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Mean-Field limit and semiclassical approximation for quantum particle systems

FEDERICA PEZZOTTI

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– Introduction

In this thesis we discuss the connection between the mean-field limit and the semiclassical approximation for a system of N identical quantum particles. More precisely, we look at a system of N identical particles (of mass $m = 1$) interacting by means of the mean-field potential:

$$U(X_N) = \frac{1}{2N}\sum_{l\neq j}^{N} \phi(x_l - x_j), \quad \phi : \mathbb{R}^3 \to \mathbb{R} \tag{I.1}$$

(where $X_N = \{x_1, \dots, x_N\},\ x_j \in \mathbb{R}^3,\ j = 1, \dots, N$) in the limit $N \to \infty$. It is well known that the effective (limiting) dynamics of such a system is ruled by the following nonlinear one-particle Schrödinger equation:

$$i\hbar\partial_t\psi_t = -\frac{\hbar^2}{2}\Delta\psi_t + \left(\phi * |\psi_t|^2\right)\psi_t, \tag{I.2}$$

where

$$\left(\phi * |\psi_t|^2\right)(x) = \int_{\mathbb{R}^3} \mathrm{d}y\ \phi(x-y)|\psi_t(y)|^2 \tag{I.3}$$

is the effective self-consistent interaction. Equation (I.2) is known as the Hartree equation. The rigorous derivation of (I.2) from the many-body evolution can be formulated in terms of convergence of j-particle Reduced Density Matrices (RDM). In fact, by considering the N-particle wave function $\Psi_{N,t} = \Psi_{N,t}(X_N)$ solution of the Schrödinger equation:

$$i\hbar\partial_t\Psi_{N,t} = -\frac{\hbar^2}{2}\sum_{i=1}^{N}\Delta_{x_i}\Psi_{N,t} + U\Psi_{N,t}, \tag{I.4}$$

with U given by (I.1) and completely factorized initial datum given by:

$$\Psi_{N,0}(X_N) = \prod_{j=1}^{N} \psi_0(x_j), \tag{I.5}$$

it can be proven that, for fixed j (with $1 \leq j \leq N$) the j-particle reduced density matrix, defined as the trace class operator with kernel

$$\rho^{(j)}_{N,t}(X_j, Y_j) = \int_{\mathbb{R}^{3(N-j)}} \mathrm{d}X_{N-j} \overline{\Psi}_{N,t}(X_j, X_{N-j}) \Psi_{N,t}(Y_j, X_{N-j}), \tag{I.6}$$

converges, in the limit $N \to \infty$, to the factorized state:

$$\rho^{(j)}_t(X_j, Y_j; t) = \prod_{k=1}^{j} \overline{\psi}_t(x_k) \psi_t(y_k), \tag{I.7}$$

where $\psi_t(x)$ solves the one-particle Hartree equation (I.2) with initial datum ψ_0. This feature is usually called “propagation of chaos”.

The previous result was originally obtained for sufficiently smooth potentials (see [2], [6], [7]); then it has been generalized to include Coulomb interactions (see [16], [17], [18]). Furthermore, some results concerning the speed of convergence of the mean-field evolution to the Hartree dynamics (for all fixed times), have been proven more recently (see [20], [21]).

The limit $N \to \infty$ for a classical system interacting by means of the same mean-field interaction (I.1), can be considered as well (see [4], [5], [9], [10] for the case of smooth potential, and [22] for more singular interactions). In fact, considering as initial state of the system a completely factorized probability distribution $F_{N,0} = F_{N,0}(X_N, V_N)\,\mathrm{d}X_N \mathrm{d}V_N$ in the N-particle phase space $\mathbb{R}^{3N} \times \mathbb{R}^{3N}$, namely:

$$F_{N,0}(X_N, V_N) = \prod_{j=1}^{N} f_0(x_j, v_j), \quad \text{for some one-particle density } f_0, \tag{I.8}$$

it is known that its evolution $F_N(X_N, V_N; t)$ at time $t > 0$, is obtained by solving the Liouville equation:

$$(\partial_t + V_N \cdot \nabla_{X_N}) F_N(t) = \nabla_{X_N} U \cdot \nabla_{V_N} F_N(t), \tag{I.9}$$

with U given by (I.1). Then, the j-particle marginal at time $t > 0$, defined as

$$F^{(j)}_N(X_j, V_j; t) = \int_{\mathbb{R}^{3(N-j)} \times \mathbb{R}^{3(N-j)}} \mathrm{d}X_{N-j} \mathrm{d}V_{N-j} F_N(X_j, X_{N-j}, V_j, V_{N-j}; t), \tag{I.10}$$

converges, as $N \to \infty$, to the product state:

$$F^{(j)}\left(X_j, V_j; t\right) = \prod_{k=1}^{j} f\left(x_k, v_k; t\right), \tag{I.11}$$

where $f(x, v; t)$ is the solution of the Vlasov equation:

$$\left(\partial_t + v \cdot \nabla_x\right) f(t) = \left(\nabla_x \phi * f(t)\right) \cdot \nabla_v f(t), \tag{I.12}$$

(the convolution above is with respect to both the variables x and v) with initial datum f_0. Equation (1.1.8) is the classical analogue of the Hartree equation (I.2).

Although the mean-field limit $N \to \infty$ is well understood for both classical and quantum systems, there is a question which is still open, namely, does that limit hold for quantum systems uniformly in $\hbar$, at least for systems having a reasonable classical analogue?

The proofs which are available up to now exhibit an error vanishing when $N \to \infty$ but diverging as $\hbar \to 0$, although in [8], [24], [26], [27] some efforts in the direction of a better control of the error term have been done.

If one wants to deal with the classical and quantum case simultaneously, it is natural to work in the classical phase space by using the Wigner formalism.

The one-particle Wigner function associated with the wave function $\psi_t(x)$ is given by:

$$f^{\hbar}\left(x, v; t\right) = (2\pi)^{-3} \int_{\mathbb{R}^3} \mathrm{d}y\ e^{iy\cdot v} \overline{\psi}_t \left(x + \frac{\hbar y}{2}\right) \psi_t \left(x - \frac{\hbar y}{2}\right), \tag{I.13}$$

and, similarly, the N-particle Wigner function associated with the wave function $\Psi_{N,t}(X_N)$ is defined as:

$$\begin{aligned} &W_N^{\hbar}\left(X_N, V_N; t\right) = \\ &= (2\pi)^{-3N} \int_{\mathbb{R}^{3N}} \mathrm{d}Y_N\ e^{iY_N \cdot V_N} \overline{\Psi}_{N,t} \left(X_N + \frac{\hbar Y_N}{2}\right) \Psi_{N,t} \left(X_N - \frac{\hbar Y_N}{2}\right). \end{aligned} \tag{I.14}$$

Then, by using that $\psi_t(x)$ and $\Psi_{N,t}(X_N)$ solve equations (I.2) and (I.4) respectively, we find the equations:

$$\left(\partial_t + v \cdot \nabla_x\right) f^{\hbar}(t) = T^{\hbar} f^{\hbar}(t) \tag{I.15}$$

and

$$\left(\partial_t + V_N \cdot \nabla_{X_N}\right) W_N^{\hbar}(t) = T_N^{\hbar} W_N^{\hbar}(t), \tag{I.16}$$

where $T^{\hbar}$ and $T_N^{\hbar}$ are suitable pseudodifferential operators.

The initial data for equations (I.15) and (I.16) are

$$f_0^{\hbar}(x,v) = (2\pi)^{-3}\int_{\mathbb{R}^3} \mathrm{d}y\; e^{iy\cdot v}\overline{\psi}_0\left(x+\frac{\hbar y}{2}\right)\psi_0\left(x-\frac{\hbar y}{2}\right), \tag{I.17}$$

and

$$\begin{aligned} &W_{N,0}^{\hbar}(X_N,V_N) = \\ &= (2\pi)^{-3N}\int_{\mathbb{R}^{3N}} \mathrm{d}Y_N e^{iY_N\cdot V_N}\overline{\Psi}_{N,0}\left(X_N+\frac{\hbar Y_N}{2}\right)\Psi_{N,0}\left(X_N-\frac{\hbar Y_N}{2}\right) = \\ &= \prod_{j=1}^{N} f_0^{\hbar}(x_j,v_j), \end{aligned} \tag{I.18}$$

respectively.

One can easily rephrase the result of [7] by showing that the j-particle Wigner function

$$W_{N,j}^{\hbar}(X_j,V_j;t)=\int_{\mathbb{R}^{3(N-j)}\times\mathbb{R}^{3(N-j)}} \mathrm{d}X_{N-j}\mathrm{d}V_{N-j}W_N^{\hbar}(X_j,X_{N-j},V_j,V_{N-j};t) \tag{I.19}$$

converges, in a suitable sense, to

$$f_j^{\hbar}(X_j,V_j;t) = \prod_{k=1}^{j} f^{\hbar}(x_k,v_k;t) \quad \text{for any } t>0. \tag{I.20}$$

However, the error in approximating the N-particle dynamics by the limiting one is diverging when $\hbar\to 0$ (for example, for sufficiently small times $t<t_0$ it is of the form $\frac{C_j}{N}e^{\frac{c}{\hbar}}$). The reason is that the operator $T_N^{\hbar}$ appearing in (I.16) is bounded on the space in which we can prove the convergence of (I.19), but its norm diverges as $\frac{c}{\hbar}$ when $\hbar\to 0$. On the other hand, the classical counterpart of this problem has been solved, so that it seems natural to look for an asymptotic expansion for the j-particle "marginals" $W_{N,j}^{\hbar}$, namely:

$$W_{N,j}^{\hbar}(t) = W_{N,j}^{(0)}(t) + \hbar W_{N,j}^{(1)}(t) + \hbar^2 W_{N,j}^{(2)}(t) + \dots, \tag{I.21}$$

and for an analogous expansion for the j-fold product of solutions of the equation (I.15), namely:

$$f_j^{\hbar}(t) = \left(f^{\hbar}\right)^{\otimes j}(t) = f_j^{(0)}(t) + \hbar f_j^{(1)}(t) + \hbar^2 f_j^{(2)}(t) + \dots \tag{I.22}$$

The zeroth order term in (I.21) is expected to correspond to what we previously denoted by $F_{N,t}^{(j)}$, namely, the j-particle marginals associated to the Liouville equation (I.9), while the function $f_j^{(0)}(t)$ appearing in (I.22) is expected to be the j-fold product of solutions of the Vlasov equation (I.12). Therefore, if at order zero in $\hbar$ we obtain the classical quantities, the classical mean-field theory ensures that the convergence of $W_{N,j}^{(0)}(t)$ to $f_j^{(0)}(t)$ is well established for all t and j. Then, it looks natural trying to show the convergence

$$W_{N,j}^{(k)}(t) \to f_j^{(k)}(t)\,, \text{ as } N \to \infty, \text{ for any } k > 0. \tag{I.23}$$

This is the main goal of the present research.

A complete proof of the uniformity in $\hbar$ of the limit $N \to \infty$ would require a control of the remainder of the expansion (I.21), but we are not able to provide it. However, in proving (I.23) we characterize the quantum corrections to the classical mean-field limit and we prove that they are expressed in terms of classical quantities only.

The plan of the thesis is the following.

In Sections 1 and 2 we discuss the mean-field model both in the classical framework and in the quantum context. First we introduce notation and technical tools that are needed to formulate the mean-field results to which we referred previously. Then, we give an outlook of the known results by discussing briefly the main approaches in facing the problem both for smooth and singular interactions. Thus, we focus on the case of sufficiently regular potential by showing in detail the proof of the validity of "propagation of chaos" both in the classical and in the quantum case, accenting the main differences in the methods and, primarily, the inadequacy of the "BBGKY hierarchy method" in facing the classical mean-field limit although in the quantum framework it plays a crucial role. Furthermore, we highlight the non uniformity with respect to $\hbar$ of the error in the quantum mean-field approximation and we analyze in detail which is the estimate that, providing a bound which diverges as $\hbar \to 0$, is responsible for that.

In Section 3 we introduce the Wigner formalism. We accent first of all why it is appropriate in looking at the semiclassical behavior of quantum systems. Also, we point out the main difficulties of this formalism with respect to the wave function (Schrödinger) and the density matrix (Heisenberg) formulations introduced in Section 2. Moreover, we rephrase the quantum mean-field result in the Wigner formalism and we note that the error in the mean-field approximation is still not uniform with respect to $\hbar$ and diverging when $\hbar \to 0$. This "bad" behavior is due to the failure of the same estimate we detected in Section 3, suitably rephrased in the Wigner framework. Finally, we discuss some known results concerning the connection between mean-field limit and semiclassical approximation.

In Section 4 we prove our main result, namely, the convergence (I.23). More precisely, we do the semiclassical expansion both for the N-particle mean-field system (see (I.21)) and for the Hartree dynamics (I.22) deriving explicitly what are the equations solved by the coefficients at each order in $\hbar$. Then, we introduce the initial datum as a suitable mixtures of coherent states. This choice guarantees that the zeroth order coefficient of the N-particle expansion is a factorized probability distribution. Finally, we identify the higher order N-particle terms to be the expectation of certain derivatives of the empirical measure. Such an expectation is with respect to the probability distribution that we previously obtained from the N-particle zeroth order coefficient. By virtue of that, we obtain the limit $N \to \infty$ by using the classical mean-field results presented in Section 1 and appropriate properties of the derivatives of the classical trajectories associated with the mean-field interaction.

In the last Section we present possible applications of our result (presented in Section 4) in considering suitable mixtures of WKB states (instead of coherent ones) and in dealing with other (related) problems.

I wish to thank my advisor, Prof. Mario Pulvirenti, for suggesting me a problem which I considered challenging from the very first moment, for offering me his precious experience and considering me not only as a student but indeed as a co-worker.

1 – Classical Mean-Field limit

In this Section we analyze the mean-field limit for a many-body classical system. More precisely, we are looking at a system constituted by N identical particles interacting by the potential

$$U^{cl}(X_N) = \frac{1}{2N} \sum_{k \neq l}^{N} \phi(x_k - x_l), \tag{1.1}$$

where we used the notation $X_N = (x_1, \ldots, x_N) \in \mathbb{R}^{3N}$ for the positions of the N particles (here and henceforth we put the superscripts "*cl*" and "*Q*" to distinguish between classical and quantum quantities denoted by the same symbol). We note that U^{cl} is given by a sum over all interactions among pair of particles; the two-body interactions are governed by the potential ϕ which we assume to be spherically symmetric (as it is in all reasonable physical situations), namely $\phi(x) = \phi(|x|)\ \forall\ x \in \mathbb{R}^3$. We set the dimension to be equal to 3 but the results we are going to discuss hold in any dimension. Sometimes we will refer to the system under consideration as "mean-field system".

We want to characterize the dynamics when the number of particles N is very big. In this sense we speak about "macroscopic" or "effective" dynamics and from a mathematical point of view that purpose is realized by taking the limit $N \to \infty$.

As a second step, it is also important to describe the dynamics of the fluctuations of the N-particle evolution around the limiting one, but here we do not discuss in detail this topic which is analyzed, for example, in [4].

1.1 – Setting of the problem: general features and known results

A mean-field system is described by an N-body Hamiltonian of the form

$$H_N^{cl,V}(X_N, V_N) = \sum_{k=1}^{N}\left(\frac{v_k^2}{2} + V^{cl}(x_k)\right) + U^{cl}(X_N), \tag{1.1.1}$$

where we used the notation $V_N = (v_1, \dots, v_N) \in \mathbb{R}^{3N}$ to indicate the velocities of the N particles and, for the sake simplicity, the mass of the (identical) particles is chosen equal to one. The first part of the Hamiltonian is simply the sum of the one-body Hamiltonians associated with the motion of each particle (the function V^{cl} describes an external potential which acts in the same way on all N particles), while the remaining term involving U^{cl} describes the interaction among the particles. For the sake of simplicity we assume that the force experienced by each particle is only that arising from the many-body interaction, namely, the one-particle potential V^{cl} is assumed to be equal to zero. We can do that without loss of generality because the results we are going to discuss can be generalized easily to the case $V^{cl} \neq 0$.
Thus the Hamiltonian we consider is

$$H_N^{cl}(X_N, V_N) = \sum_{k=1}^{N}\frac{v_k^2}{2} + U^{cl}(X_N), \tag{1.1.2}$$

and we note that H_N^{cl} is symmetric with respect to any permutation of the labeling.

The factor $1/N$ in the potential U^{cl} (see (1.1)) forces the energy per particle to remain finite in the limit $N \to \infty$ and this is the crucial feature in order to obtain a well-defined but non-trivial limiting dynamics. Moreover we observe that U^{cl} is such that the interaction among the particles is quite weak when N is very big (the strength of the pair interaction is of the order $1/N$) but it is long range (because the pair interaction potential ϕ is unscaled, thus its support remains of order one in the limit $N \to \infty$). Therefore when N becomes large (for example, in the applications related to the gas dynamics we have $N \approx 10^{23}$) the mutual interaction turns to be weaker and weaker but the total effect of such an interaction is not negligible (the force experienced by a fixed particle because of the presence of all the others is proportional to $(N-1)/N \approx O(1)$) . We will see that these two features are responsible for the validity of "propagation of chaos" and of the nonlinearity of the macroscopic equation we find in the limit (see Sections 1.3 and 1.4).

The dynamics of an N-particle system associated with the Hamiltonian (1.1.2) is governed by the Newton equations

$$\begin{cases} \dot{x}_i = v_i, \\ \dot{v}_i = -\dfrac{1}{N}\displaystyle\sum_{k\neq i}^{N} \nabla_{x_i}\phi(x_i - x_k), \quad i = 1, \dots, N \end{cases} \tag{1.1.3}$$

Thus we know that given an initial configuration $Z_N := (X_N, V_N) \in \mathbb{R}^{3N} \times \mathbb{R}^{3N}$ in the N-particle phase-space, the time-evolved configuration $Z_N(t)$ up to some $t > 0$ is obtained solving (1.1.3) with initial datum Z_N.

As we have already noticed, in many interesting physical situations the number N is very big thus it is not possible (and even not particularly relevant for the applications) to know which are the positions and the velocities of all particles at a certain time. In other words, it is quite difficult to determine a unique initial N-particle configuration for the time-evolution defined by (1.1.3) and, even if one was able to provide that, it would be impossible to solve such a huge number of equations, even by using numerical methods. Nevertheless, one can provide collective and more useful informations such as the probability to find N_1 particles ($N_1 \leq N$) in a region $\Lambda_1 \subset \mathbb{R}^{3N}$, the probability that N_2 particles ($N_2 \leq N$) have velocities belonging to some $\Lambda_2 \subset \mathbb{R}^{3N}$ or the probability to find N_3 particles ($N_3 \leq N$) with positions belonging to some $\Lambda_3^x \subset \mathbb{R}^{3N}$ and velocities belonging to some $\Lambda_3^v \subset \mathbb{R}^{3N}$. In other words, one can give the N-particle probability distribution in the phase-space $\mathbb{R}^{3N} \times \mathbb{R}^{3N}$. Therefore, denoting by $F_{N,0}(Z_N)\mathrm{d}Z_N$ such a distribution, we have that $F_{N,0}$ is symmetric with respect to any permutation of the variables, $F_{N,0} \geq 0$ and:

$$\int \mathrm{d}Z_N F_{N,0}(Z_N) = 1. \tag{1.1.4}$$

Moreover, by computing the marginals of $F_{N,0}(Z_N)$ with respect to the velocities V_N and to the positions X_N one obtains respectively the spatial and the velocity probability density.

The time-evolved probability density $F_N(t) := F_N(Z_N; t)$ is obtained by solving the Liouville equation

$$(\partial_t + V_N \cdot \nabla_{X_N}) F_N(t) = \nabla_{X_N} U \cdot \nabla_{V_N} F_N(t), \tag{1.1.5}$$

with initial condition $F_{N,0}$, where U is the potential defined in (1.1). By denoting as $\Phi^t(X_N, V_N)$ the Hamiltonian flow associated with equations (1.1.3), it is easy to verify that the solution of equation (1.1.5) is obtained by propagating the initial datum $F_{N,0}$ through the characteristic curves of $\Phi^t(X_N, V_N)$, namely

$$F_N(t) = F_{N,0}\left(\Phi^{-t}\left(X_N, V_N\right)\right). \tag{1.1.6}$$

Thus we are guaranteed that starting from an N-particle probability density at time $t = 0$, we have a probability density for each time $t > 0$ and the evolution preserves also the symmetry with respect to permutations of the variables (because the Hamiltonian H_N^{cl} is symmetric with respect to permutations).

In the classical framework observables of the N-particle system are represented by real functions defined on the phase-space $\mathbb{R}^{3N} \times \mathbb{R}^{3N}$. Then, if we know that the configuration of the system at a certain time τ is $Z_N(\tau)$, the value of the observable associated with a certain function u_N at time τ, is given by $u_N(Z_N(\tau))$. On the other side, if what we have is the N-particle probability distribution at a certain time τ_1, namely $F_N(\tau_1)$, we are able to give probabilistic predictions about the value of the observables at time τ_1. More precisely, the expectation of the observable associated with a certain function u_N at time τ_1, is given by

$$\langle u_N \rangle_{F_N(\tau_1)} := \int \mathrm{d}Z_N u_N(Z_N) F_N(Z_N; \tau_1). \tag{1.1.7}$$

By (1.1.3) it is clear that to guarantee existence and uniqueness of the flow $\Phi^t(X_N, V_N)$ for each t we need to assume $\phi \in \mathcal{C}_b^2(\mathbb{R}^3)$[(1)]. Therefore the first rigorous results concerning the analysis of the limit $N \to \infty$ for the N-particles mean-field system have been proven under suitable smoothness assumption on the pair interaction potential ϕ (see for example [4] and [10]). Nevertheless, several systems of physical interest are described by more singular potential. For example, a system of gravitating particles can be described by the potential (1.1) where ϕ is the Coulomb interaction among the particles and, in that case, the factor of $1/N$ in front of the potential energy can be justified by the smallness of the gravitational constant.

Mean-Field systems with singular interactions are clearly hard to face because one has to deal with a system of ODE (namely, (1.1.3)) with non regular fields. Quite recently some progress have been done in [22] where the mean-field limit is realized by only assuming $\nabla_x \phi \approx 1/|x|^\alpha, \quad \alpha < 1$ for the pair interaction ϕ. On the other side, the assumptions on the initial datum are very strong and they are quite good for numerical purposes but not satisfying from a statistical physics point of view (for example, "chaotic" initial data are not admissible, namely it is not possible to consider initially factorized N-particle distribution). The problem involving the Coulomb potential is still open.

Here we will not discuss the "singular case" because for our purposes we need to deal with a smooth interaction potential and with a classical mean-field result involving "chaotic" initial data (see Section 3 and 4), thus from now on we will focus on the mean-field limit in the "smooth case".

In [4] and [10] it is proved that the effective single particle dynamics of a mean-field system with smooth interaction potential ($\phi \in \mathcal{C}_b^2(\mathbb{R}^3)$) in the limit $N \to \infty$ is governed by the Vlasov equation:

$$(\partial_t + v \cdot \nabla_x) f(t) = (\nabla_x \phi * f(t)) \cdot \nabla_v f(t), \tag{1.1.8}$$

where $f(t) = f(x, v; t)$ for each time $t \geq 0$ is a one-particle probability density and here and in the rest of the section we denote by $*$ the convolution with

[(1)] Here and henceforth we denote by $\mathcal{C}_b^k(\mathbb{R}^d)$ the space of functions on $\mathbb{R}^d$ with continuous and uniformly bounded derivatives up to the order k

respect to both position and velocity. By computing the marginals of $f(x, v; t)$ with respect to the velocity v and the position x one finds respectively the spatial and the velocity probability density.

It is remarkable that the results proven in [4] describe both the continuum limit of the point particle dynamics associated with the mean-field interaction, as we specified previously, and the so called "propagation of chaos" for the many-body mean-field system. Moreover, in [4] it has been proven that the fluctuations of a certain class of observables (called "intensive observables") converge to a gaussian stochastic process. We will not discuss this last feature, on the contrary we will show in detail the emergence of the Vlasov dynamics as the limit of the N-particle evolution and the proof of propagation of chaos.

1.2 – The Vlasov equation

Let us consider a one-particle density $f_0 \in C^1(\mathbb{R}^6)$ and let us look at the solution $f(t)$ of the Vlasov equation (1.1.8) with initial datum f_0. Denoting by $\Phi_V^t(x, v)$ the flow associated with the system:

$$\begin{cases} \dot{x} = v, \\ \dot{v} = -\nabla_x \phi * f(t), \end{cases} \tag{1.2.1}$$

one can easily verify that $f(t)$ is obtained by propagating $f_0(x, v)$ through the characteristic curves of the flow $\Phi_V^t(x, v)$, namely

$$f(t) = f(x, v; t) = f_0\left(\Phi_V^{-t}(x, v)\right). \tag{1.2.2}$$

Therefore in proving existence and uniqueness of the solution of (1.1.8) one has to deal with a system of ODE with a self-consistent field (see (1.2.1)) and the smoothness of the potential ϕ is not sufficient to make a standard fixed point argument to be successful. One needs a more involved analysis and it has been done by R.L. Dobrushin in [5]. It is remarkable that the Vlasov equation (1.1.8) makes sense even for a generic probability measure ν because $\nabla\phi * \nu$ is sufficiently smooth (thanks to the regularity of ϕ) then the proof presented in [5] ensures existence and uniqueness of the solution in this framework. In particular, if the initial datum is an absolutely continuous measure with respect to the Lebesgue measure in $\mathbb{R}^3 \times \mathbb{R}^3$ with a smooth density f_0 (which is the case we discussed previously), the solution $f(t)$ is a strong solution whose regularity depends on that of f_0 and ϕ ($f_0 \in C^1(\mathbb{R}^6)$ and $\phi \in C_b^2(\mathbb{R}^3)$, at least). Furthermore, introducing the Wasserstein distance $\mathcal{W}$, in [5] it has been proven the following stability result for solutions of the Vlasov equation:

$$\mathcal{W}(\nu_1^t, \nu_2^t) \leq e^{Ct}\mathcal{W}(\nu_1^0, \nu_2^0) \tag{1.2.3}$$

where ν_1^0 and ν_2^0 are two probability measures and ν_1^t and ν_2^t are the weak solutions of the Vlasov equation with initial data given by ν_1^0 and ν_2^0 respectively. The metric induced by $\mathcal{W}$ on the space of probability measures on $\mathbb{R}^3 \times \mathbb{R}^3$ is equivalent to the weak topology of probability measures, namely we have to look at measures tested versus functions in $\mathcal{C}_b^0(\mathbb{R}^3 \times \mathbb{R}^3)$ (the space of continuous and uniformly bounded functions). Thus by (1.2.3) it follows that

$$\int u(x,v)\nu_n^0(\mathrm{d}x\mathrm{d}v) \to \int u(x,v)\nu^0(\mathrm{d}x\mathrm{d}v) \text{ as } n \to \infty,\ \forall\, u \in \mathcal{C}_b^0(\mathbb{R}^3 \times \mathbb{R}^3) \tag{1.2.4}$$

implies

$$\int u(x,v)\nu_n^t(\mathrm{d}x\mathrm{d}v) \to \int u(x,v)\nu^t(\mathrm{d}x\mathrm{d}v) \text{ as } n \to \infty,\ \forall\, u \in \mathcal{C}_b^0(\mathbb{R}^3 \times \mathbb{R}^3), \tag{1.2.5}$$

where $\{\nu_n^0\}_{n\geq 0}$ is a sequence of probability measures converging to some ν^0 when the parameter n goes to infinity and ν_n^t and ν^t are the weak solutions of the Vlasov equation with initial data given by ν_n^0 and ν^0 respectively. In the sequel we will denote the weak convergence of probability measures by the symbol $\overset{M}{\to}$.

1.3 – The Vlasov dynamics as the continuum limit of the N-particle Mean-Field dynamics

Let us introduce the empirical measure associated with an N-particle configuration Z'_N

$$\mu_N(z|Z'_N) = \frac{1}{N}\sum_{i=1}^{N} \delta\left(z - z'_i\right), \tag{1.3.1}$$

where $z := (x,v)$ is the generic point in the one-particle phase-space $\mathbb{R}^3 \times \mathbb{R}^3$ and $Z'_N = (z'_1, \ldots, z'_N) \in \mathbb{R}^{3N} \times \mathbb{R}^{3N}$. By definition μ_N is a measure on the one-particle phase-space but, as it is clear by (1.3.1), it depends on all the configuration Z'_N. Then let us consider an initial N-particle configuration Z_N for equations (1.1.3) distributed according to a factorized (smooth) N-particle measure $F_{N,0}\mathrm{d}Z_N$, namely

$$F_{N,0}(Z_N) = \prod_{i=1}^{N} f_0(z_i) = f_0^{\otimes N}, \quad f_0 \in C^1(\mathbb{R}^6). \tag{1.3.2}$$

We denote by μ_N^0 the empirical measure associated with Z_N and by considering the empirical measure $\mu_N(t) = \mu_N(z|Z_N(t))$ associated with the time-evolved configuration $Z_N(t)$ (solution of equations (1.1.3) with initial datum Z_N), it is easy to verify that $\mu_N(t)$ is the unique (weak) solution of the Vlasov equation (1.1.8) with initial datum μ_N^0. In fact, by integrating versus $\mu_N(t)$ versus a smooth test function $u = u(x, v)$, we find:

$$(u, \mu_N(t)) = \int \mathrm{d}z \ \mu_N(z|Z_N(t)) = \frac{1}{N}\sum_{i=1}^{N} u(z_i(t)) = \frac{1}{N}\sum_{i=1}^{N} u(x_i(t), v_i(t)). \tag{1.3.3}$$

Then, we obtain

$$\begin{aligned}\frac{d}{dt}(u, \mu_N(t)) &= \frac{1}{N}\sum_{i=1}^{N} \frac{d}{dt} u(x_i(t), v_i(t)) = \\ &= \frac{1}{N}\sum_{i=1}^{N} [\nabla_x u(x_i(t), v_i(t))\dot{x}_i(t) + \nabla_v u(x_i(t), v_i(t))\dot{v}_i(t)],\end{aligned} \tag{1.3.4}$$

that, by virtue of (1.1.3), implies

$$\begin{aligned}\frac{d}{dt}(u, \mu_N(t)) = \frac{1}{N}\sum_{i=1}^{N} &\nabla_x u(x_i(t), v_i(t)) v_i(t) - \\ &- \frac{1}{N}\sum_{i=1}^{N} \nabla_v u(x_i(t), v_i(t)) \left(\frac{1}{N}\sum_{k\neq i}^{N} \nabla_{x_i}\phi(x_i - x_k)\right).\end{aligned} \tag{1.3.5}$$

Following (1.3.3), the equation (1.3.5) becomes

$$\frac{d}{dt}(u, \mu_N(t)) = (v \cdot \nabla_x u, \mu_N(t)) - ((\nabla\phi * \mu_N(t)) \cdot \nabla_v u, \mu_N(t)), \tag{1.3.6}$$

where

$$\begin{aligned}(\nabla\phi * \mu_N(t))(x) &= \int \mathrm{d}y \mathrm{d}w \nabla_x \phi(x-y) \left(\frac{1}{N}\sum_{k=1}^{N} \delta(y - x_k(t))\delta(w - v_k(t))\right) = \\ &= \frac{1}{N}\sum_{k=1}^{N} \int \mathrm{d}y \nabla_x \phi(x-y)\delta(y - x_k(t)) = \\ &= \frac{1}{N}\sum_{k=1}^{N} \nabla_x \phi(x - x_k(t)).\end{aligned} \tag{1.3.7}$$

Therefore, $\mu_N(t)$ verifies (1.3.6) for any function u sufficiently smooth and

$$(u, \mu_N(t))|_{t=0} = (u, \mu_N^0) = \frac{1}{N}\sum_{i=1}^{N} u(x_i, v_i). \tag{1.3.8}$$

In other words, $\mu_N(t)$ satisfies the following weak equation

$$\partial_t \mu_N(t) + v \cdot \nabla_x \mu_N(t) = (\nabla_x \phi * \mu_N(t)) \cdot \nabla_v \mu_N(t), \tag{1.3.9}$$

with initial datum μ_N^0, and we note that (1.3.9) is precisely the Vlasov equation (1.1.8).

