar)^3$ yields for the evolution of the single-particle density (V.1a) the equation

$$\begin{aligned} &\frac{\partial f_1(t, \vec{r}_1, \vec{p}_1)}{\partial t} + \vec{v}_1 \cdot \vec{\nabla}_{\vec{r}_1} f_1(t, \vec{r}_1, \vec{p}_1) + \vec{F}_1 \cdot \vec{\nabla}_{\vec{p}_1} f_1(t, \vec{r}_1, \vec{p}_1) \\ &\qquad + \sum_{j=2}^{N} \frac{1}{(2\pi\hbar)^3} \int \vec{K}_{1j} \cdot \vec{\nabla}_{\vec{p}_1} \rho_N\big(t, \{\vec{r}_i\}, \{\vec{p}_i\}\big) \, \mathrm{d}^{6(N-1)}\mathcal{V}(2, \ldots, N) = 0, \end{aligned}$$

where the notation $\mathrm{d}^{6(N-1)}\mathcal{V}(2, \ldots, N)$ emphasizes the labels of the particles which are integrated out. In the integral in the second line, it is convenient to write

$$\mathrm{d}^{6(N-1)}\mathcal{V}(2, \ldots, N) = \frac{1}{N-1} \frac{\mathrm{d}^3\vec{r}_j \, \mathrm{d}^3\vec{p}_j}{(2\pi\hbar)^3} \, \mathrm{d}^{6(N-2)}\mathcal{V}(2, \ldots, j-1, j+1, \ldots, N)$$

to isolate particle j from the $N-2$ particles $i \neq j$. The latter are then straightforwardly dealt with: integrating over their phase-space coordinates yields, together with the factor $1/(2\pi\hbar)^6 = \alpha_{N,2}$, precisely the two-particle phase-space density $f_2(t, \vec{r}_1, \vec{p}_1, \vec{r}_j, \vec{p}_j)$, i.e.

$$\frac{1}{(2\pi\hbar)^3}\int \vec{K}_{1j}\cdot\vec{\nabla}_{\vec{p}_1}\rho_N\big(t,\{\vec{r}_i\},\{\vec{p}_i\}\big)\,\mathrm{d}^{6(N-1)}\mathcal{V}(2,\ldots,N) = \frac{1}{N-1}\int \vec{K}_{1j}\cdot\vec{\nabla}_{\vec{p}_1} f_2(t,\vec{r}_1,\vec{p}_1,\vec{r}_j,\vec{p}_j)\,\mathrm{d}^3\vec{r}_j\,\mathrm{d}^3\vec{p}_j.$$

Thanks to the indistinguishability of the particles, the remaining integral over $\mathrm{d}^3\vec{r}_j\,\mathrm{d}^3\vec{p}_j$ is actually independent of the value of the index j: the sum over j gives $N-1$ times the same contribution, which may be rewritten with the dummy integration variables $\vec{r}_2, \vec{p}_2$, while the factor $N-1$ cancels that coming from the denominator of $\mathrm{d}^{6(N-1)}\mathcal{V}$. All in all, one thus obtains

$$\left(\frac{\partial}{\partial t} + \vec{v}_1\cdot\vec{\nabla}_{\vec{r}_1} + \vec{F}_1\cdot\vec{\nabla}_{\vec{p}_1}\right) f_1(t,\vec{r}_1,\vec{p}_1) = -\int \vec{K}_{12}\cdot\vec{\nabla}_{\vec{p}_1} f_2(t,\vec{r}_1,\vec{p}_1,\vec{r}_2,\vec{p}_2)\,\mathrm{d}^3\vec{r}_2\,\mathrm{d}^3\vec{p}_2. \tag{V.14a}$$

That is, the equation governing the evolution of the single-particle density f_1 involves the two-particle density f_2.

By integrating out $N-2$ particles in the Liouville equation (V.12), one finds in a similar manner the evolution equation for the dynamics of the reduced two-particle density[(76)]

$$\begin{aligned}\left[\frac{\partial}{\partial t} + \vec{v}_1\cdot\vec{\nabla}_{\vec{r}_1} + \vec{v}_2\cdot\vec{\nabla}_{\vec{r}_2} + \vec{F}_1\cdot\vec{\nabla}_{\vec{p}_1} + \vec{F}_2\cdot\vec{\nabla}_{\vec{p}_2} + \vec{K}_{12}\cdot\big(\vec{\nabla}_{\vec{p}_1} - \vec{\nabla}_{\vec{p}_2}\big)\right] f_2(t,\vec{r}_1,\vec{p}_1,\vec{r}_2,\vec{p}_2) = \\ -\int \big(\vec{K}_{13}\cdot\vec{\nabla}_{\vec{p}_1} + \vec{K}_{23}\cdot\vec{\nabla}_{\vec{p}_2}\big) f_3(t,\vec{r}_1,\vec{p}_1,\vec{r}_2,\vec{p}_2,\vec{r}_3,\vec{p}_3)\,\mathrm{d}^3\vec{r}_3\,\mathrm{d}^3\vec{p}_3.\end{aligned} \tag{V.14b}$$