By the Strong Law of Large Numbers (SLLN) we know that

$$\mu_N^0 \stackrel{M}{\to} f_0 \text{ as } N \to \infty, \text{ a.e with respect to the product measure } f_0^{\otimes\infty}, \tag{1.3.10}$$

therefore, by (1.3.10), by knowing that $\mu_N(t)$ solves the Vlasov (weak) equation (1.3.9) and by (1.2.3), it follows that

$$\mu_N(t) \stackrel{M}{\to} f(t) \text{ as } N \to \infty, \text{a.e with respect to the product measure} f_0^{\otimes\infty}, \tag{1.3.11}$$

where $f(t)$ is the (strong) solution of the Vlasov equation (1.1.8) with initial datum f_0.

From now on, we will say that a configuration Z_N is "typical" with respect to the measure f_0 if the empirical measure μ_N^0 associated with Z_N verifies

$$\mu_N^0 \stackrel{M}{\to} f_0 \text{ as } N \to \infty. \tag{1.3.12}$$

1.4 – Hierarchies and Propagation of Chaos

In the previous paragraph we proved that the Vlasov equation arises from the continuum limit of a system of N particles interacting by the mean-field potential (1.1). This is precisely what convergence (1.3.11) tells us and it can be seen as a one-particle effect, namely (1.3.11) provides the equation governing the single-particle dynamics in the limit.

Now we want to show how (1.3.11) works in order to characterize the effective dynamics of a subsystem made by a fixed number j of particles. This is a natural approach in looking at the macroscopic behavior of many-body systems because we want to look at the limit $N \to \infty$ and we need to deal with quantities depending on a number of variables which remains finite in the limit.

In this perspective, for any $j = 1, \ldots, N$ we introduce the "j-particle marginal density" (or simply "j-particle marginal") associated with an N-particle density $F_N(X_N, V_N)$ as

$$F_N^{(j)}(X_j, V_j) = \int_{\mathbb{R}^{3(N-j)} \times \mathbb{R}^{3(N-j)}} \mathrm{d}X_{N-j} \mathrm{d}V_{N-j} F_N(X_N, V_N), \tag{1.4.1}$$

where we used the notation $X_j = (x_1, \ldots, x_j), V_j = (v_1, \ldots, v_j) \in \mathbb{R}^{3j}$ and $X_{N-j} = (x_{j+1}, \ldots, x_N)$, $V_{N-j} = (v_{j+1}, \ldots, v_N) \in \mathbb{R}^{3(N-j)}$. Indeed, the marginal $F_N^{(j)}$ is obtained by integrating F_N with respect to the "last" $N-j$ variables thus it is a j-particle probability density (we remind that all quantities under consideration are symmetric with respect to permutations of the variables then, without loss of generality, in order to refer to any subsystem made by $N-j$ particles we can consider the last $N-j$). Clearly if $j = N$ we have $F_N^{(N)} = F_N$.

For fixed $j < N$, the j-particle marginal does not contain the full information about the N-particle configuration described by F_N. Knowledge of the j-particle marginal $F_N^{(j)}$, however, is sufficient to compute the expected value of every j-particle observable in the configuration described by the probability distribution $F_N \mathrm{d}Z_N$. In fact, if u_j denotes an arbitrary continuous and uniformly bounded function on $\mathbb{R}^{3j}$, and if $u_j \otimes 1_{N-j}$ denotes the function on $\mathbb{R}^{3N}$ which is associated with the N-particle observable corresponding to u_j for the first j particles and to 1_{N-j} for the last $(N-j)$ particles, we have

$$
\begin{aligned}
\langle u_j \otimes 1_{N-j} \rangle_{F_N} &= \int \mathrm{d}Z_N u_j(Z_j) F_N(Z_N) = \\
&= \int \mathrm{d}Z_j u_j(Z_j) F_N^{(j)}(Z_j) = \langle u_j \rangle_{F_N^{(j)}} ,
\end{aligned}
\tag{1.4.2}
$$

where we denoted by $\langle u_j \otimes 1_{N-j} \rangle_{F_N}$ the expected value of the N-particle observable corresponding to $u_j \otimes 1_{N-j}$ with respect to the distribution $F_N \mathrm{d}Z_N$ and with $\langle u_j \rangle_{F_N^{(j)}}$ the expected value of the j-particle observable corresponding to u_j with respect to $F_N^{(j)} \mathrm{d}Z_j$. Thus, $F_N^{(j)}$ is sufficient to compute the expectation of arbitrary observables which depend non-trivially on at most j particles (because of the permutation symmetry, it is not important on which particles it acts, just that it acts at most on j particles).

We are interested in characterizing the time-evolution of the marginals $F_N^{(j)}(t) := F_N^{(j)}(Z_j; t)$ associated with the solution $F_N(t)$ of the Liouville equation (1.1.5). By integrating the Liouville equation versus the variables $Z_{N-j} = (X_{N-j}, V_{N-j})$ we find the following family of equations (one for each $j = 1, \ldots, N$)

$$
(\partial_t + V_j \cdot \nabla_{X_j}) F_N^{(j)}(t) = T_{N,j}^{cl} F_N^{(j)}(t) + \frac{N-j}{N} C_{j,j+1}^{cl} F_N^{(j+1)}(t),
\tag{1.4.3}
$$

where $T_{N,j}^{cl}$ is precisely the j-particle Liouville operator, namely $T_{N,j}^{cl} \nabla_{X_j} U^{cl}(X_j) \cdot \nabla_{V_j}$, while the operator $C_{j,j+1}^{cl}$ maps $j+1$-particle densities in j-particle ones (if $j = N$ we find $C_{N,N+1}^{cl} \equiv 0$). The family of equations (1.4.3) is known as BBGKY hierarchy (in honor of the authors who independently derived it: Born, Bogoliubov, Green, Kirkwood, Yvon) and it is called "hierarchy" because we can see that the equation for the j-particle marginal is linked to the subsequent one by the term $C^{cl}_{j,j+1}F_N^{(j+1)}(t)$. The physical meaning is clear: the variation in time of $F_N^{(j+1)}(t)$ is due to the free motion of the j particles, which is encoded in the free-transport term $V_j \cdot \nabla_{X_j} F_N^{(j)}(t)$, to the interaction among themselves, which is modeled by the term $T^{cl}_{N,j}F_N^{(j)}(t)$, and to the interaction among the j-particle subsystem and the remaining $N-j$ particles, which is encoded in the term $\frac{N-j}{N}C^{cl}_{j,j+1}F_N^{(j+1)}(t)$ (the factor $1/N$ is precisely the factor appearing in the potential U^{cl} (see (1.1)) while the interaction with the last $N-j$ particles can be modeled by $N-j$ times the interaction with the $j+1$-th because of the symmetry with respect to permutations of the labeling (which follows from the fact that we are dealing with N identical par ticles).

Writing explicitly the action of the operators $T^{cl}_{N,j}$ and $C^{cl}_{j,j+1}$, we find:

$$\left(T^{cl}_{N,j}F_N^{(j)}\right)(X_j,V_j) = \frac{1}{N}\sum_{k\neq l}^{j} \nabla_{x_k}\phi(x_k-x_l)\cdot\nabla_{v_k}F_N^{(j)}(X_j,V_j), \tag{1.4.4}$$

and

$$\begin{aligned}&\left(C^{cl}_{j,j+1}F_N^{(j+1)}\right)(X_j,V_j) =\\ &= \sum_{k=1}^{j}\int_{\mathbb{R}^3\times\mathbb{R}^3} \mathrm{d}x_{j+1}\mathrm{d}v_{j+1}\nabla_{x_k}\phi(x_k-x_{j+1})\cdot\nabla_{v_k}F_N^{(j+1)}(X_j,x_{j+1},V_j,v_{j+1}).\end{aligned} \tag{1.4.5}$$

By these expressions we can argue that the operator $T^{cl}_{N,j}$ gives a vanishing contribution in the limit because it is of size j^2/N, while the operator $C^{cl}_{j,j+1}$ is of order one in the limit and the factor $(N-j)/N$ appearing in (1.4.3) is also of order one. Therefore denoting by $F^{(j)}(t)$ the expected limit of $F_N^{(j)}(t)$ when $N\to\infty$, the formal limit of the BBGKY hierarchy (1.4.3) is

$$(\partial_t + V_j\cdot\nabla_{X_j})F^{(j)}(t) = C^{cl}_{j,j+1}F^{(j+1)}(t), \tag{1.4.6}$$

which in the case $j=1$ is equal to:

$$(\partial_t+v_1\cdot\nabla_{x_1})F^{(1)}(t) = \int \mathrm{d}x_2\mathrm{d}v_2\nabla_{x_1}\phi(x_1-x_2)\cdot\nabla_{v_1}F^{(2)}(x_1,x_2,v_1,v_2;t). \tag{1.4.7}$$

We observe that the Vlasov equation (1.1.8) can be rewritten as

$$(\partial_t + v\cdot\nabla_x)f^t = \int \mathrm{d}x_2\mathrm{d}v_2\nabla_x\phi(x-x_2)\cdot\nabla_v f^t(x,v)f^t(x_2,v_2). \tag{1.4.8}$$

Replacing (x,v) by (x_1,v_1), f^t by $F^{(1)}(t)$ and the product $f^t\, f^t$ by $F^{(2)}$ we realize that (1.4.8) is precisely the same of (1.4.7). Thus the equation of the hierarchy

(1.4.6) corresponding to $j = 1$ is properly the Vlasov equation, provided that the the two-particle distribution $F^{(2)}(t)$ is factorized, and for this reason (1.4.6) (which is an infinite hierarchy because j can be equal to any positive number) is usually called "Vlasov hierarchy". More precisely, by considering (1.4.6) and by assuming the marginals $\{F^{(j)}(t)\}_{j\geq 1}$ to be factorized, namely

$$F^{(j)}(t) = f(t)^{\otimes j} \ \forall\, j, \tag{1.4.9}$$

it is easy to verify that $f(t)$ has to solve the Vlasov equation. Conversely, if we consider a time dependent one-particle density $f(t)$ solving the Vlasov equation and we take the j-particle densities $F^{(j)}(t) = f(t)^{\otimes j}$, for $j = 1, 2\ldots$, we find that the sequence $\{F^{(j)}(t)\}_{j\geq 1}$ solves the hierarchy (1.4.6).

An interesting problem is that of the uniqueness of the solution of the Vlasov hierarchy which plays an important role in facing the mean field limit when a generic (namely, non factorized) initial datum is considered for the many-body dynamics (such a case is also studied in [4]). This topic has been discussed in [8], under strong smoothness assumptions on the interaction potential, and in [9] by assuming $\phi \in \mathcal{C}_b^2(\mathbb{R}^3)$. Here we will not enter into details because we are going to show that in the present context there is no need to prove the uniqueness of the solution of the Vlasov hierarchy in order to establish the validity of propagation of chaos. (In the next section we will see that the situation in the quantum case can be very different).

First of all let us explain what we mean by "propagation of chaos".

As we have already specified, we consider as initial datum for the Liouville equation (1.1.5) the factorized N-particle probability density (1.3.2). This choice means that we are assuming that the particles are identically and independently distributed at time $t = 0$, or equivalently, the particles are initially uncorrelated. This is quite reasonable from the physical point of view and this is what is usually called "hypotheses of molecular chaos". Because of the interaction among the particles, the factorization (1.3.2) is not preserved by the time evolution because some correlations are introduced by the dynamics; in other words, the evolved N-particle density $F_N(t)$ is not given by the product of one-particle densities, if $t \neq 0$. However, due to the mean-field character of the interaction each particle interacts very weakly (we remind that the strength of the interaction is of the order $1/N$) with all other $(N-1)$ particles. For this reason, we may expect that, in the limit of large N, the total interaction force experienced by a typical particle in the system can be effectively replaced by an averaged, mean-field, force, and therefore that factorization is approximately, and in an appropriate sense, preserved by the time evolution. In other words, we may expect that, in a sense to be made precise,

$$F_N(t) \approx f(t)^{\otimes N} \text{ as } N \to \infty \tag{1.4.10}$$

for an evolved one-particle density $f(t) = f(x, v; t)$. This asymptotic factorization is precisely what is called "propagation of chaos". Assuming (1.4.10), it is simple to derive a self-consistent equation for the time-evolution of the one-particle density $f(t)$. In fact, (1.4.10) states that, for every fixed time t, the N particles are independently distributed in space according to the density $\rho(x;t) = \int \mathrm{d}v f(x, v; t)$. If this is true, the total force experienced, for example, by the first particle can be approximated by

$$\begin{aligned}\frac{1}{N}\sum_{k\geq 2}\nabla_{x_1}\phi(x_1 - x_k) &\approx \frac{1}{N}\sum_{k\geq 2}\int \mathrm{d}y\nabla_{x_1}\phi(x_1 - y)\rho(y;t) = \\ &= \frac{N-1}{N}\int \mathrm{d}y\mathrm{d}w\nabla_{x_1}\phi(x_1 - y)f(y, w; t) = \\ &= \frac{N-1}{N}(\nabla_{x_1}\phi * f(t)) \approx (\nabla_{x_1}\phi * f(t)),\end{aligned} \tag{1.4.11}$$

as $N \to \infty$. It follows that, if (1.4.10) holds true, the one-particle density $f(t)$ must satisfy the self-consistent equation

$$(\partial_t + v \cdot \nabla_x)f(t) = (\nabla_x\phi * f(t)) \cdot \nabla_v f(t) \tag{1.4.12}$$

with initial data $f(t)|_{t=0} = f_0$ given by (1.3.2). Equation (1.4.12) is precisely the Vlasov equation and we have just presented an heuristic argument to explain how it is related to the propagation of chaos. We observe that the Vlasov equation is a nonlinear Liouville equation on $\mathbb{R}^3 \times \mathbb{R}^3$. Therefore starting from the linear Liouville equation (1.1.5) on $\mathbb{R}^{3N} \times \mathbb{R}^{3N}$, we obtain, for the evolution of factorized densities, a nonlinear Liouville equation on $\mathbb{R}^3 \times \mathbb{R}^3$; the nonlinearity in the Vlasov equation is a consequence of the many-body effects in the linear dynamics.

The validity of propagation of chaos (namely, the precise statement concerning the asymptotic factorization (1.4.10)) is expressed in terms of convergence of the j-particle marginal densities associated with the solution of the Liouville equation (1.1.5) to the j-fold product of solutions of the Vlasov equation when $N \to \infty$. We are going to show that it is a straightforward consequence of the convergence (1.3.11) (e.g. [4]).

Let us consider the j-particle marginal $F_N^{(j)}(t)$ associated with the solution $F_N(t)$ of the Liouville equation with factorized initial datum $F_{N,0}$ given by (1.3.2).

We want to look at the behavior of $F_N^{(j)}(t)$ when $N \to \infty$. Denoting by $\mathbb{E}_N$ the expectation with respect to the initial N-particle distribution $F_{N,0}(Z_N)$, after straightforward computations, we obtain:

$$\begin{aligned}&\mathbb{E}_N\left[\mu_N(z_1'|Z_N(t))\dots\mu_N(z_j'|Z_N(t))\right] = \\ &= \frac{N(N-1)\dots(N-j+1)}{N^j}\, F_N^{(j)}(Z_j';t) + O\left(\frac{1}{N}\right),\end{aligned} \tag{1.4.13}$$

where $F_N^{(j)}(Z'_j;t) = F_N^{(j)}(\Phi^{-t}(Z'_j) = F_N^{(j)}(Z'_j(-t))$ (see (1.1.6)). Consider now a typical sequence Z_N with respect to f_0, namely such that (1.3.12) holds. By the Strong Law of Large Numbers (1.3.10) we know that (1.3.12) holds a.e. with respect to the product measure $f_0^{\otimes\infty}$. Then, by (1.3.11) and (1.4.13) we have:

$$\begin{aligned}&\lim_{N\to\infty} \mathbb{E}_N\left[\mu_N(z'_1|Z_N(t))\dots\mu_N(z'_j|Z_N(t))\right] = \\ &= \lim_{N\to\infty} F_N^{(j)}(Z'_j;t) = \prod_{k=1}^{j} f(z'_k;t),\end{aligned} \tag{1.4.14}$$

in the weak topology of probability measures, where $f(z'_k;t) = f(t)$ solves the Vlasov equation with initial datum f_0. Thus propagation of chaos holds. In the end, we found that starting from an initial uncorrelated state (1.3.2) for the N-particle system, for times $t > 0$ we loose the factorization, but it is recovered in the limit because the correlations created by the dynamics are smaller and smaller when $N \to \infty$. On the other side, the effect of the many-body interaction is "translated" into the self-consistent force appearing in the Vlasov equation.

The convergence (1.4.14) of $F_N^{(j)}(t)$ to $f(t)^{\otimes j}$ implies that:

$$\langle u_j \otimes 1_{N-j}\rangle_{F_N(t)} = \langle u_j\rangle_{F_N^{(j)}(t)} \to \langle u_j\rangle_{f(t)^{\otimes j}} \ \text{ as } N\to\infty, \tag{1.14.15}$$

for each $u_j \in \mathcal{C}_b^0(\mathbb{R}^{3j}\times\mathbb{R}^{3j})$. In other words, we are able to compute the "macroscopic" expected value of j-particle observables.

A remarkable fact is that the validity of propagation of chaos has been proven without using the hierarchies and this is really a big advantage because to deal with the hierarchies (1.4.3), (1.4.6) seems to be quite difficult. A priori, one could think to prove the convergence (1.14.15) of the marginals $F_N^{(j)}(t)$ to the products $f(t)^{\otimes j}$, by using that the first ones solve the BBGKY hierarchy (1.4.3) and the second ones solve the Vlasov hierarchy (1.4.6). Thus, if one would be able to prove the convergence of solutions of the N-dependent hierarchy to the Vlasov one, by knowing that the limiting hierarchy has factorized solutions arising from the Vlasov equation (as we previously discussed), the final step for proving the propagation of chaos would be to show the uniqueness of the solution of the Vlasov hierarchy over the class in which one is able to prove convergence. As regard to the "convergence problem" the difficulty is that the BBGKY hierarchy involve s operators which are unbounded, at least in reasonable spaces, thus it does not seem possible to apply any compactness argument to ensure the convergence of the solution. On the other side, concerning the "uniqueness problem" for the limiting hierarchy (1.4.6), the crucial point is the connection between the space in which one could show convergence and those in which it would be possible to prove uniqueness. Therefore, the problem of realizing the classical mean-field limit by dealing with the hierarchies is quite hard. On the other side, we have just seen that it can be faced more naturally by using two crucial tools: the Law of Large Numbers (1.3.10) and the continuity of solutions of the Vlasov equations with respect to the weak convergence of measures (1.2.3).

In the next section we will see that in the quantum case to deal with hierarchies is not so difficult and a possible approach to realize the limit (indeed the one that has been used more in the last years) is properly the one we have just described (convergence + uniqueness), particularly to deal with singular pair interaction potentials.

2 – Quantum Mean-Field limit

This section is devoted to the analysis of the macroscopic properties of the dynamics of a quantum system constituted by N identical particles interacting by a mean-field potential in the limit $N \to \infty$. As in the previous section, we set the dimension of the system equal to 3 but the main results we are going to discuss hold in any dimension.

The mean-field interaction potential is represented by the (right hand side) multiplication operator

$$U^Q(X_N) = \frac{1}{2N} \sum_{k \neq l}^{N} \phi(x_k - x_l), \tag{2.1}$$

where, as in the previous section, we denote by $X_N = (x_1, \ldots, x_N) \in \mathbb{R}^{3N}$ the positions of the N particles and we assume ϕ to be spherically symmetric. We want to characterize the effective dynamics of such a system for large N.

The problem of investigating the error in the approximation of the many-body evolution with the limiting macroscopic dynamics, which we do not discuss here, has been studied in [20] and [21].

2.1 – Setting of the problem: general features and known results

The state of an N-particle quantum mechanical system in $\mathbb{R}^3$ can be described by a complex valued wave function $\Psi_N \in L^2(\mathbb{R}^{3N})$. Physically the absolute value squared of $\Psi_N(x_1, \ldots, x_N)$ is interpreted as the probability density for finding particle one at x_1, particle two at x_2, and so on. Moreover the absolute value squared of the Fourier transform $\hat{\Psi}_N(v_1, \ldots, v_N)$ is interpreted as the probability density for having particle one with velocity v_1, particle two with velocity v_2, and so on (for the sake simplicity we always consider identical particles with mass $m = 1$ thus velocities are always equal to momenta). Because of this probabilistic interpretation, we will always consider wave functions Ψ_N with L^2-norm equal to one.

In nature there exist two different types of particles; bosons and fermions. Bosonic systems are described by wave functions which are symmetric with respect to permutations, in the sense that

$$\Psi_N(x_{\pi(1)},\dots,x_{\pi(N)}) = \Psi_N(x_1,\dots,x_N), \tag{2.1.1}$$

for every permutation π acting on $1,\dots,N$. Fermionic systems, on the other hand, are described by antisymmetric wave functions satisfying

$$\Psi_N(x_{\pi(1)},\dots,x_{\pi(N)}) = (-1)^{\sigma(\pi)}\Psi_N(x_1,\dots,x_N), \tag{2.1.2}$$

for every permutation π acting on $1,\dots,N$ where $\sigma(\pi)=0$ if π is even (in the sense that it can be written as the composition of an even number of transpositions) and $\sigma(\pi)=1$ if it is odd. In the sequel we will denote by $L^2_s(\mathbb{R}^{3N})$ the space of bosonic wave functions (namely the subspace of $L^2(\mathbb{R}^{3N})$ consisting of all functions satisfying (2.1.1)).

Equations (2.1.1) and (2.1.2) are responsible for substantial differences between an N-particle bosonic system and a fermionic one. Actually these features determine a different way to look at the limit $N\to\infty$ in the mean-field context, the use of different techniques leading to (a bit) different effective dynamics (see paragraph "Joint limit $N\to\infty$ and $\varepsilon\to 0$" in Section 3.4). Furthermore, the different nature of bosons and fermions is crucial in the perspective of looking at the connection between mean-field limit and semiclassical approximation (as we will observe in Section 3.4) and, at least from this point of view, bosonic systems seem to be more difficult to treat.

Anyway, here and henceforth we consider undistinguishable quantum particles by neglecting the statistics. In particular, in some cases the states we consider are indeed admissible for bosons.

We know that the observables of an N-particle system are represented by self adjoint operators A on $L^2(\mathbb{R}^{3N})$, then the expectation

$$\langle A\rangle_{\Psi_N} =<\Psi_N, A\Psi_N>=\int \bar{\Psi}_N(X_N)(A\Psi_N)(X_N)\mathrm{d}X_N \tag{2.1.3}$$

gives the value of the observable represented by A in the state described by Ψ_N.

The Hamiltonian of an N-particle system interacting by (2.1), assuming the mass of the particles to be equal to one, is the standard quantization of (1.1.1), namely

$$H_N^{Q,V} = -\sum_{k=1}^{N}\left(\frac{\varepsilon^2\Delta_k}{2}+V^Q(x_k)\right)+U^Q(X_N), \tag{2.1.4}$$

where we denoted by Δ_k the Laplace operator acting on the variable x_k, $k=1,2,\dots,N$ and here and henceforth we denote the Planck constant by ε. The potentials V^Q and ϕ (appearing in (2.1) are such that the Hamiltonian $H_N^{Q,V}$ is guaranteed to be a self-adjoint operator acting on the Hilbert space $L^2(\mathbb{R}^{3N})$ and it is invariant with respect to any permutation of the labeling (namely, the Hamiltonian is symmetric in the exchange of particle names). The first part of $H_N^{Q,V}$ is a sum of one-body operators (operators acting on one particle only); the sum of the Laplacians is the kinetic part of the Hamiltonian. The function V^Q describes an external potential which acts in the same way on all N particles. The second part of the Hamiltonian describes the interaction among the particles.

As in the classical case, we can assume without loss of generality that the potential experienced by each particle is only that arising from the many-body interaction, namely, the one-particle potential V^Q is assumed to be equal to zero. Thus the Hamiltonian we consider is

$$H_N^Q = -\sum_{k=1}^{N} \frac{\varepsilon^2 \Delta_k}{2} + U^Q(X_N). \tag{2.1.5}$$

The Hamiltonian (2.1.5) is the observable associated with the energy of the N-particle system interacting by the mean-field potential (2.1), thus the expectation

$$\left\langle H_N^Q \right\rangle_{\Psi_N} =< \Psi_N, H_N^Q \Psi_N >= \int \mathrm{d}X_N \bar{\Psi}_N(X_N) \left(H_N^Q \Psi_N \right)(X_N) \tag{2.1.6}$$

gives the energy of the system in the state described by the wave function Ψ_N.

The considerations we did in the previous section as regard to the scaling of the potential hold also in the quantum context. Therefore we are guaranteed that the energy per particle is of order one for large N, as it is crucial in looking for a non-trivial and well-defined limiting dynamics, and we realize that the basic features of the model are that the mutual interaction among the particles is weak (again of size $1/N$) and of long range type (unscaled support of ϕ). Again, as a consequence of such two effects we will have propagation of chaos and nonlinearity of the equation governing the limiting one-particle dynamics respectively (see Section 2.2).

The time evolution of a wave function $\Psi_N \in L^2(\mathbb{R}^{3N})$ associated with the N-particle system whose Hamiltonian is (2.1.5) is governed by the linear Schrödinger equation

$$i\varepsilon \partial_t \Psi_{N,t} = H_N^Q \Psi_{N,t}, \tag{2.1.7}$$

and, since H_N^Q is a self-adjoint operator, the time-evolution associated with the equation (2.1.7) preserves the L^2-norm of the wave function.

The solution to (2.1.7), with initial condition $\Psi_{N,t}|_{t=0} = \Psi_{N,0} \in L^2(\mathbb{R}^{3N})$, can be written by means of the unitary group generated by H_N^Q as

$$\Psi_{N,t} = e^{-i\frac{t}{\varepsilon} H_N^Q} \Psi_{N,0} \text{ for all } t \in \mathbb{R}. \tag{2.1.8}$$

The global well-posedness of (2.1.7) is not an issue here. The study of (2.1.7) is focused, therefore, on other questions concerning the qualitative and quantitative behavior of the solution $\Psi_{N,t}$. Despite the linearity of the equation, these questions are usually quite hard to answer, because in physically interesting situation the number of particles N is very large; for example, in applications related to the study of boson stars we have $N \approx 10^{30}$. For such huge values of N, it is of course impossible to compute the solution (2.1.7) explicitly; numerical methods are completely useless as well (unless the interaction among the particles is switched off).

Fortunately, also from the point of view of physics, it is not so important to know the precise solution to (2.1.7); it is much more important, for physicists performing experiments, to have information about the macroscopic properties of the system, which describe the typical behavior of the particles, and result from averaging over a large number of particles. Restricting the attention to macroscopic quantities simplifies the study of the solution $\Psi_{N,t}$, but it still does not make it accessible to mathematical analysis. To further simplify matters, we are going to let the number of particles N tend to infinity. The macroscopic properties of the system, computed in the limiting regime $N \to \infty$, are then expected to be a good approximation for the macroscopic properties observed in experiments, where the number of particles N is very large, but finite (explicit bounds on the difference between the limiting behavior as $N \to \infty$ and the behavior for large but finite N are obtained in [20] and [21]).

2.1.1 – The density matrix formalism

To consider the limit of large N, we are going to make use of the Reduced (or Marginal) Density Matrices (RDM) associated with an N-particle wave function $\Psi_N \in L^2(\mathbb{R}^{3N})$. First of all, we define the density matrix $\hat{\rho}_N = |\Psi_N >< \Psi_N|$ associated with Ψ_N as the orthogonal projection onto Ψ_N; we use here and henceforth the notation $|\psi >< \psi|$ to indicate the orthogonal projection onto ψ (Dirac bracket notation). Therefore $\hat{\rho}_N$ is a non-negative integral operator acting from $L^2(\mathbb{R}^{3N})$ to $L^2(\mathbb{R}^{3N})$ with kernel given by

$$\rho_N(X_N; Y_N) = \bar{\Psi}_N(X_N)\Psi_N(Y_N), \tag{2.1.9}$$

where $Y_N = (y_1, \dots, y_N) \in \mathbb{R}^{3N}$. Note that, by virtue of the L^2- normalization of Ψ_N, we have

$$\begin{aligned} \mathtt{Tr}\hat{\rho}_N = \int \mathrm{d}X_N \rho_N(X_N; X_N) = \int \mathrm{d}X_N \bar{\Psi}_N(X_N)\Psi_N(X_N) = \\ = \|\Psi_N\|^2_{L^2(\mathbb{R}^{3N})} = 1. \end{aligned} \tag{2.1.10}$$

Thus $\hat{\rho}_N \in \mathcal{L}^1(L^2(\mathbb{R}^{3N}))$, where $\mathcal{L}^1(L^2(\mathbb{R}^{3N}))$ is the Banach space (with respect to the norm $\|\cdot\|_{\mathcal{L}^1(L^2(\mathbb{R}^{3N}))} = \mathtt{Tr}\,|\cdot|$) of the trace class operators acting on $L^2(\mathbb{R}^{3N})$. Moreover, the positivity of $\hat{\rho}_N$ implies $\|\hat{\rho}_N\|_{\mathcal{L}^1(L^2(\mathbb{R}^{3N}))} = \mathtt{Tr}\hat{\rho}_N = 1$.

It turns out that the state of a quantum mechanical system can be equivalently represented in the wave function (Schrödinger) picture and in the density matrix (Heisenberg) formalism and the expectation $\langle A\rangle_{\Psi_N} =< \Psi_N, A\Psi_N >$ of an observable A in the state described by Ψ_N, expressed through the density matrix $\hat{\rho}_N$, can be written as $\mathtt{Tr}A\hat{\rho}_N$. For example, the energy of the mean-field system in the state described by $\hat{\rho}_N$ is

$$\left\langle H_N^Q \right\rangle_{\Psi_N} =< \Psi_N, H_N^Q \Psi_N >= \mathtt{Tr} H_N^Q \hat{\rho}_N, \tag{2.1.11}$$

H_N^Q defined in (2.1.5).

The time evolution of a density matrix describing the state of the N-particle mean-field system is governed by the linear equation

$$i\varepsilon\partial_t \hat{\rho}_{N,t} = \left[H_N^Q, \hat{\rho}_{N,t}\right], \tag{2.1.12}$$

where $\left[H_N^Q, \hat{\rho}_{N,t}\right]$ denotes the commutator between H_N^Q and $\hat{\rho}_{N,t}$, namely $\left[H_N^Q, \hat{\rho}_{N,t}\right] = H_N^Q\hat{\rho}_{N,t} - \hat{\rho}_{N,t}H_N^Q$. Equation (2.1.12) is usually called Heisenberg equation and, by knowing that $\hat{\rho}_{N,t} = |\Psi_{N,t} >< \Psi_{N,t}|$, it can be derived easily by the Schrödinger equation (2.1.7) solved by $\Psi_{N,t}$. The self-adjointness of the Hamiltonian H_N^Q, responsible for conservation of the L^2-norm of the wave function, implies that positivity and trace of the density matrix are also preserved in time.

We remind that we are looking at systems constituted by undistinguishable particles. Then we consider density matrices $\hat{\rho}_N$ such that their kernel $\rho_N(x_1, \ldots, x_N; y_1 \ldots, y_N)$ is symmetric in the exchange of particle names, namely

$$\rho_N(x_{\pi(1)}, \ldots, x_{\pi(N)}; y_{\pi(1)}, \ldots, y_{\pi(N)}) = \rho_N(x_1, \ldots, x_N; y_1, \ldots, y_N), \tag{2.1.13}$$

for every permutation π acting on $1, \ldots, N$. By the definition of the time-evolution (2.1.12) it is easy to verify that this property is preserved in time.

The solution to (2.1.12), with initial condition $\hat{\rho}_{N,t}|_{t=0} = \hat{\rho}_{N,0}$, can be written by means of the unitary group generated by H_N^Q as

$$\hat{\rho}_{N,t} = e^{-i\frac{t}{\varepsilon}H_N^Q}\hat{\rho}_{N,0}e^{i\frac{t}{\varepsilon}H_N^Q} \text{ for all } t \in \mathbb{R}. \tag{2.1.14}$$

The main advantage in describing the state and the dynamics of an N-particle system by using the density matrix formalism is that it gives the possibility to investigate the properties of subsystems made by a fixed number of variables. The way to do that is to introduce the Reduced Density Matrices (RDM). For $j = 1, \dots, N$, we define the j-particle marginal density $\hat{\rho}_N^{(j)}$ associated with $\hat{\rho}_N$ as the partial trace of $\hat{\rho}_N$ over the degrees of freedom of the last $(N-j)$ particles:

$$\hat{\rho}_N^{(j)} = \mathtt{Tr}_{j+1}\hat{\rho}_N \tag{2.1.15}$$

where $\mathtt{Tr}_{j+1}$ denotes the partial trace over the particles $j+1, j+2, \dots, N$. In other words, $\hat{\rho}_N^{(j)}$ is defined as the non-negative trace class operator on $L^2(\mathbb{R}^{3j})$ with kernel given by

$$\rho_N^{(j)}(X_j; Y_j) = \int \mathrm{d}X_{N-j}\rho_N(X_j, X_{N-j}; Y_j, X_{N-j}). \tag{2.1.16}$$

The last equation can be considered as the definition of partial trace. As in the previous section, we used the notation $X_j = (x_1, \dots, x_j), Y_j = (y_1, \dots, y_j) \in \mathbb{R}^{3j}$ and $X_{N-j} = (x_{j+1}, \dots, x_N) \in \mathbb{R}^{3(N-j)}$. By definition, $\mathtt{Tr}\hat{\rho}_N^{(j)} = 1$ for all N and for all $j = 1, \dots, N$ (clearly, if $j = N$ we find $\hat{\rho}_N^{(N)} = \hat{\rho}_N$) thus $\hat{\rho}_N^{(j)} \in \mathcal{L}^1(L^2(\mathbb{R}^{3j}))$ for all N and for all j.

Remark 2.1.1. Note that, in the physics literature, one normally uses a different normalization for the reduced density matrices. If the statistics are taken into account, the reduced density matrices are defined as expectation of bosonic and fermionic fields in the framework of the "second quantization formalism".

For fixed $j < N$, the j-particle density matrix does not contain the full information about the state described by $\hat{\rho}_N$. Knowledge of the j-particle marginal $\hat{\rho}_N^{(j)}$, however, is sufficient to compute the expectation of every j-particle observable in the state described by the density matrix $\hat{\rho}_N$. In fact, if $A^{(j)}$ denotes an arbitrary bounded operator on $L^2(\mathbb{R}^{3j})$, and if $A^{(j)} \otimes 1^{(N-j)}$ denotes the operator on $L^2(\mathbb{R}^{3N})$ which acts as $A^{(j)}$ on the first j particles, and as the identity on the last $(N-j)$ particles, we have

$$\mathtt{Tr}(A^{(j)} \otimes 1^{(N-j)})\hat{\rho}_N = \mathtt{Tr}A^{(j)}\hat{\rho}_N^{(j)}. \tag{2.1.17}$$

Thus, $\hat{\rho}_N^{(j)}$ is sufficient to compute the expectation of arbitrary observables which depend non-trivially on at most j particles (because of the permutation symmetry, it is not important on which particles it acts, just that it acts at most on j particles).

Marginal densities play an important role in the analysis of the $N \to \infty$ limit because, in contrast to the wave function Ψ_N and to the density matrix $\hat{\rho}_N$, the j-particle marginal $\hat{\rho}_N^{(j)}$ can have, for every fixed $j \in \mathbb{N}$, a well-defined limit as $N \to \infty$ (because, if we fix $j \in \mathbb{N}$, $\{\hat{\rho}_N^{(j)}\}_N$ defines a sequence of operators all acting on the same space $L^2(\mathbb{R}^{3j})$). In other words, $\hat{\rho}_N^{(j)}$ is a function of a fixed number of variables (which remains finite in the limit $N \to \infty$), while Ψ_N and $\hat{\rho}_N$ are functions of N variables thus in the limit we would have to deal with functions of an infinite number of variables and clearly it prevents the possibility to find a well-defined limit for them.

– **Mixed states**

In the previous analysis we have always considered systems whose state is described by a density matrix $\hat{\rho} \in \mathcal{L}^1(L^2(\mathbb{R}^{3d}))$ which is the orthogonal projection onto a wave function $\Psi \in L^2(\mathbb{R}^{3d})$ with $\mathtt{Tr}\hat{\rho} = \|\Psi\|_{L^2(\mathbb{R}^{3d})} = 1$ (we had $d = N$). Such kind of states are called “pure” states. Indeed, we say that a system is in a pure state whenever we know that it is described by a uniquely determined wave function with probability equal to one. As a consequence, the density matrix describing a “pure” state is a rank-one projection on $L^2(\mathbb{R}^{3d})$, namely $|\Psi >< \Psi|$. Nevertheless, in some cases it is not possible to know precisely (namely, with probability equal to one) which is the wave function describing the state of a system but one only has probabilistic predictions about that. For example, one can have a certain number (possibly infinite) k of known wave functions $\Psi^1, \dots, \Psi^k \in L^2(\mathbb{R}^{3d})$, with $\left\|\Psi^1\right\|_{L^2(\mathbb{R}^{3d})} = \cdots = \left\|\Psi^k\right\|_{L^2(\mathbb{R}^{3d})} = 1$, and a sequence of non-negative numbers $\lambda_1, \dots, \lambda_k$ such that it is known that the state can be described by Ψ^1 with probability equal to λ_1, by Ψ^2 with probability equal to λ_2 and so on..., where $\lambda_s \leq 1$ for $s = 1, \dots, k$ and $\sum_s \lambda_s = 1$. These kind of states are called “mixed” states (or equivalently, one can say that the state “associated with” the sequence $\Psi^1, \dots, \Psi^k$ is a “mixture” of the pure states $\Psi^1, \dots, \Psi^k$).

It turns out that one of the advantages of the density matrix formalism is that it encodes both the case of pure states and the case of mixtures. In fact, denoting by $\hat{\rho}_s$ the orthogonal projection onto Ψ^s, for $s = 1, \dots, k$, the density matrix $\hat{\rho}_{\mathrm{mix}}$ associated with the system under consideration is given by

$$\hat{\rho}_{\mathrm{mix}} = \sum_{s=1}^{k} \lambda_s \hat{\rho}_s = \sum_{s=1}^{k} \lambda_s \left|\Psi^s >< \Psi^s\right|. \tag{2.1.18}$$

Then, since $\|\Psi^s\|_{L^2(\mathbb{R}^{3d})} = 1$ for any s, we have

$$\mathtt{Tr}\hat{\rho}_{\mathrm{mix}} = \sum_{s=1}^{k} \lambda_s \mathtt{Tr}\hat{\rho}_s = \sum_{s=1}^{k} \lambda_s \|\Psi^s\|_{L^2(\mathbb{R}^{3d})} = \sum_{s=1}^{k} \lambda_s = 1, \tag{2.1.19}$$

namely, $\hat{\rho}_{\mathrm{mix}} \in \mathcal{L}^1(L^2(\mathbb{R}^{3d}))$ and $\|\hat{\rho}_{\mathrm{mix}}\|_{\mathcal{L}^1(L^2(\mathbb{R}^{3d}))} = 1$.

Clearly, a mixed state reduces to a pure state if $\lambda_{\bar{s}} = 1$ for some $\bar{s}$ and $\lambda_s = 0$ for $s \neq \bar{s}$.

By virtue of (2.1.19), it turns out that the analysis done previously by starting from a pure state can be generalized straightforward to the case of mixtures.

Furthermore, there are also states that are made by a "continuum" mixture of pure states. Indeed, let us take the parameter s in (2.1.18) as a continuum variable varying in a certain set $\Lambda \subset \mathbb{R}^n$, for some n (for example, in the initial state considered in Section 4.5 we have $s = (x_0, v_0) \in \Lambda = \mathbb{R}^6$), and let us consider a function $g = g(s)$ such that $g\mathrm{d}s$ is a probability distribution on Λ. If we have a family of L^2-normalized wave functions $\{\Psi^s\}_{s\in\Lambda}$ on $\mathbb{R}^d$ (for example, in Section 4.5 we considered the family of coherent states "centered" in (x_0, v_0)), we can costruct a mixed state which is the "continuum" mixture of the pure states $\{\Psi^s\}_{s\in\Lambda}$ through the probability distribution $g\mathrm{d}s$. It turns out that the kernel ρ_{mix} of the density matrix $\hat{\rho}_{\mathrm{mix}}$ describing the mixed state under consideration is

$$\rho_{\mathrm{mix}}(X;Y) = \int_\Lambda \mathrm{d}s\ g(s)\rho^s(X;Y) = \int_\Lambda \mathrm{d}s\ g(s)\overline{\Psi}^s(X)\Psi^s(Y), \tag{2.1.20}$$

where $X \in \mathbb{R}^d,\ Y \in \mathbb{R}^d$. Clearly, all considerations we did for "discrete" mixtures hold also in that case.

2.1.2 – The limit $N \to \infty$

We will discuss several known results about the study of the limiting dynamics when $N \to \infty$ for a mean-field system and we will see that what has been established, by using different techniques and various formalisms, is that the effective single-particle dynamics is governed by a cubic nonlinear Schrödinger equation

$$i\varepsilon\partial_t\psi_t = -\frac{\varepsilon^2}{2}\Delta\psi_t + (\phi * |\psi_t|^2)\psi_t \tag{2.1.21}$$

which is known as Hartree equation. Clearly, in that case the symbol "$*$" denotes the convolution with respect to the spatial variable, namely

$$\left(\phi * |\psi_t|^2\right)(x) = \int \mathrm{d}y\ \phi(x-y)|\psi_t(y)|^2. \tag{2.1.22}$$

The first rigorous results establishing a relation between the many body Schrödinger evolution and the nonlinear Hartree dynamics were obtained by K. Hepp in [2] (for smooth interaction potentials) and then generalized by J. Ginibre and G. Velo to singular potentials in [6]. These works were inspired by techniques used in quantum field theory. We will not discuss this method because we want to focus on other techniques which are more related to the topic we are going to face in the next sections (the connection between mean-field limit and semiclassical approximation).

The first proof of the emergence of the Hartree dynamics by using the RDM formalism ("RDM-convergence") was obtained by H. Spohn in [7], for bounded potentials (see Theorem 2.3.1 in Section 2.3). The method introduced by Spohn was then extended to singular potentials: in [17], L. Erdös and H. T. Yau faced the RDM- convergence for a Coulomb potential $\phi(x) = \pm 1/|x|$; partial results for this kind of interaction were also obtained by C. Bardos, F. Golse and N. Mauser in [16] (note that recently a new proof in the case of a Coulomb interaction has been proposed by J. Fröhlich, A. Knowles, and S. Schwarz in [28]).

A different approach to the proof of the rigorous derivation of the Hartree equation from a mean-field bosonic system has been proposed by Fröhlich, Schwarz and Graffi in [26]. By using the Wigner formalism (see Section 3) they can consider the mean-field limit uniformly in the Planck constant ε (up to an exponential error depending on time); this allows them to combine the semiclassical limit and the mean field limit by assuming restrictive assumptions on the pair interaction potential (we will come back on this result in Section 3). It is also interesting to remark that the mean-field limit can be interpreted as a Egorov-type theorem; this was observed in [27] for sufficiently smooth potentials and in [28] for the Coulomb interaction.

2.2 – Quantum BBGKY hierarchy and its formal limit as $N \to \infty$

We have already remarked that, for any $j = 1, \dots, N$, the marginal densities $\hat{\rho}^{(j)}_{N,t}$ associated with the solution $\hat{\rho}_{N,t}$ of the equation (2.1.12), are crucial tools in studying the mean-field limit because they can have, for every fixed j, a well-defined limit as $N \to \infty$. Thus, we are interested in their time-evolution as $N \to \infty$.

By taking the partial trace over the degrees of freedom of the last $N - j$ particles in the Heisenberg equation (2.1.12) we find the following family of equations (one for each $j = 1, \dots, N$)

$$(2.2.1) \qquad i\varepsilon\partial_t \hat{\rho}^{(j)}_{N,t} = \sum_{k=1}^{j} \left[-\frac{\varepsilon^2}{2}\Delta_k, \hat{\rho}^{(j)}_{N,t} \right] + T^Q_{N,j}\hat{\rho}^{(j)}_{N,t} + \frac{N-j}{N} C^Q_{j,j+1}\hat{\rho}^{(j)}_{N,t},$$

where the operator $T^Q_{N,j}$ acts on $\mathcal{L}^1(L^2_s(\mathbb{R}^{3j}))$ while the operator $C^Q_{j,j+1}$ maps $j+1$-particle densities in j-particle ones (if $j = N$ we find $C^Q_{N,N+1} \equiv 0$). The family of equations (2.2.1) is called BBGKY hierarchy in analogy to the classical case and, again, it is called "hierarchy" because we can see that the equation for the j-particle marginal density is linked to the subsequent one by the term $C^Q_{j,j+1}\hat{\rho}^{(j)}_{N,t}$. The physical meaning is the same we discussed in the classical case:

the variation in time of $\hat{\rho}^{(j)}_{N,t}$ is due to the free motion of the j particles, to their interaction among themselves and to the interaction among the j-particle subsystem and the remaining $N-j$ particles. The first effect is modeled by the l.h.s and by the first term in the r.h.s of (2.2.1), the second one is encoded in $T^Q_{N,j}\hat{\rho}^{(j)}_{N,t}$), while the interaction between the j-particle subsystem and the remaining $N-j$ particles is modeled by $\frac{N-j}{N}C^Q_{j,j+1}\hat{\rho}^{(j)}_{N,t}$. The factor $1/N$ in front of $C^Q_{j,j+1}\hat{\rho}^{(j)}_{N,t}$ arises from the scaling of the p otential U^Q (see (2.1) while the factor $N-j$ is due to the symmetry with respect to permutations of the labeling (we remind that we are dealing with N identical particles): indeed, the interaction of the j particles under consideration with the last $N-j$ can be modeled by $N-j$ times the interaction with the $j+1$-th particle.

Writing explicitly the action of the operators $T^Q_{N,j}$ and $C^Q_{j,j+1}$, we find:

$$T^Q_{N,j}\hat{\rho}^{(j)}_{N,t} = \frac{1}{2N}\sum_{k\neq l}^{j}\left[\phi(x_k-x_l),\hat{\rho}^{(j)}_{N,t}\right], \tag{2.2.2}$$

and

$$C^Q_{j,j+1}\hat{\rho}^{(j)}_{N,t} = \sum_{k=1}^{j}\mathtt{Tr}_{j+1}\left\{\left[\phi(x_k-x_{j+1}),\hat{\rho}^{(j+1)}_{N,t}\right]\right\}. \tag{2.2.3}$$

By (2.2.2) we can argue that the operator $T^Q_{N,j}$ gives a vanishing contribution in the limit because it is of size j^2/N, while the operator $C^Q_{j,j+1}$ is of order one in the limit and the factor $(N-j)/N$ appearing in (2.2.1) is also of order one. Therefore denoting by $\hat{\rho}^{(j)}_t$ the expected limit of $\hat{\rho}^{(j)}_{N,t}$ when $N\to\infty$, the formal limit of the BBGKY hierarchy (2.2.1) is

$$i\varepsilon\partial_t\hat{\rho}^{(j)}_t = \sum_{k=1}^{j}\left[-\frac{\varepsilon^2}{2}\Delta_k,\hat{\rho}^{(j)}_t\right] + C^Q_{j,j+1}\hat{\rho}^{(j+1)}_t, \tag{2.2.4}$$

which in the case $j=1$ is equal to:

$$i\varepsilon\partial_t\hat{\rho}^{(1)}_t = \left[-\frac{\varepsilon^2}{2}\Delta_1,\hat{\rho}^{(1)}_t\right] + \mathtt{Tr}_2\left\{\left[\phi(x_1-x_2),\hat{\rho}^{(2)}_t\right]\right\}. \tag{2.2.5}$$

We observe that the Hartree equation (2.1.21) in the density matrix formalism ("Heisenberg form") is

$$i\varepsilon\partial_t\hat{\rho}_t = \left[-\frac{\varepsilon^2}{2}\Delta,\hat{\rho}_t\right] + \mathtt{Tr}_2\left\{\left[\phi(x-x_2),\hat{\rho}_t\otimes\hat{\rho}_t\right]\right\}. \tag{2.2.6}$$

Replacing x by x_1, $\hat{\rho}_t$ by $\hat{\rho}_t^{(1)}$ and the product $\hat{\rho}_t \otimes \hat{\rho}_t$ by $\hat{\rho}_t^{(2)}$ we realize that (2.2.6) is precisely the same of (2.2.5). Thus the equation of the hierarchy (2.2.4) corresponding to $j = 1$ is properly the Hartree equation, provided that the the two-particle density $\hat{\rho}_t^{(2)}$ is factorized, and for this reason (2.2.4) is usually called "Hartree hierarchy". More precisely, by considering (2.2.4) and by assuming the reduced density matrices $\hat{\rho}_t^{(j)}$, $j = 1, 2, \ldots$, to be factorized, namely

$$\hat{\rho}_t^{(j)} = \hat{\rho}_t^{\otimes j} \ \forall\, j, \tag{2.2.7}$$

it is easy to verify that $\hat{\rho}_t$ has to solve the Hartree equation. Conversely, if we consider a time dependent one-particle density $\hat{\rho}_t$ solving the Hartree equation (2.2.6) and we take the j-particles densities $\hat{\rho}_t^{(j)} = \hat{\rho}_t^{\otimes j}$, $j = 1, 2 \ldots$, we find that the sequence $\{\hat{\rho}_t^{(j)}\}_{j \geq 1}$ solves the hierarchy (2.2.4).

An interesting problem is that of the uniqueness of the solution of the Hartree hierarchy. The situation in the quantum case is quite different from that of the classical one. In fact, as we will see in the next section, the Hartree hierarchy is much more controllable than the Vlasov one because the operators involved are bounded with respect to the norms appropriate to study the convergence of the sequence of reduced density matrices to the solution of the limiting hierarchy. Thus, it is possible to follow the approach we described briefly at the end of the previous section (convergence + uniqueness) in order to prove "propagation of chaos" in the quantum context, namely, asymptotic factorization of the dynamics (in the sense specified in the forthcoming paragraph). Nonetheless, the proof of uniqueness of the solution of the quantum limiting hierarchy is very far to be a trivial stuff. Indeed, in the case of bounded interaction the problem is quite easy to face and, in par ticular, by following the strategy of [7] (originally introduced by O. Lanford for the derivation (for short times) of the Boltzmann equation from the hard-sphere dynamics (see [3])) it is possible to prove "at the same time" convergence and uniqueness (see Theorem 2.3.1). On the contrary, in case of more singular interactions (as the Coulomb one), the proof of propagation of chaos consists really of two steps: proving the convergence of solutions of the BBGKY hierarchy to the Hartree hierarchy and showing the uniqueness of the solution of such a hierarchy (which implies factorization of the limiting j-particle density matrices because, as we have already remarked, the Hartree hierarchy admits factorized solutions as (2.2.7)). In the Coulomb case, the "uniqueness" problem is quite hard to deal with because of the singularity of the interaction (see [17]).

Anyway, we will come back later on the rigorous proof of propagation of chaos, analyzing in detail the case of bounded potentials. Moreover we will discuss briefly the Coulomb case, accenting which are the main new tools with respect to the bounded case, why there is need of them and in which way they make the proof harder requiring a more refined analysis of the limiting hierarchy.

Now let us clarify what we mean by "propagation of chaos" in the quantum framework.

Let us consider as initial datum for the Schrödinger equation (2.1.7) a factorized N-particle wave function

$$\Psi_{N,0} = \psi_0^{\otimes N}, \quad \text{for some} \quad \psi_0 \in L^2(\mathbb{R}^3). \tag{2.2.8}$$

This assumption, rephrased in the density matrix formalism, leads to consider the following factorized N-particle density matrix

$$\hat{\rho}_{N,0} = |\Psi_{N,0} >< \Psi_{N,0}| = \hat{\rho}_0^{\otimes N}, \quad \text{with} \quad \hat{\rho}_0 = |\psi_0 >< \psi_0|, \tag{2.2.9}$$

as initial datum for the Heisenberg equation (2.1.12). As in the classical context, (2.2.8) (or equivalently (2.2.9)) is called "hypotheses of molecular chaos" because we are assuming that the particles are initially uncorrelated. Furthermore, they are all in the same (one-particle) state at time $t = 0$ and clearly $\Psi_{N,0} \in L^2_s(\mathbb{R}^{3N})$. Thus, (2.2.8) is an admissible state for bosons (while for fermions it is prevented by the Pauli exclusion principle). The physical motivation for studying the evolution of factorized wave functions is that states close to the ground state of H_N^Q (the eigenvector associated with the lowest eigenvalue), which are the most accessible and thus the most interesting states, can be approximately described by wave functions like (2.2.8) (some of the results which we are going to discuss in the following sections do not require strict factorization as in (2.2.8); instead asymptotic factorization of the initial wave function in the sense of $\mathcal{L}^1$-convergence of the RDM to the j-fold product of one-particle densities would be sufficient (see Theorem 2.3.1 and the discussion below)).

Because of the interaction among the particles, the factorization (2.2.8) (or equivalently (2.2.9)) is not preserved by the time evolution; in other words, the evolved N-particle wave function $\Psi_{N,t}$ is not given by the product of one-particle wave functions, if $t \neq 0$. All considerations done in the classical case concerning the mean-field (weak) character of the interaction hold, then we may expect that, in the limit of large N, the total interaction potential experienced by a typical particle in the system can be effectively replaced by an averaged, mean-field, potential, and therefore that factorization is approximately, and in an appropriate sense, preserved by the time evolution. In other words, we may expect that, in a sense to be made precise,

$$\Psi_{N,t} \approx \psi_t^{\otimes N} \quad \text{as} \quad N \to \infty \tag{2.2.10}$$

or

$$\hat{\rho}_{N,t} \approx \hat{\rho}_t^{\otimes N} \text{ as } N \to \infty, \text{ with } \hat{\rho}_{N,t} = |\Psi_{N,t} >< \Psi_{N,t}|, \ \hat{\rho}_t = |\psi_t >< \psi_t| \tag{2.2.11}$$

for an evolved one-particle wave function ψ_t. This asymptotic factorization is precisely what is called "propagation of chaos". Assuming (2.2.10), it is simple to derive a self-consistent equation for the time-evolution of the wave function ψ_t. In fact, (2.2.10) states that, for every fixed time t, the N bosons are independently distributed in space according to the density $|\psi_t(x)|^2$. If this is true, the total potential experienced, for example, by the first particle can be approximated by

$$\begin{aligned}\frac{1}{N}\sum_{k\geq 2}\phi(x_1-x_k) &\approx \frac{1}{N}\sum_{k\geq 2}\int \mathrm{d}y\phi(x_1-y)|\psi_t(y)|^2 = \\ &= \frac{N-1}{N}(\phi * |\psi_t|^2) \approx (\phi * |\psi_t|^2),\end{aligned} \tag{2.2.12}$$

as $N \to \infty$. It follows that, if (2.2.10) holds true, the one-particle wave function ψ_t must satisfy the self-consistent equation

$$i\varepsilon\partial_t\psi_t = -\frac{\varepsilon^2}{2}\Delta\psi_t + \left(\phi * |\psi_t|^2\right)\psi_t \tag{2.2.13}$$

with initial datum ψ_0 given by (2.2.8). Equation (2.2.13) is precisely the Hartree equation and we have just presented an heuristic argument to explain how it is related to the propagation of chaos. We observe that the Hartree equation is a nonlinear Schrödinger equation on $\mathbb{R}^3 \times \mathbb{R}^3$. Therefore starting from the linear Schrödinger equation (2.1.7) on $\mathbb{R}^{3N} \times \mathbb{R}^{3N}$, we obtain, for the evolution of factorized densities, a nonlinear Schrödinger equation on $\mathbb{R}^3 \times \mathbb{R}^3$; the nonlinearity in the Hartree equation is a consequence of the many-body effects in the linear dynamics.

The validity of propagation of chaos (namely, the precise statement concerning the asymptotic factorization (2.2.10) or (2.2.11)) is expressed in terms convergence in $\mathcal{L}^1(L^2(\mathbb{R}^{3j}))$ of the j-particle marginal densities associated with the solution of the Heisenberg equation (2.1.12) to the j-fold product of solutions of the Hartree equation when $N \to \infty$, namely

$$\left\|\hat{\rho}_{N,t}^{(j)} - \hat{\rho}_t^{\otimes j}\right\|_{\mathcal{L}^1(L^2(\mathbb{R}^{3j}))} \to 0, \text{ as } N \to \infty, \tag{2.2.14}$$

$\hat{\rho}_t \in \mathcal{L}^1(L^2(\mathbb{R}^3))$ solving the Hartree equation (in the "Heisenberg form") (2.2.6) with initial datum $\hat{\rho}_0$ given by (2.2.11). Clearly, $\hat{\rho}_t = |\psi_t >< \psi_t|$, ψ_t solving the Hartree equation (2.2.13) with initial datum ψ_0 given by (2.2.10).

We have already remarked that, for fixed $j < N$, the j-particle RDM $\hat{\rho}_{N,t}^{(j)}$ does not contain the full information about the N-particle system described by $\hat{\rho}_{N,t}$. Nonetheless, $\hat{\rho}_{N,t}^{(j)}$ is sufficient to compute the expectation of arbitrary observables of the form $A_j \otimes 1_{N-j}$ which depend non-trivially on at most j particles (because of the permutation symmetry, it is not important on which particles it acts, just that it acts at most on j particles).

Therefore the convergence (2.2.14) implies that:

$$\begin{aligned}\langle A_j \otimes 1_{N-j} \rangle_{\Psi_{N,t}} &= \mathtt{Tr}(A_j \otimes 1_{N-j})\hat{\rho}_{N,t} = \mathtt{Tr} A_j \hat{\rho}^{(j)}_{N,t} \; \rightarrow \; \mathtt{Tr} A_j \hat{\rho}_t^{\otimes j} = \\ &= \langle A_j \rangle_{\psi_t^{\otimes j}} \text{ as } N \rightarrow \infty,\end{aligned} \tag{2.2.15}$$

for each bounded operator A_j acting on $L^2(\mathbb{R}^{3j})$. In other words, (2.2.14) allows to know the "macroscopic" expected value of j-particle observables for an N-particle system interacting by a men-field potential.

2.3 – Mean-Field limit for bounded potentials

We consider, in this section, the dynamics generated by the mean field Hamiltonian (2.1.5) under the assumption that the interaction potential is a bounded operator. We will assume, in other words, that $\phi \in L^\infty(\mathbb{R}^3)$ (recall that the operator norm of the multiplication operator $\phi(x_k - x_l)$ is given by the L^∞-norm of the function ϕ).