In turn, the evolution equation for f_2 involves the three-particle phase-space density f_3.

> The only trick in deriving this form of the evolution equation consists in using relation (V.10c) to rewrite $\vec{K}_{21}\cdot\vec{\nabla}_{\vec{p}_2}$ as $-\vec{K}_{12}\cdot\vec{\nabla}_{\vec{p}_2}$.

This generalizes to the equation of motion for the reduced k-particle density f_k—obtained by integrating out $N-k$ particles in the Liouville equation (V.12)—, which is not closed, but depends on the $(k+1)$-particle density f_{k+1} for $1 \leq k < N$:

$$\begin{aligned}\left[\frac{\partial}{\partial t} + \sum_{j=1}^{k}\Big(\vec{v}_k\cdot\vec{\nabla}_{\vec{r}_j} + \vec{F}_j\cdot\vec{\nabla}_{\vec{p}_j}\Big) + \sum_{1\leq i<j\leq k}\vec{K}_{ij}\cdot\big(\vec{\nabla}_{\vec{p}_i} - \vec{\nabla}_{\vec{p}_j}\big)\right] f_k(t,\vec{r}_1,\vec{p}_1,\ldots,\vec{r}_k,\vec{p}_k) = \\ -\int\sum_{j=1}^{k}\vec{K}_{j,k+1}\cdot\vec{\nabla}_{\vec{p}_j} f_{k+1}(t,\vec{r}_1,\vec{p}_1,\ldots,\vec{r}_k,\vec{p}_k,\vec{r}_{k+1},\vec{p}_{k+1})\,\mathrm{d}^3\vec{r}_{k+1}\,\mathrm{d}^3\vec{p}_{k+1}.\end{aligned} \tag{V.14c}$$

The meaning of this equation is rather clear: The left-hand side describes the "free", or *streaming* evolution of f_k, involving only the k particles under consideration—including their reciprocal interactions. On the other hand, the right-hand side is a *collision term* describing the interaction between any of these k particles and a partner among the group of the other, not measured particles.

Eventually, the N-particle phase-space density f_N is simply ρ_N multiplied by a normalization factor, so that the evolution equation for f_N is closed, since it is the Liouville equation (V.12) itself

$$\left[\frac{\partial}{\partial t} + \sum_{j=1}^{N}\Big(\vec{v}_j\cdot\vec{\nabla}_{\vec{r}_j} + \vec{F}_j\cdot\vec{\nabla}_{\vec{p}_j}\Big) + \sum_{1\leq i<j\leq N}\vec{K}_{ij}\cdot\big(\vec{\nabla}_{\vec{p}_i} - \vec{\nabla}_{\vec{p}_j}\big)\right] f_N(t,\vec{r}_1,\vec{p}_1,\ldots,\vec{r}_N,\vec{p}_N) = 0. \tag{V.14d}$$

[(76)] Note that there is an erroneous factor of $\frac{1}{2}$ in Eq. (3.60) of Ref. [54].

Together, the coupled equations (V.14a)–(V.14d) constitute the so-called *BBGKY hierarchy*, where the initials stand for Bogolioubov[(bs)]–Born[(bt)]–Green[(bu)]–Kirkwood[(bv)]–Yvon[(bw)] (in alphabetical and reverse chronological order).

The system of equations (V.14) is exact, in the sense that it is strictly equivalent to the Liouville equation for the probability density in Γ-space. Yet since the hierarchy involves all reduced densities, and accordingly N equations, one loses the simplification aimed at when considering single-or two-particle densities only. To recover some simplicity—and thereby be able to actually compute the evolution of the system—, one has to choose a closure procedure, based on physical arguments, which amounts to truncating the hierarchy at some level. This is most often done after Eq. (V.14a), sometimes after Eq. (V.14b).