In the sequel we will use the notation $\phi_{kl} := \phi(x_k - x_l)$.

Theorem 2.3.1 [Spohn 1980]. *Let the pair interaction potential ϕ be in $L^\infty(\mathbb{R}^3)$ and the initial state of the system be described by a factorized N-particle wave function $\Psi_{N,0} \in L^2_s(\mathbb{R}^{3N})$, namely*

$$\Psi_{N,0} = \psi_0^{\otimes N}, \quad \textit{for some} \quad \psi_0 \in L^2(\mathbb{R}^3): \quad \|\psi_0\|_{L^2(\mathbb{R}^3)} = 1. \tag{2.3.1}$$

This implies that the initial N-particle density matrix $\hat{\rho}_{N,0} \in \mathcal{L}^1(L^2(\mathbb{R}^{3N}))$ is given by

$$\hat{\rho}_{N,0} = |\Psi_{N,0} >< \Psi_{N,0}| = \hat{\rho}_0^{\otimes N}, \quad \hat{\rho}_0 = |\psi_0 >< \psi_0|. \tag{2.3.2}$$

Then, for any fixed j,

$$\left\| \hat{\rho}^{(j)}_{N,t} - \hat{\rho}_t^{\otimes j} \right\|_{\mathcal{L}^1(L^2(\mathbb{R}^{3j}))} \longrightarrow 0, \quad \textit{as} \quad N \rightarrow \infty, \tag{2.3.3}$$

where $\hat{\rho}^{(j)}_{N,t}$ solves the BBGKY hierarchy (2.2.1) *with initial datum $\hat{\rho}_0^{\otimes j}$ and $\hat{\rho}_t \in \mathcal{L}^1(L^2(\mathbb{R}^3))$ is the solution of the Hartree equation (in the "Heisenberg form")*

$$i\varepsilon \partial_t \hat{\rho}_t = \left[-\frac{\varepsilon^2}{2}\Delta, \hat{\rho}_t \right] + \mathtt{Tr}_2\{[\phi(x - x_2), \hat{\rho}_t \otimes \hat{\rho}_t]\}, \tag{2.3.4}$$

with initial datum $\hat{\rho}_0$. In terms of wave functions, we find that $\hat{\rho}_t = |\psi_t >< \psi_t|$, ψ_t solving the Hartree equation (2.1.21) *with initial datum ψ_0.*

PROOF. Let $\hat{\rho}^{(N)} \in \mathcal{L}^1(L^2(\mathbb{R}^{3N}))$ be a trace class operator with kernel $\rho^{(N)}$ invariant under permutations of the labeling. For fixed j, let $\hat{\rho}_j^{(N)} \in \mathcal{L}^1(L^2(\mathbb{R}^{3j}))$ be

$$\hat{\rho}_j^{(N)} = \mathtt{Tr}_{j+1}\hat{\rho}^{(N)}. \tag{2.3.5}$$

Then, by considering the time-evolution $\hat{\rho}^{(N)}(t) = e^{-\frac{i}{\varepsilon}H_N^Q t}\hat{\rho}^{(N)}e^{\frac{i}{\varepsilon}H_N^Q t}$, H_N^Q defined in (2.1.5), it is also invariant under permutations of the labeling and the j-particle trace class operator $\hat{\rho}_j^{(N)}(t) = \mathtt{Tr}_{j+1}\hat{\rho}^{(N)}(t)$ satisfies the differential equation

$$\begin{aligned} i\varepsilon\partial_t\hat{\rho}_j^{(N)}(t) = &\left[\sum_{k=1}^{j}\left(-\frac{\varepsilon^2}{2}\Delta_k\right) + \frac{1}{2N}\sum_{k\neq l}^{j}\phi_{kl}, \hat{\rho}_j^{(N)}(t)\right] + \\ &+\left(\frac{N-j}{N}\right)\sum_{k=1}^{j}\mathtt{Tr}_{j+1}\left\{\left[\phi_{kj+1}, \hat{\rho}_{j+1}^{(N)}(t)\right]\right\}. \end{aligned} \tag{2.3.6}$$

This is what we previously called BBGKY hierarchy (see (2.2.1)) as it can be seen by using the "compact" notation

$$\begin{aligned} \partial_t\hat{\rho}_j^{(N)}(t) = &-\frac{i}{\varepsilon}\left[\sum_{k=1}^{j}\left(-\frac{\varepsilon^2}{2}\Delta_k\right), \hat{\rho}_j^{(N)}(t)\right] - \frac{i}{\varepsilon}T_{N,j}^Q\hat{\rho}_j^{(N)}(t) - \\ &-\frac{i}{\varepsilon}\left(\frac{N-j}{N}\right)C_{j,j+1}^Q\hat{\rho}_{j+1}^{(N)}(t), \end{aligned} \tag{2.3.7}$$

$T_{N,j}^Q$ and $C_{j,j+1}^Q$ as in (2.2.2) and (2.2.3) respectively.

Let $S_j^{(N)}(t)$ is the flow associated with the equation:

$$\partial_t\hat{\rho}_j^{(N)}(t) = -\frac{i}{\varepsilon}\left[H_{N,j}^Q, \hat{\rho}_j^{(N)}(t)\right], \tag{2.3.8}$$

with

$$H_{N,j}^Q := \sum_{k=1}^{j}\left(-\frac{\varepsilon^2}{2}\Delta_k\right) + T_{N,j}^Q. \tag{2.3.9}$$

Thus, $S_j^{(N)}(t)\hat{\rho}_j = e^{-\frac{i}{\varepsilon}H_{N,j}^Q t}\hat{\rho}_j e^{\frac{i}{\varepsilon}H_{N,j}^Q t}$, for any $\hat{\rho}_j \in \mathcal{L}^1(L^2(\mathbb{R}^{3j}))$. By the Duhamel formula, the solution of (2.3.7) can be written as

$$\begin{aligned} \hat{\rho}_j^{(N)}(t) = &S_j^{(N)}(t)\hat{\rho}_j^{(N)} + \\ &+\left(\frac{N-j}{N}\right)\left(-\frac{i}{\varepsilon}\right)\int_0^t \mathrm{d}t_1\, S_j^{(N)}(t-t_1)C_{j,j+1}^Q\hat{\rho}_{j+1}^{(N)}(t_1). \end{aligned} \tag{2.3.10}$$

Iterating the integral equation (2.3.10), we obtain the series

$$\begin{aligned}\hat\rho_j^{(N)}(t) = S_j^{(N)}(t)\hat\rho_j^{(N)} + {} & + \sum_{n=1}^{N-j} \int_{0\le t_n\le\cdots\le t_1\le t} \mathrm{d}t_n \ldots \mathrm{d}t_1 S_j^{(N)}(t-t_1)\times \\ & \times \left(\frac{N-j}{N}\right)\left(-\frac{i}{\varepsilon}\right) C^Q_{j,j+1}\cdots\left(\frac{N-j-n+1}{N}\right) \\ & \times \left(-\frac{i}{\varepsilon}\right) C^Q_{j+n-1,j+n} S^{(N)}_{j+n}(t_n)\hat\rho^{(N)}_{j+n}.\end{aligned} \tag{2.3.11}$$

Let $\|\cdot\|_j$ denote the trace norm in $\mathcal{L}^1(L^2(\mathbb{R}^{3j}))$. Since $S_j^{(N)}(t)$ preserves the $\|\cdot\|_j$ norm (because $H^Q_{N,j}$ is a self-adjoint operator on $L^2(\mathbb{R}^{3j})$), by the expression (2.2.3) for $C^Q_{j,j+1}$, it is easy to verify that the n-th term of the series (2.3.11) is bounded by

$$\frac{t^n}{n!}\, j(j+1)\ldots(j+n-1)\left(\frac{2\,\|\phi\|_{L^\infty}}{\varepsilon}\right)^n \left\|\hat\rho^{(N)}_{j+n}\right\|_{j+n}. \tag{2.3.12}$$

If one assumes

$$\mathbf{P1})\ \left\|\hat\rho_j^{(N)}\right\|_j \le a^j \quad \text{for any } j, \tag{2.3.13}$$

then the series (2.3.11) converges in trace norm for $|t|\le t_0$ with $t_0 < \frac{\varepsilon}{4\|\phi\|_{L^\infty} a}$.

For any $\hat\rho_j \in \mathcal{L}^1(L^2(\mathbb{R}^{3j}))$, let $S_j(t)\hat\rho_j = e^{-\frac{i}{\varepsilon}H_j t}\hat\rho_j e^{\frac{i}{\varepsilon}H_j t}$, where $H_j = \sum_{k=1}^j\left(-\frac{\varepsilon^2}{2}\Delta_k\right)$ is the j-particle free Hamiltonian. We note that

$$\left\|T^Q_{N,j}\hat\rho_j^{(N)}\right\| \le \frac{j(j-1)}{2N}\|[\phi,\hat\rho_j^{(N)}]\|_j \le \frac{j(j-1)}{N}\,\|\phi\|_{L^\infty}\left\|\hat\rho_j^{(N)}\right\|_j, \tag{2.3.14}$$

then by Property **P1**) we find

$$\left\|T^Q_{N,j}\right\| \le \frac{j(j-1)}{N}\,\|\phi\|_{L^\infty}\, a^j \to 0 \quad \text{as} \quad N\to\infty, \tag{2.3.15}$$

where $\|\cdot\|$ is the operator norm on $\mathcal{L}^1(L^2(\mathbb{R}^{3j}))$.

We note that, for any $\hat\rho_j\in\mathcal{L}^1(L^2(\mathbb{R}^{3j}))$,

$$\begin{aligned}\left\|S_j^{(N)}(t)\hat\rho_j - S_j(t)\hat\rho_j\right\|_j &\le \frac{1}{\varepsilon}\int_0^t \mathrm{d}\tau\,\left\|S_j(t-\tau)T^Q_{N,j}\hat\rho_j(\tau)\right\|_j \le \\ &\le \frac{1}{\varepsilon}\int_0^t \mathrm{d}\tau\,\left\|T^Q_{N,j}\hat\rho_j(\tau)\right\|_j,\end{aligned} \tag{2.3.16}$$

where we use that $S_j(t)$ preserves the trace norm. Then, from (2.3.15), it follows that

$$\lim_{N\to\infty}\left\|S_j^{(N)}(t)-S_j(t)\right\|=0. \tag{2.3.17}$$

If one assumes

$$\mathbf{P2})\ \lim_{N\to\infty}\left\|\hat\rho_j^{(N)}-\hat\rho_j\right\|_j=0, \tag{2.3.18}$$

for some $\hat\rho_j\in\mathcal{L}^1(L^2(\mathbb{R}^{3j}))$, then by (2.3.11) and (2.3.17), it follows that $\hat\rho_j^{(N)}(t)$ converges as $N\to\infty$ in trace norm to

$$\begin{aligned}\hat\rho_j(t)=\sum_{n=0}^{+\infty}\int_{0\le t_n\le\cdots\le t_1\le t}&\mathrm{d}t_n\ldots\mathrm{d}t_1\ S_j(t-t_1)\times\\ &\times\left(-\frac{i}{\varepsilon}\right)C^Q_{j,j+1}\cdots\left(-\frac{i}{\varepsilon}\right)C^Q_{j+n-1,j+n}\ S_{j+n}(t_n)\hat\rho_{j+n},\end{aligned} \tag{2.3.19}$$

for $|t|\le t_0$. We note that the n-th term of the above series in bounded in trace norm by (2.3.12), then for short times $|t|\le t_0$ we are ensures that (2.3.19) converges in trace norm.

Let $\hat\rho^{(N)}$ be a density matrix. Then $\left\|\hat\rho_j^{(N)}(t)\right\|_j=\left\|\hat\rho_j^{(N)}\right\|_j$ by preservation of positivity and trace. Therefore, if for the initial state the bound **P1**) is satisfied, it remains valid for all times, and the argument just given can be iterated to prove convergence of $\hat\rho_j^{(N)}(t)$ to $\hat\rho_j(t)$ as $N\to\infty$ for all times. Furthermore, $\hat\rho_j(t)$ is uniquely determined for all times because by iteration we prove that (2.3.19) converges in trace norm for all times.

One checks that for the particular initial state $\hat\rho_{N,0}$ in (2.3.2) the conditions **P1**) and **P2**) are satisfied with $a=1$ and $\hat\rho_j=\hat\rho_0^{\otimes j}$. Therefore, we can claim that the solution $\rho_{N,t}^{(j)}$ of the BBGKY hierarchy (2.3.7) with initial datum $\hat\rho_0^{\otimes j}$ converges in trace norm to the unique j-particle density matrix $\hat\rho_j(t)$ identified by the series (2.3.19) with $\hat\rho_{j+n}=\hat\rho_0^{\otimes j+n}\ \ \forall\ n$. Differentiating (2.3.19) with respect to t, one obtains the limiting hierarchy of equations

$$i\varepsilon\partial_t\hat\rho_j(t)=\left[\sum_{k=1}^{j}\left(-\frac{\varepsilon^2}{2}\Delta_k\right),\hat\rho_j(t)\right]+C^Q_{j,j+1}\ \hat\rho_{j+1}(t), \tag{2.3.20}$$

whose unique trace class solution is $\hat\rho_j(t)$ with initial datum $\hat\rho_0^{\otimes j}$. Moreover, (2.3.20) preserves the factorization property for all t according to the Hartree equation (in the Heisenberg form) (2.3.4). This ensures the validity of propagation of chaos, namely $\hat\rho_j(t)=\hat\rho_t^{\otimes j}$, $\hat\rho_t$ solving the nonlinear Heisenberg equation (2.3.4) with initial datum $\hat\rho_0=|\psi_0><\psi_0|$. Then, $\hat\rho_t=|\psi_t><\psi_t|$, ψ_t solving the Hartree equation (2.1.21) with initial datum ψ_0.

Remark 2.3.1. By looking at the the proof above it is clear that in order to let Theorem 2.3.1 to hold there is no need of strict factorization of the initial datum as in (2.3.2). Instead asymptotic factorization in the sense of

$$\lim_{N\to\infty}\left\|\hat{\rho}^{(j)}_{N,0}-\hat{\rho}_0^{\otimes j}\right\|_j=0 \tag{2.3.21}$$

would be sufficient. We remind that (2.3.21) is a reasonable "physical" condition because states close to the ground state of H_N^Q, which are the most accessible and thus the most interesting states, can be approximately described by factorized wave functions, and then, by factorized density matrices.

Remark 2.3.2. In proving the convergence of the series (2.3.11) to (2.3.19) the crucial tools have been the boundedness of the operator $T^Q_{N,j}:\mathcal{L}^1(L^2(\mathbb{R}^{3j}))\to\mathcal{L}^1(L^2(\mathbb{R}^{3j}))$ (see (2.3.14)) and property **P1**) for the RDM. In particular, the bound (2.3.15) on the operator norm of $T^Q_{N,j}$ provides the rate of convergence to the Hartree dynamics by means of (2.3.16).

Then, by observing that the estimate obtained in (2.3.16) is not uniform with respect to ε and it fails when $\varepsilon\to 0$, it follows that the error in approximating the N-particle dynamics with the limiting one is diverging when $\varepsilon\to 0$ (for short times it is of the form $\frac{C_j}{N}e^{Ct/\varepsilon}$).

In the next sections we will discuss some other results concerning the mean-field limit starting from factorized initial datum as in (2.3.1), both for bounded interactions and for the Coulomb potential and we will see that considerations done in Remark 2.3.2 still hold. This means that all results concerning the mean-field limit exhibit an error in approximating the N-particle dynamics by the limiting one which is not uniform with respect to ε and diverging when $\varepsilon\to 0$. This is a quite surprising feature because it seems that, roughly speaking, the accuracy of the approximation depends on "how much" the system can be considered quantum or not and, except for fermionic systems, there are no reasonable motivations for that. In fact, we will see in Section 3 that in the fermionic case it is quite natural to look at a joint limit: $N\to\infty$ and $\varepsilon\to 0$ as in [8] and [19]. On the contrary, in looking at systems of undistiguishable particles or even bosonic systems the fact that the mean-field limit and the semiclassical approximation seems to be so strictly connected is an open problem (except for specific scalings of the potential as in [24]). Furthermore, in the classical case (see Section 1) everything works, so it is quite natural to ask if, at least for quantum systems having a reasonable classical analogue, it is possible to realize the limit $N\to\infty$ uniformly with respect to ε. This is the main motivation of our research and in the next section we will focus on that topic, discussing some known results and presenting what we did in this perspective.

2.3.1 – An alternative approach

From the proof of Theorem 2.3.1 presented above, we notice that the expansion of the BBGKY hierarchy in (2.3.11) is much more involved than the corresponding expansion (2.3.19) of the infinite hierarchy (2.3.19). It turns out that it is possible to avoid the expansion of the BBGKY hierarchy making use of a simple compactness argument; this will be especially important when dealing with singular potentials. In the following we explain the main steps of this alternative proof to Theorem 2.3.1. Then, in the next section, we will illustrate how to extend it to potentials with a Coulomb singularity. The idea, which was first presented in [16], [17], [18], consists in characterizing the limit of the RDM $\hat{\rho}^{(j)}_{N,t}$ as the unique solution to the infinite hierarchy of equations (2.3.19); combined with the compactness, this information provides a proof of Theorem 2.3.1.

More precisely, the proof is divided into three main steps:

i) First of all, one shows the compactness of the sequence $\{\hat{\rho}^{(j)}_{N,t}\}_{j=1}^{N}$ with respect to an appropriate weak topology.
ii) Then, one proves that an arbitrary limit point $\{\hat{\rho}^{(j)}_{\infty,t}\}_{j\geq 1}$ of the sequence $\{\hat{\rho}^{(j)}_{N,t}\}_{j=1}^{N}$ is a solution to the infinite hierarchy (2.3.19) (one proves, in other words, the convergence to the infinite hierarchy).
iii) Finally, one shows the uniqueness of the solution to the infinite hierarchy (2.3.19).

We have already observed that the factorized family $\{\hat{\rho}_t^{\otimes j}\}_{j\geq 1}$ is a solution of the infinite hierarchy with factorized initial datum $\hat{\rho}_0^{\otimes j}$. In particular, if $\hat{\rho}_0 = |\psi_0 >< \psi_0|$, as in the present case, we find that $\hat{\rho}_t = |\psi_t >< \psi_t|$, ψ_t solving the Hartree equation (2.1.21). Then, by proving that the solution of the infinite hierarchy is unique, we are guaranteed that it is factorized according to the solution of the Hartree equation.

Therefore, by *ii)*, it follows immediately that $\hat{\rho}^{(j)}_{N,t} \to \hat{\rho}_t^{\otimes j} = (|\psi_t >< \psi_t|)^{\otimes j}$ as $N \to \infty$ (at first only in the weak topology with respect to which we have compactness; since the limit is an orthogonal rank one projection, it is however simple to check that weak convergence implies strong convergence, in the sense (2.3.3)). Next, we discuss these three main steps (compactness, convergence, and uniqueness) in some more details in order to show that, even following this approach, the estimates that ensure the convergence are not uniform with respect to ε and they fail if $\varepsilon \to 0$.

Compactness: By knowing that, for any j and N, $\left\|\hat{\rho}^{(j)}_{N,t}\right\|_{\mathcal{L}^1} = 1$ for fixed t, thanks to standard abstract and compactness results of functional analysis we prove that the sequence $\Gamma_{N,t} = \{\hat{\rho}^{(j)}_{N,t}\}_{j=1}^{N}$ is compact with respect to a suitable topology. More precisely, for an arbitrary fixed $T > 0$, we denote by $\mathcal{C}\left([0,T], \mathcal{L}^1(L^2(\mathbb{R}^{3j}))\right)$ the space of functions of $t \in [0,T]$ with values in $\mathcal{L}^1(L^2(\mathbb{R}^{3j}))$ which are continuous in time with respect to a suitable metric η_j

on $\mathcal{L}^1(L^2(\mathbb{R}^{3j}))$ (it can be constructed explicitly in such a way that the topology generated by η_j is equivalent to the weak*-topology of $\mathcal{L}^1(L^2(\mathbb{R}^{3j}))$). By η_j we can easily define a metric $\hat{\eta}_j$ on $\mathcal{C}([0,T],\mathcal{L}^1(L^2(\mathbb{R}^{3j})))$ and we consider the topology τ_{prod} on $\bigoplus_{j\geq 1}\mathcal{C}([0,T],\mathcal{L}^1(L^2(\mathbb{R}^{3j})))$ given by the product of the topologies generated by the metrics $\hat{\eta}_j$ on $\mathcal{C}([0,T],\mathcal{L}^1(L^2(\mathbb{R}^{3j})))$. The topology τ_{prod} is precisely the topology with respect to which we prove compactness of the sequence $\{\Gamma_{N,t}\}_{N\in\mathbb{N}}$ and this is equivalent to the following

Proposition 2.3.1. *Fix an arbitrary time $T>0$. For every sequence $\{M_m\}_{m\in\mathbb{N}}$ there exists a subsequence $\{N_m\}_{m\in\mathbb{N}}\subset\{M_m\}_{m\in\mathbb{N}}$ and a limit point $\Gamma_{\infty,t}=\{\hat{\rho}^{(j)}_{\infty,t}\}_{j\geq 1}$ for $\Gamma_{N_m,t}=\{\hat{\rho}^{(j)}_{N,t}\}_{j=1}^{N_m}$ such that*

$$\hat{\rho}^{(j)}_{\infty,t}\geq 0,\quad \mathtt{Tr}\hat{\rho}^{(j)}_{\infty,t}\leq 1,\ \forall\, j\geq 1, \tag{2.3.22}$$

$\hat{\rho}^{(j)}_{\infty,t}$ (for any j) is symmetric with respect to permutations of the labeling.

Let $\mathcal{K}_j\equiv\mathcal{K}(L^2(\mathbb{R}^{3j}))$ be the space of compact operators on $L^2(\mathbb{R}^{3j})$, equipped with the operator norm. The claim of Proposition 2.3.1 is equivalent to the affirm that, passing to a subsequence,

For every fixed $j\geq 1$ and for every fixed compact operator $J^{(j)}\in\mathcal{K}_j$,

$$\mathtt{Tr}\ J^{(j)}(\hat{\rho}^{(j)}_{N,t}-\hat{\rho}^{(j)}_{\infty,t})\to 0\quad\text{as}\quad N\to\infty \tag{2.3.23}$$

uniformly in t for $t\in[0,T]$.

<u>**Convergence**</u>: The second main step consists in characterizing the limit points of the (compact) sequence $\Gamma_{N,t}=\{\hat{\rho}^{(j)}_{N,t}\}_{j=1}^{N}$ as solutions to the infinite hierarchy of equations (2.3.19) with initial datum $\hat{\rho}_0^{\otimes j}$, $\hat{\rho}_0=|\psi_0><\psi_0|$.

Proposition 2.3.2. *Suppose that $\phi\in L^\infty(\mathbb{R}^3)$ such that $\phi(x)\to 0$ as $|x|\to\infty$. Assume moreover that $\Gamma_{\infty,t}=\{\hat{\rho}^{(j)}_{\infty,t}\}_{j\geq 1}\in\bigoplus_{j\geq 1}\mathcal{C}([0,T],\mathcal{L}^1(L^2(\mathbb{R}^{3j})))$ is a limit point of the sequence $\Gamma_{N,t}=\{\hat{\rho}^{(j)}_{N,t}\}_{j=1}^{N}$ in the sense (2.3.23). Then*

$$\hat{\rho}^{(j)}_{\infty,t}=S_j(t)\hat{\rho}^{(j)}_{\infty,0}+\left(-\frac{i}{\varepsilon}\right)\int_0^t \mathrm{d}t_1\ S_j(t-t_1)C^Q_{j,j+1}\,\hat{\rho}^{(j+1)}_{\infty,t_1}. \tag{2.3.24}$$

for all $j\geq 1$, with $\hat{\rho}^{(j)}_{\infty,0}=\hat{\rho}^{(j)}_{N,0}=\hat{\rho}_0^{\otimes j}$. Here $S_j(t)$ is the flow associated with the j-particle free dynamics and $C^Q_{j,j+1}$ is defined as in (2.2.3). Therefore equation (2.3.24) evaluated for all $j\geq 1$ gives rise precisely to a solution of the Hartree hierarchy (2.3.19) with factorized initial datum.

Note that in Proposition 2.3.2 we assume the potential to vanish at infinity. This condition, which was not required in Theorem 2.3.1, is not essential but it simplifies the proof and it is also satisfied by the Coulomb interaction for which the derivation of the Hartree equation has been proven (e.g. [17]) by following the present strategy (together with crucial technical tools that are necessary to deal with the singularity of the potential).

Proof. Passing to a subsequence we can assume that $\Gamma_{N,t} \to \Gamma_{\infty,t}$ as $N \to \infty$, in the sense (2.3.23); this implies immediately that $\hat\rho^{(j)}_{\infty,0} = \hat\rho^{(j)}_{N,0} = \hat\rho_0^{\otimes j}$. To prove (2.3.24), on the other hand, it is enough to show that for every fixed $j \geq 1$, and for every fixed $J^{(j)}$ from a dense subset of $\mathcal{K}_j$,

$$\begin{aligned}\mathtt{Tr} J^{(j)} \hat\rho^{(j)}_{\infty,t} &= \mathtt{Tr} J^{(j)} S_j(t) \hat\rho^{(j)}_{\infty,0} + \\ &\quad + \left(-\frac{i}{\varepsilon}\right) \int_0^t \mathrm{d}t_1 \, \mathtt{Tr} J^{(j)} S_j(t-t_1) C^Q_{j,j+1} \, \hat\rho^{(j+1)}_{\infty,t_1}.\end{aligned} \tag{2.3.25}$$

To demonstrate (2.3.25), we start from the BBGKY hierarchy (2.3.7) which leads to

$$\begin{aligned}\mathtt{Tr} J^{(j)} \hat\rho^{(j)}_{N,t} &= \mathtt{Tr} J^{(j)} S_j(t) \hat\rho^{(j)}_{N,0} + -\frac{i}{\varepsilon} \int_0^t \mathrm{d}t_1 \, \mathtt{Tr} J^{(j)} S_j(t-t_1) T^Q_{N,j} \hat\rho^{(j)}_{N,t_1} \times \\ &\times \left(-\frac{i}{\varepsilon}\right) \frac{(N-j)}{N} \int_0^t \mathrm{d}t_1 \, \mathtt{Tr} J^{(j)} S_j(t-t_1) C^Q_{j,j+1} \, \hat\rho^{(j+1)}_{N,t_1}.\end{aligned} \tag{2.3.26}$$

Since, by assumption, the l.h.s. and the first term on the r.h.s. of the last equation converge, as $N \to \infty$, to the l.h.s. and, respectively, to the first term on the r.h.s. of (2.3.25) (for every compact operator $J^{(j)}$), (2.3.24) follows if we can prove that

$$-\frac{i}{\varepsilon} \int_0^t \mathrm{d}t_1 \mathtt{Tr} J^{(j)} S_j(t-t_1) T^Q_{N,j} \hat\rho^{(j)}_{N,t_1} \to 0 \tag{2.3.27}$$

and that

$$\begin{aligned}&\left(-\frac{i}{\varepsilon}\right) \frac{(N-j)}{N} \int_0^t \mathrm{d}t_1 \, \mathtt{Tr} J^{(j)} S_j(t-t_1) C^Q_{j,j+1} \, \hat\rho^{(j+1)}_{N,t_1} \to \\ &\to \left(-\frac{i}{\varepsilon}\right) \int_0^t \mathrm{d}t_1 \, \mathtt{Tr} J^{(j)} S_j(t-t_1) C^Q_{j,j+1} \, \hat\rho^{(j+1)}_{\infty,t_1}\end{aligned} \tag{2.3.28}$$

as $N \to \infty$. Eq. (2.2.27) follows because, by the expression (2.2.2) of $T^Q_{N,j}$, we have

$$\begin{aligned}&\left| \frac{i}{\varepsilon} \mathtt{Tr} J^{(j)} S_j(t-t_1) T^Q_{N,j} \hat\rho^{(j)}_{N,t_1} \right| \leq \\ &\leq \frac{1}{\varepsilon 2N} \sum_{k \neq l}^{j} \left| \mathtt{Tr} J^{(j)} S_j(t-t_1) \left[\phi(x_k - x_l), \hat\rho^{(j)}_{N,t_1} \right] \right| \leq \\ &\leq \frac{j^2}{\varepsilon N} \left\| J^{(j)} \right\| \|\phi\| \, \mathtt{Tr} \left| \hat\rho^{(j)}_{N,t_1} \right| = \frac{j^2}{\varepsilon N} \left\| J^{(j)} \right\| \|\phi\| \to 0\end{aligned} \tag{2.3.29}$$

because the product $\left\|J^{(j)}\right\| \|\phi\|$ is finite and uniformly bounded with respect to N ($\left\|J^{(j)}\right\|$ and $\|\phi\|$ being the operator norms of $J^{(j)}$ and of the multiplication operator ϕ). To prove (2.3.28) one can use a similar argument, combined with the observation that, by the expression (2.2.3) of $C^Q_{j,j+1}$,

$$\begin{aligned}&\frac{i}{\varepsilon}\mathtt{Tr}J^{(j)}S_j(t-t_1)C^Q_{j,j+1}\left(\hat\rho^{(j+1)}_{N,t_1}-\hat\rho^{(j+1)}_{\infty,t_1}\right)=\\&=\frac{i}{\varepsilon}\sum_{1\le k\le j}\mathtt{Tr}\left[(J^{(j)}S_j(t-t_1)),\phi(x_k-x_{j+1})\right]\left(\hat\rho^{(j+1)}_{N,t_1}-\hat\rho^{(j+1)}_{\infty,t_1}\right)\to 0,\end{aligned}\tag{2.3.30}$$

as $N\to\infty$. This does not follow directly from the assumption that $\Gamma_{N,t}\to\Gamma_{\infty,t}$ in the sense (2.3.23) because the operator $\left[(J^{(j)}S_j(t-t_1)),\phi(x_k-x_{j+1})\right]$ is not compact on $L^2(\mathbb{R}^{3(j+1)})$. Instead it is necessary to apply an approximation argument which is made simpler by the assumption that $\phi(x)\to 0$ as $|x|\to\infty$ (that is the reason for which we did it). The details of this approximation argument can be found, for example, in [23]. ∎

Uniqueness: to conclude the proof of Theorem 2.3.1, we still have to prove the uniqueness of the solution to the infinite (Hartree) hierarchy (2.3.24).

Proposition 2.3.3. *Fix* $\Gamma_{\infty,0}=\{\hat\rho^{(j)}_{\infty,0}\}_{j\ge1}\in\bigoplus_{j\ge1}\mathcal{L}^1(L^2(\mathbb{R}^3))$. *Then there exists at most one solution* $\Gamma_{\infty,t}=\{\hat\rho^{(j)}_{\infty,t}\}_{j\ge1}\in\bigoplus_{j\ge1}\mathcal{C}([0,T],\mathcal{L}^1(L^2(\mathbb{R}^3)))$ *to the infinite* (*Hartree*) *hierarchy* (2.3.24) *such that* $\hat\rho^{(j)}_{\infty,t}\,|_{t=0}=\hat\rho^{(j)}_{\infty,0}$ *and* $\mathtt{Tr}\left|\hat\rho^{(j)}_{\infty,t}\right|\le 1$ *for all* $j\ge1$ *and all* $t\in[0,T]$.

Proof. The proof is exactly the same we did in proving Theorem 2.3.1. Indeed, we write the solution of the Hartree hierarchy by iterating the Duhamel formula (2.3.24) and we observe that the series we obtain is uniformly bounded in trace norm by a geometric series converging for short times $t<t_0$ (see (2.3.19)). This proves uniqueness locally in time. Then, by noting that t_0 does not depend on the initial condition (except for the trace norm of $\hat\rho_{\infty,0}$ which is clearly preserved in time) but only on the L^∞-norm of the interaction potential ϕ, we can iterate the same argument, obtaining uniqueness for all times. ∎

We realize that the estimate ensuring the convergence is (2.3.29) and, as in the proof of Theorem 2.3.1 presented in the previous paragraph, we note that it is due to the boundness of the operator $T^Q_{N,j}:\mathcal{L}^1(L^2(\mathbb{R}^{3j}))\to\mathcal{L}^1(L^2(\mathbb{R}^{3j}))$. Indeed, its norm is bounded by C/N, thus vanishing when $N\to\infty$. Nevertheless, by looking at (2.3.29) we see that there is a factor $1/\varepsilon$ in front of $T^Q_{N,j}$, thus we obtain a bound of order $1/\varepsilon$ which is diverging if $\varepsilon\to0$. Therefore, even by using this approach, it is clear that considerations done previously as regard to the uniformity of the mean-field approximation with respect to ε, still hold.

We conclude this paragraph by observing that in estimating the operator norm of $T^{Q}_{N,j}$ on $\mathcal{L}^1(L^2(\mathbb{R}^{3j}))$ we have to deal with $\frac{1}{\varepsilon}\mathtt{Tr}\left[\phi, \hat{\rho}^{(j)}_{N,t}\right]$ and we find a uniform bound with respect to N, but diverging in ε, by using that in any Hilbert space $\mathcal{H}$:

$$\mathtt{Tr}[A,B] \leq 2\,\|A\|\,\mathtt{Tr}\,|B|\,, \quad \forall \quad A \in \mathcal{L}^{\infty}(\mathcal{H})\,, B \in \mathcal{L}^{1}(\mathcal{H})\,, \tag{2.3.31}$$

where $\mathcal{L}^{\infty}(\mathcal{H})$ is the space of bounded operators on $\mathcal{H}$ ($\|\cdot\|$ being the operator norm in $\mathcal{L}^{\infty}(\mathcal{H})$) and $\mathcal{L}^{1}(\mathcal{H})$ is the space of trace class operators on $\mathcal{H}$ equipped with the norm $\mathtt{Tr}\,|\cdot|$. Essentially the crucial question in looking for an estimate of the error in the mean-field approximation (for bounded or even smooth potentials) which is uniform (or at least "better diverging") with respect to ε is: can we improve (2.3.31) by taking into account further properties of the operators A and B we have to deal with, possibly considering suitable "semiclassical" initial data?

2.3.2 – Mean-Field limit for the Coulomb potential

The result presented in [17] concerning the mean-field limit in the case of Coulomb interaction, $\phi = 1/|x|$, is formulated as in Theorem 2.3.1, except for the fact that the initial one particle wave function ψ_0 is assumed to be in $H_1(\mathbb{R}^3)$ (the Sobolev space $W^{1,2}(\mathbb{R}^3)$ of functions il $L^2(\mathbb{R}^3)$ whose derivatives are also in $L^2(\mathbb{R}^3)$) and that the theorem holds for dimensions $d \geq 2$. Even the general strategy of the proof is the same we outlined in the previous paragraph. First one proves the compactness of the sequence of marginal $\Gamma_{N,t} = \{\hat{\rho}^{(j)}_{N,t}\}_{j=1}^{N}$ with respect to an appropriate weak topology (the product topology τ_{prod} previously introduced), then one shows that an arbitrary limit point $\Gamma_{\infty,t} = \{\hat{\rho}^{(j)}_{\infty,t}\}_{j\geq 1}$ of the sequence $\Gamma_{N,t} = \{\hat{\rho}^{(j)}_{N,t}\}_{j=1}^{N}$ is a solution to the infinite hierarchy of equations

$$\hat{\rho}^{(j)}_{\infty,t} = S_j(t)\hat{\rho}^{j}_{0} + \left(-\frac{i}{\varepsilon}\right)\int_0^t \mathrm{d}t_1\; S_j(t-t_1)C^{Q}_{j,j+1}\,\hat{\rho}^{(j+1)}_{\infty,t_1}. \tag{2.3.32}$$

where S_j is the free evolution defined in Section 2.3, and the collision map $C^{Q}_{j,j+1}$ is now given by

$$C^{Q}_{j,j+1}\hat{\rho}^{(j)}_{N,t} = \lambda\sum_{k=1}^{j}\mathtt{Tr}_{j+1}\left\{\left[\frac{1}{|x_k - x_{j+1}|}, \hat{\rho}^{(j+1)}_{N,t}\right]\right\}, \tag{2.3.33}$$

where λ is a coupling constant that can be positive (as in the most interesting physical case: the attractive Coulomb interaction) or not (repulsive case). Finally, one proves the uniqueness of the solution to (2.3.32). Although the proof of the compactness and of the convergence also require several changes with respect to what we discussed in the previous paragraph, the main difficulty one has to face when the bounded potential is replaced by the Coulomb interaction is the proof of the uniqueness of the solution to the infinite hierarchy. The key idea introduced by ErdHos and Yau in [17] was to restrict the class of densities for which uniqueness must be proven. In Theorem 2.3.1, uniqueness is proven in the class of densities with $\mathtt{Tr}|\hat{\rho}_t^{(j)}| \leq 1$ for all $j \geq 1$, and all $t \in [0, T]$ (but the same argument works under the weaker assumption $Tr|\hat{\rho}_t^{(j)}| \leq C^j$, for some constant $C < +\infty$). In [17], in the case of a Coulomb potential the uniqueness of (2.3.32) has been proven in the (smaller) class of densities $\Gamma_t = \{\hat{\rho}_t^{(j)}\}_{j\geq 1}$ satisfying the a-priori bound

$$\mathtt{Tr}\left|(1-\Delta_1)^{1/2}\ldots(1-\Delta_j)^{1/2}\,\hat{\rho}_t^{(j)}\,(1-\Delta_j)^{1/2}\ldots(1-\Delta_1)^{1/2}\right| \leq C^j \tag{2.3.34}$$

for all $j \geq 1$ and for all $t \in [0, T]$.

There is, of course, a price to pay in order to restrict the proof of the uniqueness to this class of densities. In fact, to apply this uniqueness result to prove the convergence of the RDM to the j-fold product of solutions of the Hartree equation, one has to show that an arbitrary limit point $\Gamma_{\infty,t} = \{\hat{\rho}_{\infty,t}^{(j)}\}_{j\geq 1}$ of the sequence of densities $\Gamma_{N,t} = \{\hat{\rho}_{N,t}^{(j)}\}_{j=1}^N$ associated with $\hat{\rho}_{N,t}$ satisfies the a-priori bound (2.3.34). Due to the Coulomb singularity, this is actually not so simple and requires an additional approximation argument and suitable energy estimates.

Anyway, even if in the Coulomb case strong technical tools are needed in proving the mean-field result (much more with respect to the bounded interaction case), it is not difficult to realize that the estimates ensuring the convergence are not uniform with respect to ε and they fail if $\varepsilon \to 0$. To see this, for concreteness in the case $d = 3$, we observe that the Coulomb potential is controlled in three dimensions by the Laplacian (by virtue of an operator inequality of Hardy type). This is the reason for considering the class of density matrices such that (2.3.34) holds. Roughly speaking, by (2.3.34) it follows that, considering the operator $\frac{1}{|x_i - x_k|}\hat{\rho}_{N,t}^{(j)}$ (appearing both in the BBGKY and in the Hartree hierarchy) multiplied in a suitable way by some operators $(C - \Delta_k)^{1/2}$ $(C > 1)$ and taking the trace, one obtains estimates which are uniform with respect to N. Such estimates are crucial in proving the uniqueness of the solution of the Hartree hierarchy and even the convergence of the BBGKY hierarchy to the limiting one. In particular, they provide the rate of convergence to the Hartree dynamics in terms of the number of particles N and indipendently of ε. Nevertheless, by looking at the explicit computations, we find a factor $1/\varepsilon$ in front of the interaction potential, thus we have again diverging estimates when $\varepsilon \to 0$.

From now on, we will focus on the case of smooth pair interaction potential, primarily, because in this case both the quantum and the classical mean-field limit have been rigorously established, therefore it is quite reasonable to look at that situation in investigating the connection between mean-field limit and semiclassical approximation (which we are going to discuss in Section 3 and 4). On the other side, we will see that for our purposes we need to deal with a smooth potential (see Section 4).

3 – Mean-Field limit VS Semiclassical approximation

In this section we discuss the problem of "connecting" mean-field limit and semiclassical approximation which, as we saw previously, emerges quite naturally from the analysis of the quantum mean-field limit results. If one wants to deal with the classical and quantum case simultaneously, it is natural to work in the classical phase space by using the so called "Wigner formalism".

3.1 – The Wigner formulation

By the Heisenberg uncertainty principle, it follows that it is not possible to determine simultaneously the position and the momentum of a quantum particle, thus the concept of classical phase space density does not generalize directly to quantum mechanics. Nevertheless one can define a substitute for it, namely the Wigner transform. For any wave function $\psi \in L^2(\mathbb{R}^d)$ we define the Wigner transform of ψ as

$$f_\psi^\varepsilon(x,v) = (2\pi)^{-d} \int_{\mathbb{R}^d} \mathrm{d}y\, e^{iy\cdot v} \overline{\psi}\left(x + \frac{\varepsilon y}{2}\right) \psi\left(x - \frac{\varepsilon y}{2}\right), \tag{3.1.1}$$

and we still interpret it as "quantum phase space density" (see [1]). It is easy to check that f_ψ^ε is always real but in general is not positive (thus it cannot be the density of a positive measure - in coincidence with the Heisenberg principle). However, its marginals reconstruct the position and momentum space densities, as the following formulas can be easily checked:

$$\int f_\psi^\varepsilon(x,v)dv = |\psi(x)|^2, \quad \int f_\psi^\varepsilon(x,v)dx = |\hat{\psi}(v)|^2 \tag{3.1.2}$$

$\hat{\psi}(v)$ being the Fourier transform of ψ, namely, by integrating versus the velocity variable we obtain the quantum spatial probability density and by integrating with respect to the position variable we find the velocity (or momentum) probability density. In particular

$$\int f_\psi^\varepsilon(x,v)dvdx = 1 \tag{3.1.3}$$

for normalized wave functions. More generally, if $J(x, v)$ is a classical phase space observable, the scalar product

$$\left\langle J, f^{\varepsilon}_{\psi}\right\rangle = \int J(x, v) f^{\varepsilon}_{\psi}(x, v) dv dx \tag{3.1.4}$$

can be interpreted as the expected value of J in state described by ψ. Recall that "honest" quantum mechanical observables are self-adjoint operators O on $L^2(\mathbb{R}^d)$ and their expected value is given by

$$\langle O\rangle_{\psi} = \int \bar{\psi}(x)(O\psi)(x)\mathrm{d}x \tag{3.1.5}$$

For a large class of observables there is a natural relation between observables O and their phase space representations (called symbols) that are functions on the phase space like $J(x, v)$. For example, if J depends only on x or only on v, then the corresponding operator is just the standard quantization, i.e.

$$\int J(x) f^{\varepsilon}_{\psi}(x, v) dx dv = \langle \psi, J\psi\rangle \tag{3.1.6}$$

where J is a multiplication operator on the right hand side,

$$\int J(v) f^{\varepsilon}_{\psi}(x, v) dx dv = \langle \psi, J(-i\varepsilon\nabla)\psi\rangle \tag{3.1.7}$$

and similar relations hold for the Weyl quantization of any symbol $J(x, v)$. We also remark that the map $\psi \to f^{\varepsilon}_{\psi}$ is invertible, i.e. one can fully reconstruct the wave function from its Wigner transform. On the other hand, not every real function of two variables (x, v) is the Wigner transform of some wave function.

The correspondence between wave functions and their Wigner transform can be easily rephrased for density matrices. Indeed, if $\hat{\rho} = |\psi >< \psi|$ for some $\psi \in L^2(\mathbb{R}^d)$, then formula (3.1.1) can be rewritten as

$$f^{\varepsilon}_{\rho}\left(x, v\right) = (2\pi)^{-d} \int_{\mathbb{R}^3} \mathrm{d}y\; e^{iy\cdot v} \rho\left(x + \frac{\varepsilon y}{2}, x - \frac{\varepsilon y}{2}\right), \tag{3.1.8}$$

where $\rho(x, y) = \bar{\psi}(x)\psi(y)$ is the integral kernel of $\hat{\rho}$. Furthermore, formula (3.1.8) holds for any density matrix $\hat{\rho} \in \mathcal{L}^1(L^2(\mathbb{R}^d))$, even for those which are associated with mixed states and (3.1.3) holds because of positivity and trace norm normalization of the density matrix. Vice versa, starting from a quantum system whose state is described by a Wigner function $f^{\varepsilon}\left(x, v\right)$, it is possible to compute the corresponding density matrix (actually, its integral kernel) by the Weyl quantization rule

$$\rho_{f^{\varepsilon}}\left(x, y\right) = (2\pi)^{-d} \int_{\mathbb{R}^d} \mathrm{d}v\; e^{i\frac{v}{\varepsilon}\cdot(x-y)} f^{\varepsilon}\left(\frac{x+y}{2}, v\right). \tag{3.1.9}$$

Therefore the Wigner transform and the Weyl quantization rule provide an invertible map $\hat{\rho} \leftrightarrow f^{\varepsilon}_{\rho}$ between density matrices and Wigner functions and it is simple to check that

$$\|\rho\|_{L^2(\mathbb{R}^d\times\mathbb{R}^d)} = \left\|f^{\varepsilon}_{\rho}\right\|_{L^2(\mathbb{R}^d\times\mathbb{R}^d)}. \tag{3.1.10}$$

This is particularly meaningful because for any density matrix $\hat{\rho}$ we have

$$\hat{\rho} \geq 0,\ \hat{\rho} \in \mathcal{L}^1(L^2(\mathbb{R}^d)),\ \text{with}\ \|\hat{\rho}\|_{\mathcal{L}^1(L^2(\mathbb{R}^d))} = 1 \Rightarrow \|\hat{\rho}\|_{\mathcal{L}^2(L^2(\mathbb{R}^d))} \leq 1, \tag{3.1.11}$$

where $\mathcal{L}^2(L^2(\mathbb{R}^d))$ is the Hilbert space of Hilbert-Schmidt operators on $L^2(\mathbb{R}^d)$ and for any operator $\Gamma \in \mathcal{L}^2(L^2(\mathbb{R}^d))$ with kernel $\gamma = \gamma(x, y)$ we find

$$\|\Gamma\|_{\mathcal{L}^2(L^2(\mathbb{R}^d))} = \|\gamma\|_{L^2(\mathbb{R}^d\times\mathbb{R}^d)}. \tag{3.1.12}$$

Therefore by (3.1.11), (3.1.12) and by (3.1.10) it follows that

$$\begin{aligned} &\|\rho\|_{L^2(\mathbb{R}^d\times\mathbb{R}^d)} \leq 1\ \forall\ \text{density matrix} \\ &\hat{\rho} \Rightarrow \|f^{\varepsilon}\|_{L^2(\mathbb{R}^d\times\mathbb{R}^d)} \leq 1\ \forall\ \text{Wigner function}\ f \end{aligned} \tag{3.1.13}$$

Remark 3.1.1. By (3.1.9) it follows that one can fully reconstruct a density matrix from its Wigner transform but, in general, by knowing the Wigner function associated with the state of a quantum system it is not possible to reconstruct such a state in the wave function picture. More precisely, if we know that the system is in a *pure state* and we know that it is described by a certain Wigner function f^{ε}, we can reconstruct the density matrix $\hat{\rho}$ which will be given by $\hat{\rho} = |\psi><\psi|$ for some L^2-function ψ. On the contrary, if the system is in a *mixed state*, by knowing the Wigner function we can only reconstruct the density matrix but there is no way to know which are the wave functions "composing" it.

Remark 3.1.2. The correspondence between density matrices and Wigner functions is quite useful but one has to be careful in using that. In fact, by considering a density matrix $\hat{\rho}$ one can compute its Wigner transform f^{ε}_{ρ} and it will be for sure a real function on the classical phase space with the properties specified above. On the contrary, a real function on the classical phase space does not correspond necessarily to an admissible quantum state, namely, it is not necessarily the Wigner transform of a density matrix.

Let us consider a density matrix $\hat{\rho}^0 \in \mathcal{L}^1(L^2(\mathbb{R}^d))$ representing the initial state of a system whose Hamiltonian H is

$$H = -\frac{\varepsilon^2}{2}\Delta_x + U(x) \tag{3.1.14}$$

and the potential U is such that H is a self-adjoint operator on $L^2(\mathbb{R}^d)$. We know that the time evolution for the density matrix $\hat{\rho}^0$ is determined by

$$i\varepsilon\partial_t\hat{\rho}^t = [H, \hat{\rho}^t], \tag{3.1.15}$$

and it is easy to check that it preserves the Hilbert-Schmidt norm of $\hat{\rho}^0$, namely the L^2-norm of the kernel ρ^0. Thus, by looking at the initial Wigner function $f^\varepsilon_{\rho^0}(x,v)$ $(x, v \in \mathbb{R}^d)$ and at the time-evolved $f^\varepsilon_t(x,v) = f^\varepsilon_{\rho^t}(x,v)$, the L^2-norm has to be also preserved in time (by (3.1.10). We can verify this property by looking at the equation solved by f^ε_t. By applying the Wigner transform defined in (3.1.1) to (3.1.15), we find the equation

$$(\partial_t + v\cdot\nabla_x)\, f^\varepsilon_t = T^\varepsilon f^\varepsilon_t, \tag{3.1.16}$$

where

$$(T^\varepsilon f^\varepsilon_t)(x,v) = i\int_{-1/2}^{1/2} \mathrm{d}\lambda \int \mathrm{d}k\hat{U}(k)e^{i\ k\cdot x}(k\cdot\nabla_v)f^\varepsilon_t(x, v+\varepsilon\lambda k), \tag{3.1.17}$$

and we denoted by $\hat{U}$ the Fourier transforms of U, namely:

$$\hat{U}(k) = \int_{\mathbb{R}^d} \mathrm{d}x\, e^{-i\ k\cdot x}U(x). \tag{3.1.18}$$

By noting that both $v\cdot\nabla_x$ and T^ε are skewsymmetric operators and reminding that $f^\varepsilon_t(x,v) \in \mathbb{R}$ for any t, we find

$$\frac{1}{2}\frac{d}{dt}\|f^\varepsilon_t\|^2_{L^2(\mathbb{R}^d\times\mathbb{R}^d)} = (f^\varepsilon_t, \partial_t f^\varepsilon_t) = (f^\varepsilon_t, -v\cdot\nabla_x f^\varepsilon_t) + (f^\varepsilon_t, T^\varepsilon f^\varepsilon_t) = 0, \tag{3.1.19}$$

namely the L^2-norm is conserved. It can be also proved that H_s-estimates hold for (3.1.16) ($H_s(\mathbb{R}^{3N}\times\mathbb{R}^{3N})$ being the Sobolev space $W^{s,2}(\mathbb{R}^{3N}\times\mathbb{R}^{3N})$) by assuming the potential ϕ to be sufficiently smooth (see for example [25]) in the sense that the H_s-norm of the time evolved Wigner function is controlled by the H_s-norm of the initial datum, up to a constant depending on time (but finite for any time interval) and of a suitable norm of the potential.

Equation (3.1.16) looks like a classical kinetic equation but the crucial facts are that f^ε_t is not a probability density in the phase space $\mathbb{R}^d\times\mathbb{R}^d$ and we have to deal with a pseudodifferential operator instead of a differential one as it is usual in kinetic theory. It is immediate to check that

$$\int \mathrm{d}x \int \mathrm{d}v\ f^\varepsilon_t(x,v) = \int \mathrm{d}x\rho^\varepsilon_t(x) = 1\ \forall\ t>0, \tag{3.1.20}$$

with

$$\rho_t^\varepsilon(x) = \int \mathrm{d}v\ f_t^\varepsilon(x,v),\ \rho_t^\varepsilon \geq 0\ \forall\ t, \tag{3.1.21}$$
$$\rho_t^\varepsilon(x)\mathrm{d}x := \text{ spatial probability distribution,}$$

and (3.1.20) follows from conservation of "mass" and from the fact that, because of the trace norm normalization of $\hat{\rho}^0$, we have $\int \mathrm{d}x \int \mathrm{d}v\ f_{\rho^0}^\varepsilon(x,v) = \mathtt{Tr}\hat{\rho}^0 = 1$.

3.2 – The Mean-Field system in the Wigner formalism

The Wigner formalism introduced in the previous section is an alternative way of describing the state and the dynamics of a quantum system and it is precisely equivalent to the density matrix (or Heisenberg) description, and, for pure states, to the wave function (or Schrödinger) picture. As we have observed, the advantage in using the Wigner formalism in looking at semiclassical approximation of quantum systems is that Wigner functions "live" on the classical phase space and for suitable "semiclassical" quantum states the Wigner functions can have a well defined limit when $\varepsilon \to 0$ (see for example [13]).

Thus, in the perspective of looking at the semiclassical limit, we rephrase the quantum mean-field model discussed in Section 2 by using the Wigner formulation.

By applying the Wigner transform (3.1.8) to the Heisenberg equation(2.1.12) we find

$$(\partial_t + V_N \cdot \nabla_{X_N})\, W_N^\varepsilon(t) = T_N^\varepsilon W_N^\varepsilon(t), \tag{3.2.1}$$

where $W_N^\varepsilon(t) := W_N^\varepsilon(X_N, V_N; t)$ is the Wigner function describing the state of the system (namely, the Wigner transform of the density matrix $\hat{\rho}_{N,t}$),

$$X_N = (x_1, \ldots, x_N) \in \mathbb{R}^{3N}, \quad V_N = (v_1, \ldots, v_N) \in \mathbb{R}^{3N},$$

and the pair $Z_N := (X_N, V_N)$ denotes the generic point in the classical N-particle phase space. Moreover,

$$\begin{aligned}(T_N^\varepsilon W_N^\varepsilon)\,(Z_N) = \frac{i}{(2\pi)^{3N}} \int_{-1/2}^{1/2} \mathrm{d}\lambda \int \mathrm{d}K_N \hat{U}^Q(K_N) e^{iK_N\cdot V_N} \times \\ \times (K_N \cdot \nabla_{V_N})\, W_N^\varepsilon(X_N, V_N + \lambda\varepsilon K_N),\end{aligned} \tag{3.2.2}$$

where $K_N = (k_1, \ldots, k_N) \in \mathbb{R}^{3N}$, U^Q is the (mean-field) interaction potential (2.1), and $\hat{U}^Q$ is the Fourier transform of U^Q, namely:

$$\hat{U}^Q(k) = \int_{\mathbb{R}^{3N}} \mathrm{d}X_N\ e^{-i\ K_N\cdot X_N}\ U^Q(X_N). \tag{3.2.3}$$

We note that (3.2.1) is the analogue of the classical Liouville equation (1.1.5) and, roughly speaking, by setting "$\varepsilon = 0$" in (3.2.2) we obtain precisely the Liouville operator appearing in (1.1.5). From now on, we will refer to (3.2.1) as "N-particle Wigner-Liouville equation".

We remind that we are dealing with undistinguishable particles, then we consider N-particle Wigner functions W_N which are invariant in the exchange of particle names, namely

$$W_N(x_{\pi(1)},\dots,x_{\pi(N)},v_{\pi(1)},\dots,v_{\pi(N)}) = W_N(x_1,\dots,x_N,v_1,\dots,v_N), \tag{3.2.4}$$

for every permutation π acting on $1,\dots,N$. It is easy to verify that this property is preserved by the evolution (3.2.1).

3.2.1 – The Wigner BBGKY hierarchy

For any fixed j we introduce the j-particle "marginals":

$$\begin{aligned} W^{\varepsilon}_{N,j}(t) &:= W^{\varepsilon}_{N,j}(X_j,V_j;t) = \\ &= \int_{\mathbb{R}^{3(N-j)}\times\mathbb{R}^{3(N-j)}} \mathrm{d}X_{N-j}\mathrm{d}V_{N-j} W^{\varepsilon}_N(X_j,X_{N-j},V_j,V_{N-j};t). \end{aligned} \tag{3.2.5}$$

It is easy to check that $\{W^{\varepsilon}_{N,j}(t)\}_{j=1}^N$ are precisely the Wigner transforms of the RDM $\{\hat\rho^{(j)}_{N,t}\}_{j=1}^N$. Furthermore, by integrating the Wigner-Liouville equation (3.2.1) with respect to the last $N-j$ variables we find the following sequence of equations:

$$\begin{gathered} \left(\partial_t + V_j\cdot\nabla_{X_j}\right) W^{\varepsilon}_{N,j}(t) = T^{\varepsilon}_{N,j} W^{\varepsilon}_{N,j}(t) + \left(\frac{N-j}{N}\right) C^{\varepsilon}_{j,j+1} W^{\varepsilon}_{N,j+1}(t), \\ j = 1,2,\dots,N, \\ \text{with} \quad W^{\varepsilon}_{N,N}(t) = W^{\varepsilon}_N(t) \quad \text{and} \quad C^{\varepsilon}_{N,N+1} \equiv 0, \end{gathered} \tag{3.2.6}$$

which is precisely the BBGKY hierarchy (2.2.1) rephrased in the Wigner formalism and it can be seen as the quantum analogue of the classical BBGKY hierarchy (1.4.3).

The operator T^{ε}_j (for a fixed j), describing the interaction of the first j particles, is given by

$$\begin{aligned} (T^{\varepsilon}_{N,j} W^{\varepsilon}_{N,j})(X_j,V_j) = \frac{i(2\pi)^{-3N}}{N} \sum_{l\neq r}^{j} \int_{-1/2}^{1/2} \mathrm{d}\lambda \int_{\mathbb{R}^3} \mathrm{d}k \hat\phi(k) e^{ik(x_l-x_r)} (k\cdot\nabla_{v_l}) \times \\ \times W^{\varepsilon}_{N,j}(X_j, V_{l-1}, v_l + \lambda\varepsilon k, V_{j-l}), \end{aligned} \tag{3.2.7}$$

while the collision operator $C^{\varepsilon}_{j,j+1}$ is

$$\begin{aligned}(3.2.8)\quad &\big(C^{\varepsilon}_{j,j+1}W^{\varepsilon}_{N,j+1}\big)(X_j,V_j)=\\ &=i(2\pi)^{-3N}\sum_{l=1}^{j}\int_{-1/2}^{1/2}\mathrm{d}\lambda\int_{\mathbb{R}^3}\mathrm{d}k\hat{\phi}(k)\int_{\mathbb{R}^3\times\mathbb{R}^3}\mathrm{d}x_{j+1}\mathrm{d}v_{j+1}\ e^{ik\cdot(x_l-x_{j+1})}\times\\ &\times(k\cdot\nabla_{v_l})W^{\varepsilon}_{N,j+1}(X_j,x_{j+1},V_{l-1},v_l+\lambda\varepsilon k,V_{j-l},v_{j+1}),\end{aligned}$$

and in (3.2.7) and (3.2.8) we denoted by $\hat{\phi}$ the Fourier transform of the pair interaction potential ϕ, namely:

$$(3.2.9)\qquad \hat{\phi}(k)=\int_{\mathbb{R}^3}\mathrm{d}x\ e^{-i\ k\cdot x}\phi(x).$$

By using (iteratively) the Duhamel formula, the solution $W^{\varepsilon}_{N,j}(t)$ of the equations (3.2.6) with initial datum $W^{\varepsilon}_{N,j}(0)$ can be written as

$$\begin{aligned}(3.2.10)\quad W^{\varepsilon}_{N,j}(t)=&\Phi^{(N)}_j(t)W^{\varepsilon}_{N,j}(0)+\\ &+\sum_{n=1}^{N-j}\int_{0\le t_n\le\cdots\le t_1\le t}\mathrm{d}t_n\ldots\mathrm{d}t_1\ \Phi^{(N)}_j(t-t_1)\left(\frac{N-j}{N}\right)\times\\ &\times C^{\varepsilon}_{j,j+1}\cdots\left(\frac{N-j-n+1}{N}\right)C^{\varepsilon}_{j+n-1,j+n}\Phi^{(N)}_{j+n}(t_n)W^{\varepsilon}_{N,j+n}(0).\end{aligned}$$

where $\Phi^{(N)}_j$ is the flow associated with the j-particle operator $-V_j\cdot\nabla_{X_j}+T^{\varepsilon}_{N,j}$.

3.3 – The Hartree dynamics in the Wigner formalism

This section is devoted to the description of the Hartree dynamics discussed in Section 2 in terms of the Wigner formalism.

By applying the Wigner transform (3.1.8) to the Hartree equation (in the Heisenberg form) (2.2.6) we find

$$(3.3.1)\qquad (\partial_t+v\cdot\nabla_x)\,f^{\varepsilon}(t)=T^{\varepsilon}_{f^{\varepsilon}}f^{\varepsilon}(t),$$

where $f^{\varepsilon}(t):=f^{\varepsilon}(x,v;t)$ is the Wigner function describing the state of the system (namely, the Wigner transform of the density matrix $\hat{\rho}_t$ solving the Hartree equation (2.2.6)).