The most drastic closure prescription, which is discussed in § V.2.2 b below, consists in fully neglecting interactions. A similar, yet physically richer, scheme is to keep Eq. (V.14a) intact, yet to assume that the right-hand side of Eq. (V.14b) vanishes. Alternative procedures will be considered in § V.2.3 b and in the next Chapter.

Remarks:

∗ If the number of particles in the system is not fixed, i.e. in a grand-canonical description, there is no upper bound to the hierarchy.

∗ The generalization to a system consisting of several particle types, labeled a, $b\ldots$, interacting with each other over respective potentials W^{ab}, is quite straightforward. One first needs to introduce the reduced densities f_k^b, $f_k^b\ldots$, for having k particles of a given type in an infinitesimal k-particle phase-space volume, as well as "mixed" densities $f_{k_a k_b\ldots}^{ab\ldots}$ for having k_a particles of type a, k_b particles of type $b\ldots$ within corresponding phase-space volume elements. These various densities—including the mixed ones—then obey coupled equations similar to those of the hierarchy (V.14), with in addition sums over the various particle types. For instance, the evolution equation for f_1^a involves on its right-hand side not only f_2^a, but also all $f_{1,1}^{ab}$ involving the particles of type $b \neq a$ which couple to those of type a.

V.2.2 b System of non-interacting neutral particles: single-particle Liouville equation

Consider first the case where the particles in the system are not interacting, i.e. when W vanishes identically. The Hamilton function H_N can then be expressed as the sum over the N particles of a single-particle Hamiltonian $h \equiv \vec{p}^{\,2}/2m + V(t,\vec{r})$.

Under these conditions, the various equations of the BBGKY hierarchy (V.14) decouple from each other. For instance, the evolution equation (V.14a) for the dynamics of the single-particle density f_1 becomes the *single-particle Liouville equation* (or *collisionless Boltzmann equation*)

$$\frac{\partial f_1(t,\vec{r},\vec{p})}{\partial t} + \vec{v}\cdot\vec{\nabla}_{\vec{r}} f_1(t,\vec{r},\vec{p}) + \vec{F}(t,\vec{r})\cdot\vec{\nabla}_{\vec{p}} f_1(t,\vec{r},\vec{p}) = 0, \tag{V.15}$$

with $\vec{F} = -\vec{\nabla}_{\vec{r}} V$ the external force acting on particles. The contribution $\left(\vec{v}\cdot\vec{\nabla}_{\vec{r}} + \vec{F}\cdot\vec{\nabla}_{\vec{p}}\right) f_1$—which is actually the Poisson bracket in μ-space of $f_1(t,\vec{r},\vec{p})$ and the single-particle Hamilton function $h(\vec{r},\vec{p})$—is often referred to as *drift term*.

The latter implicitly defines two time scales of the system, namely

$$\tau_{\rm s} \sim \left(\vec{v}\cdot\vec{\nabla}_{\vec{r}}\right)^{-1}, \qquad \tau_{\rm e} \sim \left(\vec{F}\cdot\vec{\nabla}_{\vec{p}}\right)^{-1}. \tag{V.16}$$

$\tau_{\rm s}$ is the time for a particle to cross the typical distance over which the single-particle density f_1 is varying. As such, it is also the characteristic time scale for smoothing out spatial inhomogeneities of the single-particle distribution.

[(bs)] N. N. Bogolioubov, 1909–1992 [(bt)] M. Born, 1882–1970 [(bu)] H. S. Green, 1920–1999 [(bv)] J. G. Kirkwood, 1907–1959 [(bw)] J. Yvon, 1903–1979

In turn, τ_e is the typical time associated with the gradient imposed by the external potential V. It is thus also the characteristic time scale over which the system inhomogeneities will relax under the influence of $\vec{F}$ to the equilibrium solution matching the external potential. τ_e is generally larger than τ_s.

Remark: One sees at once that the other equations of the hierarchy involve the same two time scales, and no further one. That is, any f_k evolves with the same time scale as f_1, which will no longer be the case in the presence of interactions.

V.2.2 c Influence of inter-particle interactions

Let us now take into account the effect of interactions between particles, considering the first equation (V.14a) of the BBGKY hierarchy with a non-vanishing right-hand side. On the other hand, we assume that the right member of the second equation (V.14b) vanishes, i.e. we neglect the influence of the three-particle density on the evolution of f_2.