For any fixed g, the operator T^{ε}_g acts as follows:

$$(3.3.2)\quad T^{\varepsilon}_g f^{\varepsilon}(x,v)=(2\pi)^{-3}i\int_{-1/2}^{1/2}\mathrm{d}\lambda\int_{\mathbb{R}^3}\mathrm{d}k\hat{\phi}(k)\hat{\rho}_g(k)e^{i\ k\cdot x}(k\cdot\nabla_v)f^{\varepsilon}(x,v+\varepsilon\lambda k),$$

where

$$\rho_g(x) = \int_{\mathbb{R}^3} \mathrm{d}v\; g(x,v), \tag{3.3.3}$$

and $\hat{\rho}_g$ is the Fourier transform of ρ_g, namely:

$$\hat{\rho}_g(k) = \int_{\mathbb{R}^3} \mathrm{d}x\; e^{-i\; k\cdot x}\rho_g(x). \tag{3.3.4}$$

We observe that equation (3.3.1) is nonlinear (as we can see by (3.3.2) replacing g with f^ε) because it arises from a nonlinear Heisenberg equation. Thus in the following we will refer to (3.3.1) as "(Hartree) nonlinear Wigner-Liouville equation". Furthermore, we note that (3.3.1) is the analogue of the classical Vlasov equation (1.1.8) and, roughly speaking, by setting "$\varepsilon = 0$" in (3.3.2) we obtain precisely the Vlasov operator appearing in (1.1.8).

By the analysis we did in the previous section, we know that the linear equation (3.1.16) preserves the L^2-norm (see (3.1.19)). The same holds for the nonlinear equation (3.3.1) and, by assuming the potential to be sufficiently smooth, it can be proved that the H_s-norm is controlled for any $s > 0$. Indeed we have the following

Proposition 3.3.1. *Let $f^\varepsilon(t)$ be the solution of the nonlinear Wigner-Liouville equation* (3.3.1) *whit initial datum $f_0^\varepsilon \in H_s(\mathbb{R}^3 \times \mathbb{R}^3)$ with $s \in \mathbb{N}$. Assuming the potential ϕ to satisfy*

$$\int \mathrm{d}k\; \hat{\phi}(k)|k|^n < +\infty \qquad \forall\; n = 1,2,\ldots,s \tag{3.3.5}$$

we find that

$$\|f^\varepsilon(t)\|_{H_s(\mathbb{R}^3\times\mathbb{R}^3)} \leq e^{Ct}\, \|f_0^\varepsilon\|_{H_s(\mathbb{R}^3\times\mathbb{R}^3)}\,, \tag{3.3.6}$$

where C is a positive constant depending on s and on ϕ but not on ε. For $s = 0$ we have $C = 0$ and (3.3) *becomes an equality* (*conservation of the L^2-norm*).

Proof. For any multi index $\alpha = \{\alpha_1, \alpha_2, \alpha_3\}$, we use the standard notation

$$D_x^\alpha = \frac{\partial^{|\alpha|}}{\partial^{\alpha_1}x_1\partial^{\alpha_2}x_2\partial^{\alpha_3}x_3}, \tag{3.3.7}$$

where $|\alpha| = \alpha_1 + \alpha_2 + \alpha_3$. Analogously we set

$$D_v^\alpha = \frac{\partial^{|\alpha|}}{\partial^{\alpha_1}v_1\partial^{\alpha_2}v_2\partial^{\alpha_3}v_3}. \tag{3.3.8}$$

It is well known that $H_s(\mathbb{R}^3 \times \mathbb{R}^3)$ equipped with the scalar product

$$(f,g)_s = \sum_{\substack{\alpha,\beta\in\mathbb{N}:\\ |\alpha|+|\beta|\le s}} \left(D_v^\alpha D_x^\beta f, D_v^\alpha D_x^\beta g\right)_{L^2(\mathbb{R}^3\times\mathbb{R}^3)} \tag{3.3.9}$$

is an Hilbert space and the corresponding norm is $\|g\|_s := \|g\|_{H_s(\mathbb{R}^3\times\mathbb{R}^3)} = \sqrt{(g,g)_s}$. In order to estimate $\|f^\varepsilon(t)\|_s$, we compute the time derivative $\partial_t D_v^\alpha D_x^\beta f^\varepsilon(t)$ with $|\alpha|+|\beta|\le s$. By (3.3.1) we find:

$$\begin{aligned}\partial_t D_v^\alpha D_x^\beta f^\varepsilon(t) &= D_v^\alpha D_x^\beta(-v\cdot\nabla_x + T^\varepsilon_{f^\varepsilon})f^\varepsilon(t) =\\ &= (-v\cdot\nabla_x + T^\varepsilon_{f^\varepsilon})D_v^\alpha D_x^\beta f^\varepsilon(t) +\\ &\quad + \sum_{\substack{\alpha'<\alpha:\\ |\alpha'|=1}} C_{\alpha,\alpha'} D_v^{\alpha'} v\cdot\nabla_x D_v^{\alpha-\alpha'} D_x^\beta f^\varepsilon(t)+\\ &\quad + \sum_{\substack{\beta'<\beta:\\ |\beta'|\ge 1}} \frac{i\, C_{\beta,\beta'}}{(2\pi)^3}\int_{-1/2}^{1/2}\mathrm{d}\lambda \int \mathrm{d}k\ \hat\phi(k)\hat\rho^\varepsilon(k;t) D_x^{\beta'} e^{i\ k\cdot x}\times\\ &\quad \times (k\cdot\nabla_v) D_v^\alpha D_x^{\beta-\beta'} f^\varepsilon(x, v+\varepsilon\lambda k;t)\end{aligned} \tag{3.3.10}$$

where $C_{\alpha,\alpha'}$, $C_{\beta,\beta'}$ are suitable combinatorial coefficients, $\alpha'<\alpha$, $\beta'<\beta$ mean $\alpha'_j<\alpha_j$, $\beta'_j<\beta_j$ (for $j=1,2,3$) respectively and finally $\alpha-\alpha' = \{\alpha_j-\alpha'_j\}_{j=1}^3$, $\beta-\beta'=\{\beta_j-\beta'_j\}_{j=1}^3$.

We observe now that, by virtue of the antisymmetry of the operators $v\cdot\nabla_x$ and T_g^ε (for any function g), we have

$$(h, v\cdot\nabla_x h)_{L^2(\mathbb{R}^3\times\mathbb{R}^3)} = (h, T_g^\varepsilon h)_{L^2(\mathbb{R}^3\times\mathbb{R}^3)} = 0, \tag{3.3.11}$$

for any g and for each h smooth enough. Moreover, reminding that $f^\varepsilon(t)\in\mathbb{R}$ for all t, if $s>0$, for any $\alpha,\beta:\ 0<|\alpha|+|\beta|\le s$, we find:

$$\begin{aligned}&\frac{1}{2}\frac{d}{dt}\left(D_v^\alpha D_x^\beta f^\varepsilon(t), D_v^\alpha D_x^\beta f^\varepsilon(t)\right)_{L^2(\mathbb{R}^3\times\mathbb{R}^3)} =\\ &= \left(D_v^\alpha D_x^\beta f^\varepsilon(t), \partial_t D_v^\alpha D_x^\beta f^\varepsilon(t)\right)_{L^2(\mathbb{R}^3\times\mathbb{R}^3)},\end{aligned} \tag{3.3.12}$$

which for $s=0$ (namely $|\alpha|=|\beta|=0$) becomes:

$$\frac{1}{2}\frac{d}{dt}\left(f^\varepsilon(t), f^\varepsilon(t)\right)_{L^2(\mathbb{R}^3\times\mathbb{R}^3)} = \left(f^\varepsilon(t), \partial_t f^\varepsilon(t)\right)_{L^2(\mathbb{R}^3\times\mathbb{R}^3)}. \tag{3.3.13}$$

Inserting (3.3.10) in the right hand side of (3.3.13), by virtue of (3.3.11) we find:

$$\frac{1}{2}\frac{d}{dt}(f^\varepsilon(t), f^\varepsilon(t))_{L^2(\mathbb{R}^3\times\mathbb{R}^3)} = \frac{d}{dt}\|f^\varepsilon(t)\|_{L^2(\mathbb{R}^3\times\mathbb{R}^3)} = 0, \tag{3.3.14}$$

namely, the L^2-norm is conserved.

On the contrary, for $s>0$, we insert (3.3.10) in the right hand side of (3.3.12). We find the term involving $D_v^\alpha D_x^\beta f^\varepsilon(t)$ does not give any contribution by virtue of (3.3.11). Thus, by using the shorthand notation $(\cdot,\cdot)_{L^2(\mathbb{R}^3\times\mathbb{R}^3)} = (\cdot,\cdot)_{L^2}$, we obtain

$$\begin{aligned}
&\frac{1}{2}\frac{d}{dt}\left(D_v^\alpha D_x^\beta f^\varepsilon(t), D_v^\alpha D_x^\beta f^\varepsilon(t)\right)_{L^2} = \sum_{\substack{\alpha'<\alpha:\\ |\alpha'|=1}} \times \\
&\times C_{\alpha,\alpha'}\left(D_v^\alpha D_x^\beta f^\varepsilon(t), D_v^{\alpha'} v\cdot\nabla_x D_v^{\alpha-\alpha'} D_x^\beta f^\varepsilon(t)\right)_{L^2} + \\
&+\sum_{\substack{\beta'<\beta:\\ |\beta'|\geq 1}} \frac{i\ C_{\beta,\beta'}}{(2\pi)^3}\int_{-1/2}^{1/2}\mathrm{d}\lambda\int \mathrm{d}k\ \hat{\phi}(k)\hat{\rho}^\varepsilon(k;t)\times \\
&\times\left(D_v^\alpha D_x^\beta f^\varepsilon(t), D_x^{\beta'} e^{i\ k\cdot x}(k\cdot\nabla_v) D_v^\alpha D_x^{\beta-\beta'} f^\varepsilon(x,v+\varepsilon\lambda k;t)\right)_{L^2}.
\end{aligned} \tag{3.3.15}$$

We note that the first term on the right hand side of (3.3.15) is absent when $|\alpha|=0$. On the contrary, if $|\alpha|\geq 1$, by using the Schwartz inequality we obtain:

$$\left(D_v^\alpha D_x^\beta f^\varepsilon(t), D_v^{\alpha'} v\cdot\nabla_x D_v^{\alpha-\alpha'} D_x^\beta f^\varepsilon(t)\right)_{L^2} \leq C\left\|f^\varepsilon(t)\right\|_s^2 \tag{3.3.16}$$

because $|\alpha|-|\alpha'|+|\beta|+1=|\alpha|+|\beta|\leq s$. Analogously, we find that the second term in the right hand side of (3.3.15) is estimated by

$$\begin{aligned}
&\int \mathrm{d}k\ \hat{\phi}(k)\hat{\rho}^\varepsilon(k;t)|k|^{\beta'+1}\left\|D_v^\alpha D_x^\beta f^\varepsilon(t)\right\|_{L^2}\left\|\nabla_v D_v^\alpha D_x^{\beta-\beta'} f^\varepsilon(t)\right\|_{L^2}\leq \\
&\leq \int \mathrm{d}k\ \hat{\phi}(k)\hat{\rho}^\varepsilon(k;t)|k|^{\beta'+1}\left\|f^\varepsilon(t)\right\|_s^2,
\end{aligned} \tag{3.3.17}$$

where we used that $|\alpha|+1+|\beta|-|\beta'|\leq s$. Now we remind that $\rho^\varepsilon(x;t)$ is the spatial density associated with the Wigner function $f^\varepsilon(t)$, namely $\rho^\varepsilon(x;t)\geq 0$ for all x and t,

$$\rho^\varepsilon(x;t)=\int \mathrm{d}v f^\varepsilon(x,v;t), \tag{3.3.18}$$

then the L^1-norm of $\rho^\varepsilon(t)|_{t=0}$ is preserved by the evolution and it is equal to one. Thus, the Fourier transform $\hat{\rho}^\varepsilon(t)$ is in $L^\infty(\mathbb{R}^3\times\mathbb{R}^3)$ for all t and we find:

$$\int \mathrm{d}k\hat{\phi}(k)\hat{\rho}^\varepsilon(k;t)|k|^{\beta'+1}\leq\|\hat{\rho}^\varepsilon(t)\|_{L^\infty(\mathbb{R}^3\times\mathbb{R}^3)}\int \mathrm{d}k\hat{\phi}(k)|k|^{\beta'+1}<+\infty, \tag{3.3.19}$$

by virtue of the assumption (3.3.5) on the pair interaction potential ϕ (we remind that $1 \leq |\beta'| < |\beta| \leq s$). Finally, by (3.3.15), (3.3.16), (3.3.17) and (3.3.19) , it follows that:

$$\frac{1}{2}\frac{d}{dt}\sum_{\substack{\alpha,\beta:\\ |\alpha|+|\beta|\leq s}}(D_v^\alpha D_x^\beta f^\varepsilon(t), D_v^\alpha D_x^\beta f^\varepsilon(t))_{L^2}=\frac{1}{2}\frac{d}{dt}\|f^\varepsilon(t)\|_s^2\leq C\|f^\varepsilon(t)\|_s^2, \quad \forall\ t \tag{3.3.20}$$

C depending on ϕ and s but not on ε. We conclude straightforward by observing that inequality (3.3.20) is equivalent to (3.3.6).

3.3.1 – The Wigner infinite hierarchy

Let us consider the sequence $\{f_j^\varepsilon(t)\}_{j\geq 1}$, where $f_j^\varepsilon(t) = f_j^\varepsilon(X_j, V_j; t)$ is given by:

$$f_j^\varepsilon(X_j, V_j; t) = \prod_{k=1}^{j} f^\varepsilon(x_k, v_k; t) = (f^\varepsilon)^{\otimes j}(X_j, V_j; t) \tag{3.3.21}$$

and $f^\varepsilon(t)$ is the solution of the nonlinear Wigner-Liouville equation (3.3.1). By differentiating in time (3.3.21) we easily deduce the following (infinite) hierarchy of equations:

$$\left(\partial_t + V_j \cdot \nabla_{X_j}\right) f_j^\varepsilon(t) = C_{j,j+1}^\varepsilon f_{j+1}^\varepsilon(t), \tag{3.3.22}$$

where the operator $C_{j,j+1}^\varepsilon$ is the same of (3.2.8). This is precisely the Hartree hierarchy (2.2.4) rephrased in the Wigner formalism and it can be seen as the quantum analogue of the Vlasov hierarchy (1.4.6). Here we derived the Hartree hierarchy by considering the j-particle Wigner function (3.3.21) which is a product of solution of the nonlinear Wigner-Liouville equation (3.3.1). Conversely, as we observed in Section 2 for the Heisenberg formalism, by starting from the hierarchy (3.3.22) and assuming the solution to be factorized according to a one-particle time dependent Wigner function $f^\varepsilon(t)$, it turns out that $f^\varepsilon(t)$ has to solve equation (3.3.1).

By using (iteratively) the Duhamel formula, the solution $f_j^\varepsilon(t)$ of the equations (3.3.22) with initial datum $f_j^\varepsilon(0)$ can be written as

$$\begin{aligned} f_j^\varepsilon(t) &= \Phi_j(t) f_j^\varepsilon(0) + \\ &+ \sum_{n=1}^{N-j}\int_{0\leq t_n\leq\cdots\leq t_1\leq t} \mathrm{d}t_n \ldots \mathrm{d}t_1 \Phi_j(t-t_1)\times \\ &\times C_{j,j+1}^\varepsilon \ldots C_{j+n-1,j+n}^\varepsilon\ \Phi_{j+n}(t_n) f_{j+n}^\varepsilon(0). \end{aligned} \tag{3.3.23}$$

where Φ_j is the flow associated with the j-particle operator $-V_j \cdot \nabla_{X_j}$, namely it is the free j-particle flow

$$\Phi_j(t) f_j^\varepsilon(X_j, V_j) = f_j^\varepsilon(X_j - V_j t, V_j). \tag{3.3.24}$$

3.4 – The Limit $N \to \infty$

By the analysis done in the previous section, it is quite natural to rephrase the mean-field result discussed in Section 2 in the Wigner formalism. This will be the subject of this section and, here and in the sequel, we will always assume the interaction potential to be sufficiently smooth.

Thanks to Theorem 2.3.1, we know that, for bounded potentials, the sequence $\hat{\rho}_{N,t}^{(j)}$ of the RDM associated with the N-particle mean-field dynamics is converging in trace norm, as $N \to \infty$, to the j-fold product $\hat{\rho}_t^{\otimes j}$ of solutions of the Hartree equation. By reminding that the space $\mathcal{L}^1(L^2(\mathbb{R}^{3j}))$ of trace class operators on $L^2(\mathbb{R}^{3j})$ is a subspace of the space $\mathcal{L}^2(L^2(\mathbb{R}^{3j}))$ of Hilbert-Schmidt operators on $L^2(\mathbb{R}^{3j})$, it follows that:

$$\left\| \hat{\rho}_{N,t}^{(j)} - \hat{\rho}_t^{\otimes j} \right\|_{\mathcal{L}^2(L^2(\mathbb{R}^{3j}))} \leq \left\| \hat{\rho}_{N,t}^{(j)} - \hat{\rho}_t^{\otimes j} \right\|_{\mathcal{L}^1(L^2(\mathbb{R}^{3j}))} \to 0, \quad \text{as} \quad N \to \infty. \tag{3.4.1}$$

Therefore, by virtue of the equality (3.1.12) concerning the Hilbert-Schmidt norm and thanks to the property (3.1.10) of the Wigner function, we can conclude that

$$\begin{aligned} &\left\| W_{N,j}^\varepsilon(t) - (f^\varepsilon(t))^{\otimes j} \right\|_{L^2(\mathbb{R}^{3j} \times \mathbb{R}^{3j})} \leq \\ &\leq \left\| \hat{\rho}_{N,t}^{(j)} - \hat{\rho}_t^{\otimes j} \right\|_{\mathcal{L}^1(L^2(\mathbb{R}^{3j}))} \to 0, \quad \text{as} \quad N \to \infty, \end{aligned} \tag{3.4.2}$$

where $W_{N,j}^\varepsilon(t)$ are the time evolved Wigner marginals defined in (3.2.5) and $f^\varepsilon(t)$ is the solution of the (Hartree) nonlinear Wigner equation (3.3.1).

Therefore, the mean-field theorem ensuring the convergence in trace norm of the RDM, guarantees also the L^2-strong convergence of the corresponding Wigner marginals. Nevertheless, by looking at (3.4.2), it is clear that the error in the approximation for large N is precisely the same we saw previously, and then, it is depending on ε and diverging as $\varepsilon \to 0$.

It turns out that, in the perspective of obtaining estimates on the error in the mean-field approximation which are uniform with respect to ε or, at least, which exhibit a less singular dependence on ε, a quite natural approach is to rephrase the whole mean-field result discussed in Section 2 (by assuming the interaction to be sufficiently smooth) in the Wigner formalism.

By looking at the Wigner BBGKY hierarchy (3.2.6) we observe that the operator $T_{N,j}^\varepsilon$ is of size $O\left(\frac{j^2}{N}\right)$ while the operator $C_{j,j+1}^\varepsilon$ is $O(1)$ with respect to N and it is properly the same appearing in the infinite hierarchy (3.3.22). Therefore, in analogy to what we did in proving Theorem 2.3.1 one expects that the flow $\Phi_j^{(N)}(t)$ appearing in (3.2.10) converges in a suitable sense to the free flow $\Phi_j(t)$ as $N \to \infty$ so that, this time by using the BBGKY hierarchy, one can prove that

$$W^\varepsilon_{N,j}(t) \to f^\varepsilon_j(t), \quad \text{as} \quad N \to \infty, \tag{3.4.3}$$

in a sense to be made precise.

In Sections 1 and 2, to show the validity of propagation of chaos, we considered as initial datum for the N-particle dynamics the (bosonic) factorized state (2.2.8), or equivalently, (2.2.9). We observe that the Wigner transform f^ε_ρ defined in (3.1.8) is linear with respect to the density matrix (kernel) ρ, thus we find that the Wigner transform of the factorized state $\hat{\rho}_{N,0} = \hat{\rho}_0^{\otimes N}$ considered in Theorem 2.3.1 is also factorized, namely

$$W^\varepsilon_N(X_N, V_N) = \prod_{i=1}^N f^\varepsilon_0(x_i, v_i), \tag{3.4.4}$$

where f^ε_0 is the Wigner transform of $\hat{\rho}_0$. Moreover, being $\hat{\rho}_0 = |\psi_0 >< \psi_0|$, we find

$$f^\varepsilon_0 = f^\varepsilon_{\rho_0} \leftrightarrow \hat{\rho}_0 = |\psi_0 >< \psi_0| \tag{3.4.5}$$

and

$$\|f^\varepsilon_0\|_{L^2(\mathbb{R}^3\times\mathbb{R}^3)} = \|\rho_0\|_{L^2(\mathbb{R}^3\times\mathbb{R}^3)} = \|\psi_0\|^2_{L^2(\mathbb{R}^3)} = 1. \tag{3.4.6}$$

By taking the j-particle marginal associated with $W^\varepsilon_N(X_N, V_N)$ we straightforward obtain

$$W^\varepsilon_{N,j}(X_j, V_j) = \prod_{i=1}^j f^\varepsilon_0(x_i, v_i) = (f^\varepsilon_0)^{\otimes j}(X_j, V_j), \tag{3.4.7}$$

then, by (3.2.10), the solution of the equations (3.2.6) with initial datum (3.4.7) is given by

$$\begin{aligned} W^\varepsilon_{N,j}(t) =\ & \Phi_j^{(N)}(t)(f^\varepsilon_0)^{\otimes j} + \\ & + \sum_{n=1}^{N-j} \int_{0\le t_n \le \dots \le t_1 \le t} \mathrm{d}t_n \dots \mathrm{d}t_1\, \Phi_j^{(N)}(t-t_1) \left(\frac{N-j}{N}\right) \times \\ & \times C^\varepsilon_{j,j+1} \dots \left(\frac{N-j-n+1}{N}\right) C^\varepsilon_{j+n-1,j+n}\, \Phi^{(N)}_{j+n}(t_n)(f^\varepsilon_0)^{\otimes j+n}, \end{aligned} \tag{3.4.8}$$

while the hierarchy (3.3.23) with initial datum $(f_0^\varepsilon)^{\otimes j}$ is

$$\begin{aligned} f_j^\varepsilon(t) &= \Phi_j(t)(f_0^\varepsilon)^{\otimes j} + \\ &+ \sum_{n=1}^{N-j} \int_{0\le t_n\le\cdots\le t_1\le t} \mathrm{d}t_n \dots \mathrm{d}t_1\ \Phi_j(t-t_1)\times \\ &\times C^\varepsilon_{j,j+1}\dots C^\varepsilon_{j+n-1,j+n}\ \Phi_{j+n}(t_n)(f_0^\varepsilon)^{\otimes j+n}. \end{aligned} \tag{3.4.9}$$

Following the line of the proof of Theorem 2.3.1, to prove the convergence of the series (3.4.8) to (3.4.9) we must find a norm $|\cdot|_j$ for the marginals $W^\varepsilon_{N,j}(t)$ which plays the role of the trace norm on $L^2(\mathbb{R}^{3j})$ in Theorem 2.3.1. First of all, it has to be controlled by the flows $\Phi_j^{(N)}$ and Φ_j in the sense that for any $T>0$ and for fixed j

$$\left|\Phi_j^{(N)}(t)W^\varepsilon_{N,j}\right|_j \le C_{t,j}\left|W^\varepsilon_{N,j}\right|_j, \quad C_{t,j}>0:\ \sup_{t\in[0,T]} C_{t,j}<+\infty, \tag{3.4.10}$$

and

$$\left|\Phi_j(t)W^\varepsilon_{N,j}\right|_j \le C'_{t,j}\left|W^\varepsilon_{N,j}\right|_j, \quad C'_{t,j}>0:\ \sup_{t\in[0,T]} C'_{t,j}<+\infty, \tag{3.4.11}$$

(note that for the flows $S_j^{(N)}$ and S_j involved Theorem 2.3.1 we had properly conservation of the trace norm, actually estimates of the form (3.4.10) and (3.4.11) would have been sufficient). Thus, by (3.4.10) we could have the following bound for the n-th term of the (formal) series (3.4.8)

$$\begin{aligned} &\frac{t^n}{n!} j(j+1)\dots(j+n-1)(C_t)^n\left|(f_0^\varepsilon)^{\otimes j+n}\right|_{j+n}, \\ &C_t = C_t(\phi,j)>0:\ \forall T>0\ \sup_{t\in[0,T]} C_t<+\infty \end{aligned} \tag{3.4.12}$$

provided that the operator $C^\varepsilon_{j,j+1}$ satisfies

$$\left|C^\varepsilon_{j,j+1}W^\varepsilon_{N,j+1}\right|_j \le j\,C\left|W^\varepsilon_{N,j+1}\right|_{j+1}, \quad C=C(\phi)>0. \tag{3.4.13}$$

Clearly (3.4.12) and (3.4.13) would hold even for the n-th term of the series (3.4.9) by virtue of (3.4.11).

By (3.4.12), it would follow that $|\cdot|_j$ has to be such that

$$\left|(f_0^\varepsilon)^{\otimes j}\right|_j = (|f_0^\varepsilon|_1)^j \le a^j \quad \text{for any } j, \tag{3.4.14}$$

where a is some positive constant. Then we could conclude that the n-th term of the (formal) series (3.4.8) and the n-th term of (3.4.9) are bounded by:

$$\begin{aligned} &\frac{t^n}{n!} j(j+1)\dots(j+n-1)\,(C_t)^n a^{j+n} < t^n (C_j\ a^j)\,(2aC_t)^n, \\ &C = C(\phi) > 0 \end{aligned} \tag{3.4.15}$$

and then we would have convergence for short times $|t| < t_0$ (t_0 depending on ϕ and a) of (3.4.8) and (3.4.9) with respect to the norm $|\cdot|_j$. This would imply that the solution of the infinite hierarchy (3.3.23) with initial datum $(f_0^\varepsilon)^{\otimes j}$ is uniquely determined up to time t_0, thus, by the analysis done in the previous section, we would know that it is given by $(f^\varepsilon(t))^{\otimes j}$, $f^\varepsilon(t)$ solving the nonlinear Wigner-Liouville equation (3.3.1). Moreover, by (3.4.5) it would follow that

$$f^\varepsilon(t) = f^\varepsilon_{\rho_t} \leftrightarrow \hat{\rho}_t = |\psi_t >< \psi_t|, \tag{3.4.16}$$

ψ_t solving the Hartree equation (2.1.21) with initial datum ψ_0.

To prove convergence of (3.4.8) to (3.4.9), the norm $|\cdot|_j$ has to be such that

$$\left\| T^\varepsilon_{N,j} \right\| \to 0 \quad \text{as} \quad N \to \infty, \tag{3.4.17}$$

where $\|\cdot\|$ is the operator norm on the space of j-particle functions with finite norm $|\cdot|_j$. In fact, we observe that

$$\left| \Phi_j^{(N)}(t)\ f_j - \Phi_j(t)\ f_j \right|_j \le \int_0^t \mathrm{d}\tau \left| \Phi_j(t-\tau) T^\varepsilon_{N,j}\ f_j(\tau) \right|_j, \tag{3.4.18}$$

for any j-particle Wigner function f_j. Thus, by virtue of (3.4.11) and (3.4.17) we would obtain

$$\lim_{N\to\infty} \left\| \Phi_j^{(N)}(t) - \Phi_j(t) \right\| = 0, \tag{3.4.19}$$

implying convergence of (3.4.8) to (3.3.23) with respect to the norm $|\cdot|_j$, namely, propagation of chaos, for short times $|t| < t_0$ in the sense that, for any fixed j,

$$\left| W^\varepsilon_{N,j}(t) - (f^\varepsilon(t))^{\otimes j} \right|_j \to 0, \quad \text{as} \quad N \to \infty \quad \forall\, t < t_0. \tag{3.4.20}$$

Finally, the argument just given could be iterated to prove propagation of chaos for $t \in [t_0 - \delta, t_0 + \delta]$ (for any $\delta > 0$) if we could prove that

$$\left| f_j^\varepsilon(t_0 - \delta) \right|_j = (|f^\varepsilon(t_0 - \delta)|_1)^j \le C a^j. \quad \text{For any fixed } j. \tag{3.4.21}$$

In fact, the bound (3.4.21), together with the convergence proved previously up to time t_0, would imply estimate (3.4.14) to hold for $W^\varepsilon_{N,j}(t)$ where $t = t_0 - \delta$.

Then, by iteration we could conclude that propagation of chaos in the sense of (3.4.20) holds for all t.

By looking at the scheme we have just presented it turns out that the accuracy of the mean-field approximation would be provided by the speed of convergence of the operator norm of $T^{\varepsilon}_{N,j}$ to zero as $N \to \infty$ (see (3.4.17)). Then, if one was able to provide an estimate uniform in ε for $\left\|T^{\varepsilon}_{N,j}\right\|$, the convergence (3.4.20) would be also uniform with respect to ε and then, by iteration, we would have uniformity in ε for all times.

– **Choice of the norm** $|\cdot|$

Since by (3.4.2) we already know that the j-particle Wigner marginals are converging strongly in L^2 to the j-fold product of solutions of the (Hartree) nonlinear Wigner-Liouville equation, it would be reasonable to choose the L^2-norm as $|\cdot|$ to check if it is possible to improve the "bad" dependence of the error (in the limit $N \to \infty$) with respect to ε. Moreover, on the basis of (3.4.6) one could think to choose the L^2-norm because (3.4.14) would be satisfied (with $a = 1$) and this would hold for each t because the Hartree dynamics preserves the L^2-norm (see (3.3.14)). Furthermore, the flows $\Phi^{(N)}_j(t)$ and $\Phi_j(t)$ not only control the L^2-norm in the sense of (3.4.10) and (3.4.11) but even preserve it.

Nevertheless, it turns out that the operator $C^{\varepsilon}_{j,j+1}$ is unbounded from L^2 $(\mathbb{R}^{3(j+1)} \times \mathbb{R}^{3(j+1)})$ to $L^2(\mathbb{R}^{3j} \times \mathbb{R}^{3j})$ (it can be verified easily by looking at (3.2.8)), thus property (3.4.13) fails.