Inspecting the resulting evolution equations, one finds that there is a new time scale besides τ_s and τ_e, set by the intensity of the pairwise interaction, namely

$$\tau_\mathrm{c} \sim \left(\vec{K}\cdot\vec{\nabla}_{\vec{p}}\right)^{-1}. \tag{V.17}$$

From the evolution equation for the two-particle density f_2, the *collision duration* τ_c appears as the characteristic time scale over which collisions between two particles smooth out the differences in their respective momentum distributions. τ_c is actually the smallest time scale, much smaller than τ_s and τ_e.

As a result, the evolution of f_2 is actually quicker than that of f_1 in the non-interacting case, for this quick time scale is absent from the single-particle Liouville equation (V.15). In turn, it means that when particles are allowed to interact with each other, the pace for the evolution of f_1 is not set by its slow drift term, but by the fast collision term in the right-hand side.

Remark: One could then wonder whether the time scale for the evolution of f_2 is not governed by the collision term involving f_3, which we are neglecting here. It can be checked that this is not the case in the dilute regime in which only pairwise interactions are important.

In the derivation of the BBGKY hierarchy (V.14), we have from the start assumed that particles only interact with each other in pairs. It is quite straightforward to see what would happen if we also allowed for genuine interactions between three, four or more particles at once.

The effect of the latter is simply to add further contributions to the collision and drift terms of the equations of motion. For instance, when allowing for three-particle interactions, the equation governing the evolution of f_k would not only involve f_{k+1}, but also f_{k+2}, corresponding to the case where one particle among the k under consideration is interacting with two "outsiders". Despite this complication, one can still derive an exact hierarchy of equations.

V.2.2 d BBGKY hierarchy in position-velocity space

Instead of characterizing a pointlike particle by a point in its μ-space, i.e. by its position and canonical momentum, one sometimes rather makes use of a point in *position-velocity space*, i.e. one specifies the positions and velocities of the particles.

In that representation, one can similarly introduce k-particle densities over a k-particle position-velocity space, hereafter denoted as $f_{\vec{v},k}$, such that $f_{\vec{v},k}(t,\vec{r}_1,\vec{v}_1,\ldots,\vec{r}_k,\vec{v}_k)\,\mathrm{d}^3\vec{r}_1\,\mathrm{d}^3\vec{v}_1\cdots\mathrm{d}^3\vec{r}_k\,\mathrm{d}^3\vec{v}_k$ is the number of particles in the infinitesimal volume element $\mathrm{d}^3\vec{r}_1\,\mathrm{d}^3\vec{v}_1\cdots\mathrm{d}^3\vec{r}_k\,\mathrm{d}^3\vec{v}_k$ around the point $(\vec{r}_1,\vec{v}_1,\ldots,\vec{r}_k,\vec{v}_k)$. The density $f_{\vec{v},k}$ is related to the reduced phase-space density f_k by the relation

$$f_{\vec{v},k}(t,\vec{r}_1,\vec{v}_1,\ldots,\vec{r}_k,\vec{v}_k)\,\mathrm{d}^3\vec{r}_1\,\mathrm{d}^3\vec{v}_1\cdots\mathrm{d}^3\vec{r}_k\,\mathrm{d}^3\vec{v}_k = f_k(t,\vec{r}_1,\vec{p}_1,\ldots,\vec{r}_k,\vec{p}_k)\,\mathrm{d}^3\vec{r}_1\,\mathrm{d}^3\vec{p}_1\cdots\mathrm{d}^3\vec{r}_k\,\mathrm{d}^3\vec{p}_k. \tag{V.18}$$

In the case considered in this section of a system of particles in absence of an external vector potential, the velocity $\vec{v}$ of a particle is simply proportional to its canonical momentum $\vec{p}$, so that

$f_{\vec{v},k}$ is trivially proportional to f_k and $\vec{\nabla}_{\vec{v}}$ to $\vec{\nabla}_{\vec{p}}$. One checks at once that the position-velocity space densities obey a similar BBGKY hierarchy as the phase-space densities, the only modification being the substitutions of $\vec{\nabla}_{\vec{p}_j}$ by by $\vec{\nabla}_{\vec{v}_j}$ and $\dot{\vec{p}}_j$ by $\dot{\vec{v}}_j$. For instance, the first equation of the hierarchy reads

$$\left(\frac{\partial}{\partial t} + \vec{v}_1 \cdot \vec{\nabla}_{\vec{r}_1} + \frac{\vec{F}_1}{m} \cdot \vec{\nabla}_{\vec{v}_1}\right) f_{\vec{v},1}(t, \vec{r}_1, \vec{v}_1) = -\int \frac{\vec{K}_{12}}{m} \cdot \vec{\nabla}_{\vec{v}_1} f_{\vec{v},2}(t, \vec{r}_1, \vec{v}_1, \vec{r}_2, \vec{v}_2)\, \mathrm{d}^3\vec{r}_2\, \mathrm{d}^3\vec{v}_2. \tag{V.19}$$

The real advantage of the formulation in position-velocity space is for the case, addressed in next section, of a system of charged particles in the presence of an external vector potential.

V.2.3 System of charged particles

We now briefly introduce the subtleties that appear when the particles in the system are coupled to an external vector potential, as is for instance the case of electrically charged particles in an external (electro)magnetic field.

In this subsection, we shall exceptionally denote by $\vec{\pi}_i$ the canonical momentum conjugate to position $\vec{r}_i$, and the reduced phase-space densities by $f_{\vec{\pi},k}$.

V.2.3 a Phase-space vs. position-velocity space description

The evolution equations of the BBGKY hierarchy (V.14) have been derived starting from the Liouville equation on phase space, i.e. within the framework of a Hamiltonian formalism. A similar approach can also be adopted in the presence of an external vector field $\vec{A}(t, \vec{r})$. However, there appear two complications, which can be traced back to the expression of the canonical momentum, derived from the Hamilton equations following from the Hamilton function (V.9)

$$\dot{\vec{r}}_i = \frac{\vec{\pi}_i - q\vec{A}(t, \vec{r}_i)}{m}, \tag{V.20a}$$

$$\dot{\vec{\pi}}_i = -q\vec{\nabla}_{\vec{r}}\,\phi(t, \vec{r}_i) + q\big(\dot{\vec{r}}_i \cdot \vec{\nabla}_{\vec{r}}\big)\vec{A}(t, \vec{r}_i) + q\dot{\vec{r}}_i \times \Big[\vec{\nabla}_{\vec{r}} \times \vec{A}(t, \vec{r}_i)\Big] + \sum_{j \neq i} \vec{K}_{ij}, \tag{V.20b}$$

where in the second equation we have made use of the first one.

- The time derivatives $\vec{v}_i = \dot{\vec{r}}_i$ and $\dot{\vec{\pi}}_i$ are no longer independent of $\vec{r}_i$ or $\vec{\pi}_i$, respectively. As a consequence, the integrals (V.13)—in which $\vec{\nabla}_{\vec{p}_i}$ is to be replaced by $\vec{\nabla}_{\vec{\pi}_i}$—are no longer trivial. Yet by using the Hamilton equations, one can show at the cost of a few integration by parts that the contributions of these integrals vanish, so that the evolution of the reduced phase-space density $f_{\vec{\pi},k}$ is eventually governed by an equation with the same structure as Eq. (V.14c), although with different factors in front of the gradients.

  For example, the collisionless evolution equation for the single-particle density $f_{\vec{\pi},1}$ is

  $$\frac{\partial f_{\vec{\pi},1}(t, \vec{r}, \vec{\pi})}{\partial t} + \vec{v} \cdot \vec{\nabla}_{\vec{r}} f_{\vec{\pi},1}(t, \vec{r}, \vec{\pi}) + \dot{\vec{\pi}} \cdot \vec{\nabla}_{\vec{\pi}} f_{\vec{\pi},1}(t, \vec{r}, \vec{\pi}) = 0, \tag{V.21}$$

  which differs from Eq. (V.15) because of the Hamilton equations (V.20).

- The second issue with the evolution equations for the reduced phase-space densities derived within the Hamiltonian formalism is that they are not manifestly gauge invariant, which is quite natural since the canonical momenta $\vec{\pi}_i$ themselves are gauge-dependent, see Eq. (V.20).

To remedy the latter problem, it is convenient to consider the densities in position-velocity space, instead of phase space. The resulting equations—which take the same form as in the absence of vector potential—only involve gauge invariant quantities. For instance, the collisionless evolution equation for the single-particle density $f_{\vec{v},1}$ is

$$\frac{\partial f_{\vec{v},1}(t, \vec{r}, \vec{v})}{\partial t} + \vec{v} \cdot \vec{\nabla}_{\vec{r}} f_{\vec{v},1}(t, \vec{r}, \vec{v}) + \frac{\vec{F}_\mathrm{L}}{m} \cdot \vec{\nabla}_{\vec{v}} f_{\vec{v},1}(t, \vec{r}, \vec{v}) = 0, \tag{V.22}$$

with $\vec{F}_\mathrm{L} = q(\vec{\mathscr{E}}_\mathrm{ext} + \vec{v} \times \vec{\mathscr{B}}_\mathrm{ext})$ the Lorentz[(bx)] force due to external electromagnetic fields $(\vec{\mathscr{E}}_\mathrm{ext}, \vec{\mathscr{B}}_\mathrm{ext})$. This equation is exactly the same as Eq. (V.19) in the absence of collision term. One can check that Eqs. (V.21) under consideration of Eq. (V.20) and Eq. (V.22) are actually equivalent.