Actually, one can verify that, by assuming H_s regularity at time $t = 0$, it is propagated by the flow $\Phi^{(N)}_j(t)$ (see [25]), by the free flow $\Phi_j(t)$ and also by the nonlinear Wigner-Liouville equation (3.3.1) (according to Proposition 3.3.1). So, this choice could be appropriate for the preservation in time of property (3.4.14) but, as for the L^2-norm, the boundness of $C^{\varepsilon}_{j,j+1}$ fails.

By taking into account the (formal) analogy between the N-particle Wigner-Liouville equation (3.2.1) and the Liouville equation (1.1.5) one could think to use the L^1-norm. Indeed it is easy to check that the operators $T^{\varepsilon}_{N,j}$ and $C^{\varepsilon}_{j,j+1}$ are bounded in L^1 and it can be also verified that the flow $\Phi^{(N)}_j(t)$ controls the L^1-norm in the sense of (3.4.10). The free flow $\Phi_j(t)$ clearly preserves the L^1-norm. Furthermore, by assuming property (3.4.14) to hold , namely $f^{\varepsilon}_0 \in L^1(\mathbb{R}^3 \times \mathbb{R}^3)$, it is easy to check that it is verified for all t because the L^1-norm is controlled by the Hartree dynamics. In other words, property (3.4.21) would be satisfied and we could iterate the procedure presented above to prove convergence for all times. Therefore the L^1-norm could seem a good choice but the point is that Wigner functions are, in general, not in L^1. More precisely, by only knowing that f^{ε}_0 is the Wigner transform of a wave function $\psi_0 \in L^2(\mathbb{R}^3)$ (as in the present situation), we are not guaranteed that $f^{\varepsilon}_0 \in L^1(\mathbb{R}^3 \times \mathbb{R}^3)$. Indeed, in general the

L^1-norm of Wigner functions is not related to any norm of the wave functions from which they arise. We will come back on this topic in Remark 3.4.1.

It turns out that a fruitful approach is to use a norm which, from on side, is "good" for estimating $C^{\varepsilon}_{j,j+1}$, it is controlled by $\Phi^{(N)}_j(t)$, $\Phi_j(t)$ and even by the Hartree dynamics, and, on the other side, it somehow "relates" Wigner functions to the wave functions from which they arise.

Let us to consider the Fourier transform $\mathcal{F}_x$ of the N-particle Wigner function with respect to position variables, namely

$$(\mathcal{F}_x W^{\varepsilon}_N)(P_N, V_N) := \tilde{W}^{\varepsilon}_N(P_N, V_N) = \int \mathrm{d}X_N \; e^{-i\; P_N\cdot X_N} W^{\varepsilon}_N(X_N, V_N), \tag{3.4.22}$$

with $P_N = (p_1, \dots, p_N) \in \mathbb{R}^{3N}$ and let us define the $\tilde{L}^1$-norm as

$$\begin{aligned} \|W^{\varepsilon}_N\|_{\tilde{L}^1(\mathbb{R}^{3N}\times\mathbb{R}^{3N})} :&= \left\|\tilde{W}^{\varepsilon}_N\right\|_{L^1(\mathbb{R}^{3N}\times\mathbb{R}^{3N})} = \\ &= \int \mathrm{d}P_N \int \mathrm{d}V_N \; |\tilde{W}^{\varepsilon}_N(P_N, V_N)|. \end{aligned} \tag{3.4.23}$$

We can verify that the operator $T^{\varepsilon}_{N,j} : \tilde{L}^1(\mathbb{R}^{3j}\times\mathbb{R}^{3j}) \to \tilde{L}^1(\mathbb{R}^{3j}\times\mathbb{R}^{3j})$ is bounded under the assumption $\left\|\hat{\phi}\right\|_{L^1(\mathbb{R}^3)} < +\infty$. Indeed, by computing

$$\mathcal{F}_x(T^{\varepsilon}_{N,j} W^{\varepsilon}_{N,j})(P_j, V_j) = \int \mathrm{d}P_j \; e^{-i\; P_j\cdot X_j} \; T^{\varepsilon}_{N,j} W^{\varepsilon}_{N,j}(X_j, V_j), \tag{3.4.24}$$

by manipulating (3.2.7) we find

$$\begin{aligned} &\mathcal{F}_x(T^{\varepsilon}_{N,j} W^{\varepsilon}_{N,j})(P_j, V_j) := (\tilde{T}^{\varepsilon}_{N,j} \tilde{W}^{\varepsilon}_{N,j})(P_j, V_j) = \\ &= \frac{i(2\pi)^{-3N}}{\varepsilon N} \sum_{l\neq r}^{j} \sum_{\sigma=\pm1} \sigma \int \mathrm{d}k \; \hat{\phi}(k) \tilde{W}^{\varepsilon}_{N,j}\bigg(p_1, \dots, p_l + \\ &- k, \dots, p_j, \; v_1, \dots, v_l + \frac{\sigma\varepsilon k}{2}, \dots, v_j\bigg), \end{aligned} \tag{3.4.25}$$

then

$$\begin{aligned} \left\|T^{\varepsilon}_{N,j} W^{\varepsilon}_{N,j}\right\|_{\tilde{L}^1(\mathbb{R}^{3j}\times\mathbb{R}^{3j})} &= \left\|\tilde{T}^{\varepsilon}_{N,j} \tilde{W}^{\varepsilon}_{N,j}\right\|_{L^1(\mathbb{R}^{3j}\times\mathbb{R}^{3j})} \leq \\ &\leq \frac{1}{(2\pi)^{3N}} \frac{2j^2}{\varepsilon N} \left\|\hat{\phi}\right\|_{L^1(\mathbb{R}^3)} \left\|W^{\varepsilon}_{N,j}\right\|_{\tilde{L}^1(\mathbb{R}^{3j}\times\mathbb{R}^{3j})}. \end{aligned} \tag{3.4.26}$$

In a similar way, we verify that the operator $C^{\varepsilon}_{j,j+1} : \tilde{L}^1(\mathbb{R}^{3(j+1)} \times \mathbb{R}^{3(j+1)}) \to \tilde{L}^1(\mathbb{R}^{3j} \times \mathbb{R}^{3j})$ is bounded under the assumption $\left\|\hat{\phi}\right\|_{L^{\infty}(\mathbb{R}^3)} < +\infty$. In fact we compute

$$\mathcal{F}_x(C^{\varepsilon}_{j,j+1} W^{\varepsilon}_{N,j+1})(P_j, V_j) = \int \mathrm{d}P_j \; e^{-i\; P_j\cdot X_j} \; (C^{\varepsilon}_{j,j+1} W^{\varepsilon}_{N,j+1})(X_j, V_j), \tag{3.4.27}$$

obtaining by (3.2.8) that

(3.4.28)
$$\begin{aligned}
&\mathcal{F}_x(C^{\varepsilon}_{j,j+1}W^{\varepsilon}_{N,j+1})(P_j,V_j) := (\tilde{C}^{\varepsilon}_{j,j+1}\tilde{W}^{\varepsilon}_{N,j+1})(P_j,V_j) = \\
&= \frac{i(2\pi)^{-3N}}{\varepsilon}\left(\frac{N-j}{N}\right)\sum_{l=1}^{j}\sum_{\sigma=\pm 1}\sigma\times \\
&\times \int \mathrm{d}v_{j+1}\int \mathrm{d}k\hat{\phi}(k)\tilde{W}^{\varepsilon}_{N,j+1}\Big(p_1,\ldots,p_l+ \\
&-k,\ldots,p_j,k,\ v_1,\ldots,v_l+\frac{\sigma\varepsilon k}{2},\ldots,v_{j+1}\Big),
\end{aligned}$$

then

(3.4.29)
$$\begin{aligned}
&\left\|C^{\varepsilon}_{j,j+1}W^{\varepsilon}_{N,j+1}\right\|_{\tilde{L}^1(\mathbb{R}^{3j}\times\mathbb{R}^{3j})} = \left\|\tilde{C}^{\varepsilon}_{j,j+1}\tilde{W}^{\varepsilon}_{N,j+1}\right\|_{L^1(\mathbb{R}^{3j}\times\mathbb{R}^{3j})} \leq \\
&\leq (2\pi)^{-3N}\frac{(2j)}{\varepsilon}\left(\frac{N-j}{N}\right)\left\|\hat{\phi}\right\|_{L^\infty(\mathbb{R}^3)}\left\|W^{\varepsilon}_{N,j+1}\right\|_{\tilde{L}^1(\mathbb{R}^{3(j+1)}\times\mathbb{R}^{3(j+1)})}.
\end{aligned}$$

Furthermore, concerning the initial datum $(f_0^{\varepsilon})^{\otimes j}$, by (3.4.5) we have

(3.4.30)
$$\begin{aligned}
&\left\|(f_0^{\varepsilon})^{\otimes j}\right\|_{\tilde{L}^1(\mathbb{R}^{3j}\times\mathbb{R}^{3j})} = \left(\|f_0^{\varepsilon}\|_{\tilde{L}^1(\mathbb{R}^3\times\mathbb{R}^3)}\right)^j \leq \\
&\leq C\left(\left\|\hat{\psi}_0\right\|_{L^1(\mathbb{R}^3)}\right)^{2j} \leq C\left(\|\psi_0\|_{H_s(\mathbb{R}^3)}\right)^{2j},\ s>3/2
\end{aligned}$$

where the last inequalities are simply obtained by explicit computations. For any $t>0$, by (3.4.16) we have

(3.4.31)
$$\|f^{\varepsilon}(t)\|_{\tilde{L}^1(\mathbb{R}^3\times\mathbb{R}^3)} \leq C\left\|\hat{\psi}_t\right\|^2_{L^1(\mathbb{R}^3)} \leq C\,\|\psi_t\|^2_{H_s(\mathbb{R}^3)}, \quad s>3/2,$$

and by using standard energy methods it is easy to check that, under suitable smoothness assumption on the potential ϕ, the H_s-norm of ψ_t is controlled by the H_s-norm of ψ_0 for any s. Furthermore, even by looking at the (Hartree) nonlinear Wigner-Liouville equation (3.3.1), it is easy to check that the $\tilde{L}^1$-norm of $f^{\varepsilon}(t)$ is controlled by the $\tilde{L}^1$-norm of f_0^{ε}.

Finally, by virtue of (3.4.26), (3.4.29), (3.4.30) and (3.4.31), it follows that by setting

(3.4.32)
$$|\cdot|_j := \|\cdot\|_{\tilde{L}^1(\mathbb{R}^{3j}\times\mathbb{R}^{3j})},$$

and by assuming $\psi_0\in H_s(\mathbb{R}^3)$ with $s>3/2$ and the potential ϕ to be sufficiently smooth (in order to make all constants appearing in the estimates finite), we have

(3.4.33)
$$\left|W^{\varepsilon}_{N,j}(t)-(f^{\varepsilon}(t))^{\otimes j}\right|_j \to 0, \quad \text{as} \quad N\to\infty \quad \forall\, t.$$

Therefore, for smooth potentials, we can show propagation of chaos in the Wigner formulation by following the same strategy of Theorem 2.3.1. Nonetheless, we note that the error in the approximation (3.4.33) is still not uniform with respect to ε and diverging when $\varepsilon \to 0$ because from (3.4.26) we see that the operator norm of $T^{\varepsilon}_{N,j}$ is of order $1/\varepsilon$ (as in Theorem 2.3.1).

We conclude the present analysis by observing that (3.4.33) implies straightforward that

$$\int_{\mathbb{R}^{3j}} \mathrm{d}V_j \sup_{X_j} \left| W^{\varepsilon}_{N,j}(X_j, V_j; t) - (f^{\varepsilon}(t))^{\otimes j}(X_j, V_j) \right| \to 0, \text{ as } N \to \infty \;\forall\, t, \tag{3.4.34}$$

namely

$$\left\| W^{\varepsilon}_{N,j}(t) - (f^{\varepsilon}(t))^{\otimes j} \right\|_{L^\infty(\mathbb{R}^{3j}_{X_j}) \cap L^1(\mathbb{R}^{3j}_{V_j})} \to 0, \quad \text{as} \quad N \to \infty \quad \forall\, t. \tag{3.4.35}$$

Despite the fact that (3.4.34) is a quite "strong" convergence, it is not related to any convergence for the reduced density matrices and it does not imply any convergence for the expected value of j-particle observables (namely, it does not provide informations about macroscopic values of physically interesting quantities).

Nevertheless, one can verifies that the convergence (3.4.33) and the uniform bounds

$$\left\| W^{\varepsilon}_{N,j}(t) \right\|_{L^2(\mathbb{R}^{3j} \times \mathbb{R}^{3j})} \le 1, \quad \| f^{\varepsilon}(t) \|_{L^2(\mathbb{R}^3 \times \mathbb{R}^3)} \le 1, \tag{3.4.36}$$

imply

$$W^{\varepsilon}_{N,j}(t) \to (f^{\varepsilon}(t))^{\otimes j}, \quad \text{as} \quad N \to \infty \quad \forall t, \quad L^2 - \text{weakly}. \tag{3.4.37}$$

By virtue of property (3.1.4), (3.4.37) ensures the convergence of expected values of suitable observables. More precisely, (3.4.37) allows to compute "macroscopic" (or "effective") expected value of j-particle observables O_j whose phase space representations (symbols) are in $L^2(\mathbb{R}^{3j} \times \mathbb{R}^{3j})$ (see also [11]). Indeed, for any j-particle observable O_j with symbol $O_j(X_j, V_j)$, we have the following estimate

$$(O_j, W^{\varepsilon}_{N,j}(t))_{L^2} \approx (O_j, (f^{\varepsilon}(t))^{\otimes j})_{L^2} + \frac{C_j(\varepsilon)}{N}, \quad \forall t, \quad \text{as} \quad N \to \infty, \tag{3.4.38}$$

where $C_j(\varepsilon) \to \infty \quad$ as $\quad \varepsilon \to 0$.

Remark 3.4.1. We observe that all estimates we did by using the $\tilde{L}^1$-norm would be also valid for the L^1-norm. Thus, by assuming $f^{\varepsilon}_0 \in L^1(\mathbb{R}^3 \times \mathbb{R}^3)$ and following exactly the same strategy leading to the $\tilde{L}^1$-convergence (3.4.33), we can prove that

$$\left\|W^{\varepsilon}_{N,j}(t) - (f^{\varepsilon}(t))^{\otimes j}\right\|_{L^1(\mathbb{R}^{3j}\times\mathbb{R}^{3j})} \to 0, \quad \text{as} \quad N\to\infty \quad \forall\, t, \tag{3.4.39}$$

and, as for the $\tilde{L}^1$-convergence, it can be verified that (3.4.39) together with the uniform bounds (3.4.36) leads to the L^2-weak convergence (3.4.37) and, in particular, to the estimate (3.4.38). Then, apparently, there is no reason for considering the $\tilde{L}^1$-norm instead of the L^1-norm. In fact, in both cases we can realize the limit $N\to\infty$ in the L^2-weak sense and in both cases we find that the error in the mean-field approximation is not uniform with respect to ε, indeed diverging as $\varepsilon\to 0$ (by looking at the constant $C_j(\varepsilon)$ in (3.4.38)). Nevertheless, as we have already noticed, the crucial point is: which assumptions one has to do on the wave function ψ_0 to ensure that its Wigner transform f^{ε}_0 is in $L^1(\mathbb{R}^3\times\mathbb{R}^3)$? We remind that

$$\int \mathrm{d}x \int \mathrm{d}v f^{\varepsilon}_0(x,v) = \int \mathrm{d}x |\psi_0(x)|^2 = \mathtt{Tr}\hat{\rho}_0 = 1 \;\text{ with }\; \hat{\rho}_0 = |.\psi_0 >< \psi_0| \tag{3.4.40}$$

We know that the integral on the phase space of $f^{\varepsilon}_0(x,v)$ does not correspond to its L^1-norm being f^{ε}_0 not positive in general. But, by considering a wave function ψ_0 such that $f^{\varepsilon}_0(x,v)\geq 0$ for any x,v we could identify the L^2-norm of ψ_0 (which is taken equal to one) with the L^1-norm of f^{ε}_0 and we are guaranteed that property (3.4.14) is verified (with $a=1$). The only way for having a positive Wigner function is to choose $\psi_0 \approx e^{-x^2}$ (see for example [11]), in particular we can consider coherent states of the form $\psi(x) = N_{\varepsilon} e^{-\frac{(x-x_0)^2}{\varepsilon}} e^{i\frac{v_0 x}{\varepsilon}}$, for some $x_0, v_0 \in \mathbb{R}^3$.

In the end, we found that propagation of chaos in the mean-field limit by using the Wigner formalism can be proven, for smooth potentials, in the L^2-norm, directly by the mean-field result for the RDM (the use of the BBGKY hierarchy is prevented by the unboundedness of the operators involved). On the other side, by treating the Wigner BBGKY hierarchy, it can be proven in the L^1-norm by choosing initial gaussian states, and, in the $\tilde{L}^1$-norm, by choosing initial wave functions in H_s, $s>3/2$ (if the dimension of the system is assumed to be equal to 3; in general, in any dimension d, we have $s>d/2$). In each of the three cases we obtain convergence of expected values of j-particle observables O_j with symbol in $L^2(\mathbb{R}^{3j}\times\mathbb{R}^{3j})$. Furthermore, in each of these cases the error in the mean-field approximation is not uniform with respect to ε and it is diverging as $\varepsilon\to 0$.

3.5 – Alternative approaches

The validity of propagation of chaos in the mean-field limit has been established also in [26] by using the "second-quantization formalism". For fixed ε, the authors provide an alternative proof of the emergence of the Hartree dynamics for bounded potential ϕ and, even if obtained by using a different formalism, the general strategy of the proof is analogous to that of [7] and the result can be formulated in terms of convergence of reduced density matrices to products of solutions of the Hartree equation. Then, by passing to the Wigner formalism, for a restricted class of two-body interactions the following (distributional) estimate in $\mathcal{S}'(\mathbb{R}^{3j} \times \mathbb{R}^{3j})$ is proven

$$(3.5.1) \quad W^{\varepsilon}_{N,j}(t) \approx (f^{\varepsilon}(t))^{\otimes j} + \frac{C_j}{N} + O\left(e^{-1/\sqrt{\|\phi\|_\infty t}}\right), \quad \forall\, t, \quad \text{as} \quad N \to \infty,$$

where $\|\phi\|_\infty := \|\phi\|_{L^\infty(\mathbb{R}^3)}$, C_j is a positive constant only depending on j and $W^{\varepsilon}_{N,j}(t)$ and $f^{\varepsilon}(t)$ are defined as in (3.4.38). It turns out that the error in approximating the N-particle evolution with the Hartree dynamics is indeed uniform with respect to ε but the exponential remainder appearing in (3.5.1) is small only if $\|\phi\|_\infty t << 1$, namely, by looking at very short times or by considering an interaction potential having very small L^∞-norm.

– **Joint limit $N \to \infty$ and $\varepsilon \to 0$**

In looking at the connection between mean-field limit and semiclassical approximation, a joint limit $N \to \infty$ and $\varepsilon \to 0$ can be considered. Indeed, there are systems in which this kind of limit arises quite naturally by the scaling properties of the Hamiltonian.

A remarkable example is provided by the model considered in [19] and, previously, in [8] (with a somewhat different interpretation). The model considered in [19] is a system of N fermions interacting by the mean-field potential (2.1) with initial data localized in a cube of size of order one and at energy comparable with the ground state energy of the system. The Hamiltonian of the system is given by (2.1.5), thus all the potential energy arises from the interaction term (2.1) and it follows straightforward that the potential energy per particle is of order one. As regard to the kinetic energy, it can be verified that the kinetic energy per particle of N fermions, i.e., $-\frac{1}{2}\varepsilon^2 \Delta_{x_k} (k = 1, \dots, N)$, in a cube of size one scales like $\varepsilon^2 N^{2/3}$ in the ground state. Therefore, in order to look at the limit $N \to \infty$ keeping the kinetic energy per particle of order one, one has to multiply the kinetic energy in (2.1.5) by $N^{-2/3}$. Then, by defining the "effective Planck constant" ε_{eff} such that $\varepsilon_{eff} = \varepsilon N^{-1/3}$, the Hamiltonian of the systems becomes

$$(3.5.2) \quad H^Q_{N,eff} = -\sum_{k=1}^{N} \frac{\varepsilon^2_{eff} \Delta_k}{2} + U^Q(X_N), \quad \varepsilon_{eff} \approx N^{-1/3} \to 0 \text{ as } N \to \infty.$$

Therefore the kinetic and the potential energy per particle in the Hamiltonian $H^Q_{N,eff}$ are comparable and, as we already observed in introducing the mean-field model, this is the basic physical criterion to obtain a non trivial limiting dynamics (as $N \to \infty$) that captures the nonlinear effect of the interaction. Clearly, the limit $N \to \infty$ for the system whose Hamiltonian is $H^Q_{N,eff}$ entails the limit $\varepsilon_{eff} \to 0$ which is a semiclassical limit for (2.1.5). Thus, one expects to find a limiting dynamics which is ruled by a classical equation. On the other side, it is known (and it is validated by numerous applications) that the equation governing the macroscopic (physically observable) dynamics of a Fermi gas in states close to the ground state is the Hartree-Fock equation:

$$(3.5.3)\qquad \begin{aligned} i\varepsilon\partial_t\hat{\rho}_t = {} & \left[-\frac{\varepsilon^2}{2}\Delta, \hat{\rho}_t\right] + \mathtt{Tr}_2\left\{[\phi(x-x_2), \hat{\rho}_t \otimes \hat{\rho}_t]\right\} + \\ & - \int \mathrm{d}z\, [\phi(x-z) - \phi(y-z)]\, \rho_t(x,z)\rho_t(z,y). \end{aligned}$$

Equation (3.5.3) differs from the Hartree equation (2.2.6) because of the presence of the so called “exchange term” which is the main effect of the correlations induced by the Fermi-Dirac statistics (see (2.1.2)). In [19] it has been proven that there exists a fixed time $T > 0$ such that the difference, in a suitable weak sense, between the j-particle marginal associated with the N-particle Wigner function of this system and the solution of the (Hartree) nonlinear Wigner-Liouville equation (3.3.1) is of order $N^{-1} \approx \varepsilon^3$ for any time $t \leq T$, provided that the potential ϕ is real analytic. In other words, all ε^2 corrections come from the difference between the Vlasov equation (1.1.8) and the Hartree equation (2.2.6); hence they are related to the accuracy of the semiclassical approximation in the one-body theory. In particular it is proven that all correlation effects (the main of them is precisely the exchange term) are of order at most $O(\varepsilon^3)$.

We observe that the case of undistinguishable particles (in the sense specified by (2.1.13) and (6.2.4)) and even the bosonic case are crucially different from the fermionic case discussed above. Indeed in these situations the kinetic energy per particle , i.e., $-\frac{1}{2}\varepsilon^2\Delta_{x_k}$ ($k = 1, \ldots, N$), in a cube of size one scales like ε^2 in the ground state. Thus the Hamiltonian of an N-particle system interacting by the potential (2.1) is precisely (2.1.5) because no further scaling is needed. Therefore, there is no reason for considering a joint limit and the problem of realizing the (mean-field) limit $N \to \infty$ uniformly in ε arises quite naturally.

On the other side, even for undistinguishable particles there are models in which the scaling of the potential somewhat leads to define a rescaled Hamiltonian which exhibits an effective Planck constant going to 0 as $N \to \infty$ (as in the fermionic case). These kind of systems are taken into account in [24] (and previously in [8] with the specific scaling $\varepsilon \approx N^{-1/3}$) and an example is provided by systems interacting by Kac potentials defined below.

Example: the Kac potential. Consider a system of N identical bosons of mass $m = 1$ interacting through the (Kac) potential

$$\phi_\lambda(x) = \frac{1}{\lambda}\phi\Big(\frac{x}{\lambda}\Big), \tag{3.5.4}$$

where λ is a large parameter of the same order of N and ϕ is a given smooth potential. The Hamiltonian is:

$$H_N = -\frac{\varepsilon^2}{2}\sum_{k=1}^{N}\Delta_{x_k} + \sum_{1\le k<l\le N}\phi_\lambda(x_k - x_l). \tag{3.5.5}$$

After the rescaling $x = \lambda q$ the Hamiltonian becomes:

$$H_N = -\frac{1}{2}\left(\frac{\varepsilon}{\lambda}\right)^2\sum_{k=1}^{N}\Delta_{q_k} + \frac{1}{\lambda}\sum_{1\le k<l\le N}\phi(q_k - q_l). \tag{3.5.6}$$

Setting $\lambda = N$, and $\varepsilon_{sc} = \frac{\varepsilon}{\lambda} = \frac{\varepsilon}{N}$ we finally get:

$$H_N^{sc} = -\frac{\varepsilon_{sc}^2}{2}\sum_{k=1}^{N}\Delta_{q_k} + \frac{1}{N}\sum_{1\le k<l\le N}\phi(q_k - q_l), \tag{3.5.7}$$

where $\varepsilon_{sc} \approx 1/N \to 0$ as $N \to \infty$.

In [24] it has been proven that in all situations in which $N \to \infty$ entails $\varepsilon \to 0$ (as the case of the Kac potential), which, roughly speaking, are "asymptotically classical", the Vlasov equation is indeed recovered in the limit $N \to \infty$ even when $\varepsilon \to 0$ according to an arbitrary law. For WKB states of the form $\psi(x) = a(x)e^{iS(x)/\varepsilon}$ the result, formulated in terms of weak convergence of j-particles Wigner marginals, is local in time (as one expects from WKB analysis), while by considering suitable mixtures of WKB states, the result holds globally in time. The potential is assumed to be in $\mathcal{C}_b^2(\mathbb{R}^3)$ and the explicit rate of convergence is computed by means of a constructive method.

In [8] the same result had been proven for the specific scaling $\varepsilon \approx N^{-1/3}$ by considering more general initial data but assuming the potential to be analytic. In [8] it was also proven that the solution of the (Hartree) nonlinear Wigner-Liouville equation (3.3.1) converges in $\mathcal{S}'(\mathbb{R}^3 \times \mathbb{R}^3)$ to the solution of the Vlasov equation (1.1.8) as $\varepsilon \to 0$.

4 – Mean-Field limit and Semiclassical Expansion

In this section we describe a different approach in investigating the ε dependence of the error in the mean-field approximation, by using the Wigner formalism. It consists in looking at the semiclassical expansion of the N-particle system and proving that each term of the expansion agrees, in the limit $N \to \infty$, with the corresponding one associated with the Hartree equation (see [29]).

This idea is motivated by the following argument.

In Section 1 we recalled what is established by classical mean-field theory, namely, under suitable assumption on the potential, for any fixed j we have

$$F_N^{(j)}(t) \to (f(t))^{\otimes j}, \quad \text{as} \quad N \to \infty, \tag{4.1}$$

in the weak topology of probability measures, where $F_N^{(j)}(t)$ are the j-particle marginals associated with the solution $F_N(t)$ of the Liouville equation (1.1.5) with a factorized initial datum $f_0^{\otimes N}$ and $f(t)$ is the solution of the Vlasov equation (1.1.8) with initial datum f_0. Thus, (4.1) means that propagation of chaos holds for the classical mean-field model. On the other side, in Section 3 we proved that, under suitable assumptions on the potential and on the initial datum, the following quantum mean-field limit result holds

$$W_{N,j}^{\varepsilon}(t) \to (f^{\varepsilon}(t))^{\otimes j}, \quad \text{as} \quad N \to \infty, \quad L^2 - \text{weakly}, \tag{4.2}$$

where $W_{N,j}^{\varepsilon}(t)$ are the j-particle Wigner marginals associated with the solution $W_N^{\varepsilon}(t)$ of the N-particle Wigner-Liouville equation (3.2.1) with a factorized initial datum $(f_0^{\varepsilon})^{\otimes N}$ and $f^{\varepsilon}(t)$ is the solution of the (Hartree) nonlinear Wigner-Liouville equation (3.3.1) with initial datum f_0^{ε}. Furthermore, we found that the error in approximating $W_{N,j}^{\varepsilon}(t)$ with $(f^{\varepsilon}(t))^{\otimes j}$ is not uniform with respect to ε and diverging when $\varepsilon \to 0$.

As regard to the semiclassical limit $\varepsilon \to 0$, it is known that the N-particle quantum (mean-field) dynamics for sufficiently smooth potentials converges (for fixed N) in a suitable sense to the the N-particle classical (mean-field) evolution (see for example [12], [25]). Moreover, it has also been proven that the Hartree dynamics with smooth interaction, rephrased in the Wigner formalism, is approximated in a suitable sense by the classical Vlasov evolution (see for example [8], [14]).

So that, it seems natural to consider the solution $W_N^{\varepsilon}(t)$ of the N-particle Wigner-Liouville equation (3.2.1) with a suitable factorized initial datum $(f_0^{\varepsilon})^{\otimes N}$ and to look for an asymptotic expansion as

$$f_0^{\varepsilon} = f_0^{(0)} + \varepsilon f_0^{(1)} + \varepsilon^2 f_0^{(2)} + \dots \tag{4.3}$$

implying, for the initial j-particle marginals,

$$W_{N,j}^{\varepsilon}(0) = (f_0^{\varepsilon})^{\otimes j} = (f_0^{(0)})^{\otimes j} + \varepsilon W_{N,j}^{(1)}(0) + \varepsilon^2 W_{N,j}^{(2)}(0) + \dots \tag{4.4}$$

Then, for the time evolved marginals we expect to find an analogous expansion as

$$W^{\varepsilon}_{N,j}(t) = W^{(0)}_{N,j}(t) + \varepsilon W^{(1)}_{N,j}(t) + \varepsilon^2 W^{(2)}_{N,j}(t) + \dots \tag{4.5}$$

where the zero order term $W^{(0)}_{N,j}(t)$ is expected to be equal to the (classical) marginals associated with the solution of the Liouville equation with initial datum $(f_0^{(0)})^{\otimes N}$ determined by (4.3).

In a similar way, we consider the j-fold product $(f^{\varepsilon}(t))^{\otimes j}$ of solutions of the (Hartree) nonlinear Wigner-Liouville equation (3.3.1) with initial datum f_0^{ε} and we look for an expansion as

$$(f^{\varepsilon}(t))^{\otimes j} = f_j^{(0)}(t) + \varepsilon f_j^{(1)}(t) + \varepsilon^2 f_j^{(2)}(t) + \dots \tag{4.6}$$

where the zero order term $f_j^{(0)}$ is expected to be equal to the j-fold product $(f^{(0)}(t))^{\otimes j}$, where $f^{(0)}(t)$ solves the Vlasov equation with initial datum $f_0^{(0)}$ given by (4.3).