Alternatively, one most often works in the space spanned by the positions $\vec{r}_i$ and the *linear* momenta $\vec{p}_i = m\vec{v}_i$. The densities f_k on that space obey exactly the same equations (V.14) as in the case of neutral particles. This is obvious in case there is no vector potential—conjugate and linear momenta $\vec{\pi}_i$ and $\vec{p}_i$ then coincide—and justifies our retaining the same notation as in § V.2.2 for the densities.

V.2.3 b Vlasov equation

An important example of macroscopic system of electrically charged particles is that of a plasma—where one actually has to consider two different types of particles, with positive and negative charges respectively, to ensure the mechanical stability.

In that context, Vlasov[(by)] has introduced a closure prescription for the corresponding BBGKY hierarchy, which consists in assuming that the two-particle density factorizes into the product of single particle densities[(77)]

$$f_2(t, \vec{r}_1, \vec{p}_1, \vec{r}_2, \vec{p}_2) \simeq f_1(t, \vec{r}_1, \vec{p}_1)\, f_1(t, \vec{r}_2, \vec{p}_2). \tag{V.23}$$

Under this assumption, Eq. (V.19) becomes closed and can be rewritten as

$$\left[\frac{\partial}{\partial t} + \vec{v}_1 \cdot \vec{\nabla}_{\vec{r}_1} + \left(\vec{F}_1 + \int \vec{K}_{12} f_1(t, \vec{r}_2, \vec{p}_2)\, \mathrm{d}^3\vec{r}_2\, \mathrm{d}^3\vec{p}_2\right) \cdot \vec{\nabla}_{\vec{p}_1}\right] f_1(t, \vec{r}_1, \vec{p}_1) = 0, \tag{V.24}$$

with $\vec{F}_1 = q\big(\vec{\mathscr{E}}_\mathrm{ext} + \vec{v} \times \vec{\mathscr{B}}_\mathrm{ext}\big)$ the Lorentz force due to the external electromagnetic field. This constitutes the *Vlasov equation*.

The integral inside the brackets can be viewed as an average force exerted by the partner particle 2 on particle 1. In the specific case of an electromagnetic plasma—assuming for simplicity that the particles in the system have velocities much smaller than the speed of light, so that their mutual interaction is mostly of Coulombic[(bz)] nature—this average force is that due to the mean electrostatic field created by the other particles:

$$\left[\frac{\partial}{\partial t} + \vec{v}_1 \cdot \vec{\nabla}_{\vec{r}_1} + q\big(\vec{\mathscr{E}}' + \vec{\mathscr{E}}_\mathrm{ext} + \vec{v} \times \vec{\mathscr{B}}_\mathrm{ext}\big) \cdot \vec{\nabla}_{\vec{p}_1}\right] f_1(t, \vec{r}_1, \vec{p}_1) = 0$$

with

$$\vec{\mathscr{E}}' \equiv \frac{1}{q} \int \vec{K}_{12} f_1(t, \vec{r}_2, \vec{p}_2)\, \mathrm{d}^3\vec{r}_2\, \mathrm{d}^3\vec{p}_2.$$

The Vlasov assumption is thus an instance of *mean-field approximation*.

Remark: The Vlasov equation (V.24) is nonlinear, and thus non-trivial. In practice it must be solved in a self-consistent way, since the mean field in which f_1 evolves depends on f_1 itself.

Bibliography for Chapter V

- Huang, *Statistical Mechanics* [54], chapter 3.5.
- Landau & Lifshitz, *Course of theoretical physics. Vol. 10: Physical kinetics* [5], chapter I § 16.
- Pottier, *Nonequilibrium statistical physics* [6], chapter 4.

(77) We do not write this hypothesis as an identity with an = sign to accommodate the possible mismatch between the normalizations of f_1 and f_2.

(bx) H. A. Lorentz, 1853–1926 (by) A. A. Vlasov, 1908–1975 (bz) C. A. Coulomb, 1736–1806