Therefore, by recognizing that at zero order in ε we find the classical quantities, by (4.1) we know that $W^{(0)}_{N,j}(t)$ converges to $f_j^{(0)}(t) = (f^{(0)}(t))^{\otimes j}$ in the weak topology of probability measures. Then, it looks natural to ask if the following convergence holds

$$W^{(k)}_{N,j}(t) \to f_j^{(k)}(t)\,, \quad \text{as } N \to \infty, \text{ for any } k > 0 \tag{4.7}$$

in a suitable sense. This is what we are going to show in the present section and it is contained in our recent paper [29].

Note that the term by term convergence (4.7) does not provide the uniformity in ε of the limit $N \to \infty$ because this would require a control of the remainder of the expansion (4.5), and for the moment we are not able to do it. On the other side, in proving (4.7), we provide quantum corrections to the classical mean-field limit result and, by characterizing explicitly both coefficients $W^{(k)}_{N,j}(t)$ and $f_j^{(k)}(t)$, we prove that those corrections are given in terms of the classical Liouville flow and, in particular, of suitable derivatives of the classical trajectories.

We note that to prove (4.7) we make use of coherent states (see Section 4.5) and in that framework it is somewhat expected to find that quantum corrections to the classical dynamics can be expressed in terms of derivatives of the classical trajectories (see for example [2], [15]).

4.1 – Semiclassical expansion for the Hartree dynamics

We want to determine an expansion in power series of ε of the solution $f^\varepsilon(x,v;t)$ of the (Hartree) nonlinear Wigner-Liouville equation (3.3.1) for a given initial datum $f_0^\varepsilon(x,v)$, namely:

$$f^\varepsilon(t) = f^{(0)}(t) + \varepsilon f^{(1)}(t) + \varepsilon^2 f^{(2)}(t) + \dots \tag{4.1.1}$$

by knowing that the initial datum f_0^ε is expanded as follows

$$f_0^\varepsilon(x,v) = f_0^{(0)}(x,v) + \varepsilon f_0^{(1)}(x,v) + \varepsilon^2 f_0^{(2)}(x,v) + \dots \tag{4.1.2}$$

Indeed an expansion like (4.1.2) holds for general quantum states. For example, in [25] the semiclassical expansion for various kinds of states is presented, both gently varying with respect to ε (such as pure states whose wave function is not depending on ε) and singularly behaving as $\varepsilon \to 0$ (such as states of semiclassical type: WKB and coherent states). In the first situation we find an expansion of the form (4.1.2) where the coefficients $f_0^{(k)}$ are smooth, on the contrary, for WKB and coherent states we find distributional coefficients (precisely Dirac δ-functions and suitable derivatives of it) which apparently are more difficult to treat (with respect to the smooth case). Nevertheless, by manipulating them in a suitable way, such kinds of "singular" expansions can be very useful to deal with problems of semiclassical approximation (see Section 4.5 and Section 5).

Following [25], for a fixed g, the operator T_g^ε appearing in equation (3.3.1) can be expanded as

$$T_g^\varepsilon = T_g^{(0)} + \varepsilon T_g^{(1)} + \varepsilon^2 T_g^{(2)} + \dots \tag{4.1.3}$$

where

$$T_g^{(n)} = c_n (2\pi)^{-3} i \int_{\mathbb{R}^3} \mathrm{d}k \hat{\phi}(k) \hat{\rho}_g(k) e^{i\, k\cdot x} (k \cdot \nabla_v)^{n+1}, \tag{4.1.4}$$

$$c_n = \frac{1}{2^n (n+1)!}, \tag{4.1.5}$$

for n even and

$$T_g^{(n)} = 0, \tag{4.1.6}$$

for n odd. The operator $T_g^{(n)}$, for n even, can be also written as

$$T_g^{(n)} = (-1)^{n/2} c_n \left(D_x^{n+1} \phi * g \right) \cdot D_v^{n+1}, \tag{4.1.7}$$

where, as in (1.1.8), $*$ denotes the convolution with respect to both x and v and we used the notation:

$$D_x^n \nu \cdot D_v^n \zeta = \sum_{\substack{n_1,n_2,n_3 \in \mathbb{N}: \\ \sum_j n_j = n}} \frac{\partial^n \nu}{\partial^{n_1} x^1 \partial^{n_2} x^2 \partial^{n_3} x^3} \frac{\partial^n \zeta}{\partial^{n_1} v^1 \partial^{n_2} v^2 \partial^{n_3} v^3}, \tag{4.1.8}$$
$$\text{with} x = (x^1, x^2, x^3) \in \mathbb{R}^3 \text{ and } v = (v^1, v^2, v^3) \in \mathbb{R}^3$$

for the one-particle functions ν and ζ.

Inserting (4.1.1) in (4.1.3) and setting:

$$T_k^{(n)} = T_{f^{(k)}(t)}^{(n)}, \tag{4.1.9}$$

we readily arrive to the following sequence of problems for the coefficients $f^{(k)}(t)$ of the expansion (4.1.1):

$$\begin{cases} (\partial_t + v \cdot \nabla_x) f^{(0)}(t) = T_0^{(0)} f^{(0)}(t), \\ f^{(0)}(x, v; t)\Big|_{t=0} = f_0^{(0)}(x, v), \end{cases} \tag{4.1.10}$$

and

$$\begin{cases} (\partial_t + v \cdot \nabla_x) f^{(k)}(t) = L(f^{(0)}(t)) f^{(k)}(t) + \Theta^{(k)}(t), \\ f^{(k)}(x, v; t)\Big|_{t=0} = f_0^{(k)}(x, v), \end{cases} \tag{4.1.11}$$

for $k \geq 1$, where

$$L(h)f = T_h^{(0)} f + T_f^{(0)} h = (\nabla_x \phi * h) \cdot \nabla_v f + (\nabla_x \phi * f) \cdot \nabla_v h, \tag{4.1.12}$$

and

$$\Theta^{(k)}(t) = \sum_{\substack{l,p,r: \\ l+p+r=k \\ l<k, r<k}} T_r^{(p)} f^{(l)}(t). \tag{4.1.13}$$

Note that, as we expected, equation (4.1.10) we found at zeroth order in ε is precisely the classical Vlasov equation (1.1.8)) associated with the interaction ϕ. Thus we need to assume $\phi \in \mathcal{C}_b^2(\mathbb{R}^3)$ to guarantee that the Vlasov flow is well-defined and, as we recalled in Section 1, the Vlasov equation can be solved by means of characteristics and fixed point. Moreover, the problems (4.1.11) are linear and can be solved by a recursive argument by observing that the source terms $\Theta^{(k)}(t)$ involve only those coefficients $f^{(n)}(t)$ with $n < k$, so that they are known by the previous steps. Clearly we shall state suitable smoothness assumptions on ϕ because the operators $T_r^{(p)}$ appearing in $\Theta^{(k)}(t)$ involve derivatives of ϕ of order possibly higher than 2, depending on k.

Hypotheses H: Here and henceforth we will assume that is spherically symmetric ($\phi(x) = \phi(|x|), \forall x \in \mathbb{R}^3$) and $\phi \in C_b^\infty(\mathbb{R}^3)$(1)

Actually, in some of the results we are going to show less regularity is needed on ϕ, but for the sake of simplicity we state here "maximal" hypotheses under which we can deal both with semiclassical expansions and with the term by term convergence of the N-particle expansion (see Section 4.2 and 4.6 below). Furthermore, under the same hypotheses on ϕ, by taking the initial datum as specified in Section 4.5, we are ensured about the validity of the result proven in Section 3.4 concerning the mean-field limit for Wigner functions.

In order to simplify the notation, from now on we will denote the time evolved coefficients $f^{(k)}(t) = f^{(k)}(x, v; t)$ solving (4.1.11) by $f^{(k)}$ and the source terms $\Theta^{(k)}(x, v; t) = \Theta^{(k)}(t)$ by $\Theta^{(k)}$. Moreover, we will denote the initial coefficients $f_0^{(k)}(x, v)$ by $f_0^{(k)}$. We will specify the dependence on time and on the phase space variables just in case it is not clear from the context.

The crucial tool we shall use to give a sense to the solutions $f^{(k)}$, for $k \geq 1$, of problems (4.1.11) is the following proposition whose proof will be given in Appendix A (see also [29]).

Proposition 4.1.1. *Consider the initial value problem:*

$$\begin{cases} (\partial_t + v \cdot \nabla_x)\, \gamma = L(h)\gamma + \Theta, \\ \gamma(x, v; t)|_{t=0} = \gamma_0(x, v), \end{cases} \tag{4.1.14}$$

where $\gamma_0 \in L^1(\mathbb{R}^3 \times \mathbb{R}^3)$, $h = h(x, v; t)$ *is such that* $|\nabla_v h| \in \mathcal{C}^0(L^1(\mathbb{R}^3 \times \mathbb{R}^3), \mathbb{R}^+)$, $\Theta = \Theta(x, v; t)$ *is such that* $\Theta \in \mathcal{C}^0(L^1(\mathbb{R}^3 \times \mathbb{R}^3), \mathbb{R}^+)$.

Then there exists a unique solution $\gamma = \gamma(x, v; t)$ *of* (4.1.14), *such that* $\gamma \in \mathcal{C}^0(L^1(\mathbb{R}^3 \times \mathbb{R}^3), \mathbb{R}^+)$, *given by an explicit series expansion.*

Furthermore, denoting by Σ_h *the flow generated by* $L(h)$, *we have that* $\Sigma_h(t, 0)\gamma_0 \in \mathcal{C}^d(\mathbb{R}^3 \times \mathbb{R}^3)$ *provided that* $\nabla_v h \in \mathcal{C}^d(\mathbb{R}^3 \times \mathbb{R}^3)$ *and* $\gamma_0 \in \mathcal{C}^d(\mathbb{R}^3 \times \mathbb{R}^3)$.

By looking at the problems (4.1.11), we realize that the coefficients $f^{(k)}$, for $k \geq 1$, play the role of $\gamma(x, v; t)$ in Proposition 4.1.1, while the time evolved zero-order coefficient $f^{(0)}$ and the source term $\Theta^{(k)}$ play the role of the functions $h(x, v; t)$ and $\Theta(x, v; t)$ respectively. Clearly the initial datum $\gamma_0(x, v)$ in this case is given by $f_0^{(k)}(x, v)$, $k \geq 1$.

(1) Here and henceforth we denote by $C_b^\infty(\mathbb{R}^d)$ the space of infinitely differentiable functions on $\mathbb{R}^d$ with uniformly bounded derivatives.

Therefore, by applying Proposition 4.1.1 to identify the coefficients $f^{(k)}$, $k \geq 1$, as the unique solutions of (4.1.11) in $\mathcal{C}^0(L^1(\mathbb{R}^3 \times \mathbb{R}^3), \mathbb{R}^+)$, we have to consider an initial Wigner function $f_0^\varepsilon(x,v)$ such that $f_0^{(k)} \in L^1(\mathbb{R}^3 \times \mathbb{R}^3)$ for $k \geq 1$ and $f_0^{(0)}$ is sufficiently smooth to ensure $f^{(0)}, |\nabla_v f^{(0)}| \in \mathcal{C}^0(L^1(\mathbb{R}^3 \times \mathbb{R}^3), \mathbb{R}^+)$. Concerning the source terms $\{\Theta^{(k)}\}_{k\geq 1}$, we have to prove that, with our choice of the initial datum, $\Theta^{(k)} \in \mathcal{C}^0(L^1(\mathbb{R}^3 \times \mathbb{R}^3), \mathbb{R}^+)$ for $k \geq 1$.

We take the initial Wigner function $f_0^\varepsilon(x,v)$ in such a way that

$$f_0^{(k)} \in \mathcal{S}(\mathbb{R}^3 \times \mathbb{R}^3) \text{ for any } k \geq 0, \tag{4.1.15}$$

in particular $f_0^{(k)} \in L^1(\mathbb{R}^3 \times \mathbb{R}^3)$ for any k. In Section 4.5 and in Section 5 we will give explicit examples of Wigner functions verifying this property (see also [29]). Then, by (4.1.15) we find

$$f^{(0)} \in \mathcal{C}^0\left(\mathcal{S}(\mathbb{R}^3 \times \mathbb{R}^3), \mathbb{R}^+\right) \tag{4.1.16}$$

(because of the smoothness of the Vlasov flow as discussed in Section 1.2) and, in particular

$$|\nabla_v f^{(0)}| \in \mathcal{C}^0\left(\mathcal{C}^\infty \cap L^1(\mathbb{R}^3 \times \mathbb{R}^3), \mathbb{R}^+\right). \tag{4.1.17}$$

As a consequence, from Proposition 4.1.1 we find

$$\begin{aligned} &\Sigma_{f^{(0)}}(t,s) : \mathcal{C}^0\left(\mathcal{C}^\infty \cap L^1(\mathbb{R}^3 \times \mathbb{R}^3), \mathbb{R}^+\right) \to \\ &\to \mathcal{C}^0\left(\mathcal{C}^\infty \cap L^1(\mathbb{R}^3 \times \mathbb{R}^3), \mathbb{R}^+\right) \quad \forall\, s \in [0,t]. \end{aligned} \tag{4.1.18}$$

Moreover, by looking at the series expansion associated with the solution of the homogeneous version of problem (4.1.14) (see Appendix B below and [29]), we realize that

$$\Sigma_{f^{(0)}}(t,s) : \mathcal{C}^0(\mathcal{S}(\mathbb{R}^3 \times \mathbb{R}^3), \mathbb{R}^+) \to \mathcal{C}^0(\mathcal{S}(\mathbb{R}^3 \times \mathbb{R}^3), \mathbb{R}^+) \quad \forall\, s \in [0,t], \tag{4.1.19}$$

provided that $f^{(0)}(t) \in \mathcal{S}(\mathbb{R}^3 \times \mathbb{R}^3)$ for each t and that suitable smoothness assumptions on the potential ϕ are satisfied. In particular, under our assumptions, we are guaranteed that (4.1.19) holds.

As regard to the source terms, from (4.1.13) it is easy to check that $\Theta^{(1)} = 0$ then $f^{(1)}(t) = \Sigma_{f^{(0)}}(t,0) f_0^{(1)} \in L^1(\mathbb{R}^3 \times \mathbb{R}^3)$ for each t by virtue of the fact that $f_0^{(1)} \in \mathcal{S}(\mathbb{R}^3 \times \mathbb{R}^3) \subset L^1(\mathbb{R}^3 \times \mathbb{R}^3)$ and thanks to Proposition 4.1.1. Moreover, by (4.1.19) we have also

$$f^{(1)} \in \mathcal{C}^0(\mathcal{S}(\mathbb{R}^3 \times \mathbb{R}^3), \mathbb{R}^+). \tag{4.1.20}$$

On the contrary, for $k \geq 2$ we have $\Theta^{(k)} \neq 0$ and by (4.1.13), (4.1.5) and (4.1.7) we find that the norm of $\Theta^{(k)}$ $(k \geq 2)$ in $\mathcal{C}^0(L^1(\mathbb{R}^3 \times \mathbb{R}^3), \mathbb{R}^+)$ ($\mathcal{C}^0(L^1)$-norm in the sequel) is bounded by

$$\begin{aligned}
&\sup_{\tau\in[0,t]} \left\|\Theta^{(k)}(\tau)\right\|_{L^1(\mathbb{R}^3\times\mathbb{R}^3)} = \sup_{\tau\in[0,t]} \sum_{\substack{l,p,r:\\ l+p+r=k\\ l<k,r<k}} \left\|T_r^{(p)} f^{(l)}(\tau)\right\|_{L^1(\mathbb{R}^3\times\mathbb{R}^3)} \leq \\
&\leq \sum_{\substack{r,p,l:\\ l+p+r=k\\ l<k,r<k}} c_p \sup_{\tau\in[0,t]} \times \\
&\times \left\{\left\|D_x^{p+1}\phi * f^{(r)}(\tau)\right\|_{L^\infty(\mathbb{R}^3\times\mathbb{R}^3)} \left\|D_v^{p+1} f^{(l)}(\tau)\right\|_{L^1(\mathbb{R}^3\times\mathbb{R}^3)}\right\} \leq \\
&\leq \sum_{\substack{l,p,r:\\ l+p+r=k\\ r<k,l<k}} c_p \left\|D_x^{p+1}\phi\right\|_{L^\infty(\mathbb{R}^3\times\mathbb{R}^3)} \sup_{\tau\in[0,t]} \times \\
&\times \left\{\left\|f^{(r)}(\tau)\right\|_{L^1(\mathbb{R}^3\times\mathbb{R}^3)} \left\|D_v^{p+1} f^{(l)}(\tau)\right\|_{L^1(\mathbb{R}^3\times\mathbb{R}^3)}\right\}.
\end{aligned} \tag{4.1.21}$$

Let us check if it is possible to use a recursive argument to prove that $\Theta^{(k)} \in \mathcal{C}^0(L^1(\mathbb{R}^3 \times \mathbb{R}^3), \mathbb{R}^+)$ (for $k \geq 2$). By (4.1.21) it follows that if we knew that

$$\sup_{\tau\in[0,t]} \left\{\left\|f^{(r)}(\tau)\right\|_{L^1(\mathbb{R}^3\times\mathbb{R}^3)} \left\|D_v^{p+1} f^{(l)}(\tau)\right\|_{L^1(\mathbb{R}^3\times\mathbb{R}^3)}\right\} < +\infty \tag{4.1.22}$$

for each $l, p, r : l+p+r = k$ and $l < k, r < k$, being the potential as in Hypotheses H, we would find that the $\mathcal{C}^0(L^1)$-norm of $\Theta^{(k)}$ is finite and we could conclude that for each $T > 0$:

$$\sup_{t\in[0,T]} \left\|f^{(k)}(t)\right\|_{L^1(\mathbb{R}^3\times\mathbb{R}^3)} < +\infty \quad \forall\, k \geq 2. \tag{4.1.23}$$

Thus, we note that a recursive argument is not "well-posed" because it is not possible to provide a uniform bound for the $\mathcal{C}^0(L^1)$-norm of $f^{(k)}$, by assuming the same to hold for $f^{(n)}$ with $n < k$. Indeed, by (4.1.22), we see that we would need to assume even that the L^1-norm of any derivative of $f^{(n)}$ with $n < k$ is bounded uniformly in time.

On the contrary, we realize that we can use an induction procedure in $\mathcal{C}^0(\mathcal{S}(\mathbb{R}^3 \times \mathbb{R}^3), \mathbb{R}^+)$. Indeed, by the expression of $\Theta^{(k)}$ and by the regularity of ϕ we know that $\Theta^{(k)} \in \mathcal{C}^0(\mathcal{S}(\mathbb{R}^3 \times \mathbb{R}^3), \mathbb{R}^+)$ if all coefficients $f^{(n)}$ up to $n = k-1$

are in $\mathcal{C}^0(\mathcal{S}(\mathbb{R}^3 \times \mathbb{R}^3), \mathbb{R}^+)$. Then, by (4.1.19), we obtain

$$\begin{aligned} & f^{(n)} \in \mathcal{C}^0(\mathcal{S}(\mathbb{R}^3 \times \mathbb{R}^3), \mathbb{R}^+) \quad \text{for all } n < k \\ & \Downarrow \\ & \Theta^{(k)} \in \mathcal{C}^0(\mathcal{S}(\mathbb{R}^3 \times \mathbb{R}^3), \mathbb{R}^+) \\ & \Downarrow \\ & f^{(k)} \in \mathcal{C}^0(\mathcal{S}(R^3 \times \mathbb{R}^3), \mathbb{R}^+), \end{aligned} \tag{4.1.24}$$

and thanks to (4.1.16) and (4.1.20) the induction procedure is “closed”. Therefore, we have well-posedeness of problems (4.1.11) in $L^1(\mathbb{R}^3 \times \mathbb{R}^3)$ and, in particular, the coefficients $f^{(k)}(t)$ are also in $\mathcal{S}(\mathbb{R}^3 \times \mathbb{R}^3)$ for all t. Actually, we could relax our assumption on the initial datum f_0^ε obtaining less smooth coefficients, but in the present context this not an issue because we want to focus on the structure of the expansion and not on minimal regularity properties of the solutions.

4.2 – Semiclassical expansion for the N-particle dynamics

In this section we determine an expansion in power series of ε of the solution $W_N^\varepsilon(t) = W_N^\varepsilon(X_N, V_N; t)$ of the N-particle Wigner-Liouville equation equation (3.2.1) for the factorized initial datum

$$W_{N,0}^\varepsilon(X_N, V_N) = \prod_{j=1}^{N} f_0^\varepsilon(x_j, v_j), \tag{4.2.1}$$

where f_0^ε is the same one-particle Wigner function we chose as initial datum for the nonlinear Wigner-Liouville equation (3.3.1). Thus, we know that f_0^ε is expanded as in (4.1.2) and it turns out that, for the N-fold product $(f_0^\varepsilon)^{\otimes N}$, we find

$$(f_0^\varepsilon)^{\otimes N} = W_{N,0}^{(0)} + \varepsilon W_{N,0}^{(1)} + \varepsilon^2 W_{N,0}^{(2)} + \dots \tag{4.2.2}$$

with

$$W_{N,0}^{(0)}(X_N, V_N) = \prod_{j=1}^{N} f_0^{(0)}(x_j, v_j), \tag{4.2.3}$$

$$W_{N,0}^{(k)}(X_N, V_N) = \sum_{\substack{s_1 \dots s_N \\ 0 \le s_j \le k \\ \sum_j s_j = k}} \prod_{j=1}^{N} f_0^{(s_j)}(x_j, v_j) \quad \text{for } k \ge 1. \tag{4.2.4}$$

Note that $W_{N,0}^{(k)}$ is factorized only for $k = 0$.

For the sake of simplicity, here and henceforth we will make explicit the dependence on time and on the phase space variables only if not clear from the context.

Following [25], the operator T_N^ε appearing in (3.2.1) can be expanded as

$$T_N^\varepsilon = T_N^{(0)} + \varepsilon T_N^{(1)} + \varepsilon^2 T_N^{(2)} + \dots \tag{4.2.5}$$

where, for n even we have

$$T_N^{(n)} = i(2\pi)^{-3N} C_n \int_{\mathbb{R}^{3N}} \mathrm{d}K_N \hat{U}(K_N) e^{iK_N \cdot X_N} \left(K_N \cdot \nabla_{V_N}\right)^{n+1}, \tag{4.2.6}$$

C_n being constants depending on n, and $\hat{U}$ being the Fourier transform of the potential in (2.1) (to simplify the notations we omit the superscript "Q"). For n odd, we find

$$T_N^{(n)} = 0. \tag{4.2.7}$$

Looking for a semiclassical expansion

$$W_N^\varepsilon(t) = W_N^{(0)}(t) + \varepsilon W_N^{(1)}(t) + \varepsilon^2 W_N^{(2)}(t) + \dots, \tag{4.2.8}$$

by (4.2.2), (4.2.6) and (4.2.7) we arrive to the sequence of problems:

$$\begin{cases} \left(\partial_t + V_N \cdot \nabla_{X_N}\right) W_N^{(0)}(t) = T_N^{(0)} W_N^{(0)}(t), \\ W_N^{(0)}(X_N, V_N; t)\Big|_{t=0} = W_{N,0}^{(0)}(X_N, V_N), \end{cases} \tag{4.2.9}$$

and

$$\begin{cases} \left(\partial_t + V_N \cdot \nabla_{X_N}\right) W_N^{(k)}(t) = T_N^{(0)} W_N^{(k)}(t) + \Theta_N^{(k)}(t), \\ W_N^{(k)}(X_N, V_N; t)\Big|_{t=0} = W_{N,0}^{(k)}(X_N, V_N), \end{cases} \tag{4.2.10}$$

for $k \geq 1$, where

$$\Theta_N^{(k)}(t) = \sum_{0 \leq l < k} T_N^{(k-l)} W_N^{(l)}(t). \tag{4.2.11}$$

Note that $T_N^{(0)} = \nabla_{X_N} U_N \cdot \nabla_{V_N} = \frac{1}{N} \sum_{i \neq j}^{N} \nabla_{x_i} \phi(x_i - x_j) \cdot \nabla_{v_i}$ is the classical Liouville operator, while the source terms $\Theta_N^{(k)}(t)$, at each order k, are known by the previous steps. As we recalled in Section 1, under smoothness assumptions on the interaction potential ϕ, equation (4.2.9) can be solved by considering the Hamiltonian flow $\Phi^t(X_N, V_N)$ associated with the Newton equations (1.1.3). Thus we find

$$W_N^{(0)}(X_N, V_N; t) = S_N(t) W_{N,0}^{(0)}(X_N, V_N) = W_{N,0}^{(0)}\left(\Phi^{-t}(X_N, V_N)\right), \tag{4.1.12}$$

where, from now on, we denote by S_N the flow generated by the Liouville operator $T_N^{(0)}$. On the other side, equations (4.2.10) can be solved by recurrence thanks to the Duhamel formula:

$$W_N^{(k)}(t) = S_N(t) W_{N,0}^{(k)} + \int_0^t \mathrm{d}t_1\, S_N(t-t_1)\Theta_N^{(k)}(t_1). \tag{4.2.13}$$

We conclude this section by expressing the operators $T_N^{(n)}$ (n even) in terms of the variables X_N, V_N. From (4.2.6), we find that:

$$T_N^{(n)} = \hat{T}_N^{(n)} + R_N^{(n)}, \tag{4.2.14}$$

where

$$\hat{T}_N^{(n)} = c_n \frac{(-1)^{n/2}}{N} \sum_{l \neq j}^{N} D_x^{n+1} \phi(x_l - x_j) \cdot D_{v_l}^{n+1}, \tag{4.2.15}$$

where c_n is the same of (4.1.5), and

$$R_N^{(n)} = \frac{1}{N} \sum_{l \neq j}^{N} \sum_{\substack{k_1, k_2 \in \mathbb{N}^3 \\ |k_1| + |k_2| = n+1}} C_{k_1,k_2} \frac{\partial^{n+1}}{\partial_{x_l}^{|k_1|} \partial_{x_j}^{|k_2|}} \phi(x_l - x_j) \cdot \frac{\partial^{n+1}}{\partial_{v_l}^{|k_1|} \partial_{v_j}^{|k_2|}}, \tag{4.2.16}$$

where, for $i = 1, 2$, $k_i = (k_{i,1}, k_{i,2}, k_{i,3})$, $|k_i| = k_{i,1} + k_{i,2} + k_{i,3}$, and

$$\begin{gathered} \frac{\partial^{n+1}}{\partial_{x_l}^{|k_1|} \partial_{x_j}^{|k_2|}} = \frac{\partial^{|k_1|}}{\partial^{k_{1,1}} x_l^1 \partial^{k_{1,2}} x_l^2 \partial^{k_{1,3}} x_l^3} \; \frac{\partial^{|k_2|}}{\partial^{k_{2,1}} x_j^1 \partial^{k_{2,2}} x_j^2 \partial^{k_{2,3}} x_j^3}, \\ \text{with } x_j = (x_j^1, x_j^2, x_j^3),\; x_l = (x_l^1, x_l^2, x_l^3), \end{gathered} \tag{4.2.17}$$

while C_{k_1,k_2} are suitable coefficients. The same holds for the derivatives with respect to the velocities.

We observe that, by the expression (4.2.16), we mean that the derivative of order $|k_1|$ is distributed over the three components of x_l in the same way in which it is distributed over the three components of v_l, and the same holds for the derivative of order $|k_2|$.

4.3 – Structure of the j-particles limiting marginals

Let us consider the sequence $\{f_j^\varepsilon(t)\}_{j\geq 1}$, where $f_j^\varepsilon(t) = f_j^\varepsilon(X_j, V_j; t)$ is given by

$$f_j^\varepsilon(t) = (f^\varepsilon(t))^{\otimes j} \tag{4.3.1}$$

and $f^\varepsilon(t)$ is the solution of the nonlinear Wigner-Liouville equation (3.3.1) with initial datum f_0^ε chosen as in Section 4.1. By the one-particle expansion (4.1.1), it turns out that

$$f_j^\varepsilon(t) = (f^\varepsilon(t))^{\otimes j} = f_j^{(0)}(t) + \varepsilon f_j^{(1)}(t) + \varepsilon^2 f_j^{(2)}(t) + \dots, \tag{4.3.2}$$

with

$$f_j^{(0)}(X_j, V_j; t) = \prod_{i=1}^{j} f^{(0)}(x_i, v_i; t) \tag{4.3.3}$$

$$f_j^{(k)}(X_j, V_j; t) = \sum_{\substack{s_1 \dots s_j : \\ 0 \leq s_r \leq k \\ \sum_r s_r = k}} \prod_{r=1}^{j} f^{(s_r)}(x_r, v_r; t) \quad \text{for } k \geq 1, \tag{4.3.4}$$

where the one-particle functions $f^{(s_r)}(x_r, v_r; t)$ solve equation (4.1.10), if $s_r = 0$, and (4.1.11), for $s_r > 0$. Note that $f_j^{(k)}(t)$ is factorized only for $k = 0$.

Thus by (4.3.3) we find that, as expected, the zero order term of the expansion of $(f^\varepsilon(t))^{\otimes j}$ is given by the j-fold product $(f^{(0)}(t))^{\otimes j}$ of solutions of the Vlasov initial value problem (4.1.10).

By the analysis done in Section 3, we know that $\{f_j^\varepsilon(t)\}_{j\geq 1}$ solves the infinite (Hartree) hierarchy (3.3.22) with factorized initial datum $\{(f_0^\varepsilon)^{\otimes j}\}_{j\geq 1}$. On the other hand, the sequence of j-particle marginals $\{W_{N,j}^\varepsilon(t)\}_{j=1}^N$ associated with the solution of the N-particle Wigner-Liouville equation (3.2.1) with factorized initial datum $(f_0^\varepsilon)^{\otimes N}$, solves the Wigner BBGKY hierarchy (3.2.6) with initial datum $\{(f_0^\varepsilon)^{\otimes j}\}_{j=1}^N$. Moreover, in Section 3 we proved also that, for any j, $W_{N,j}^\varepsilon(t) \to (f^\varepsilon(t))^{\otimes j}$ L^2-weakly as $N \to \infty$ and the error in approximating the N-particle dynamics with the limiting one is not uniform with respect to ε and diverging as $\varepsilon \to 0$. We recall that the reason for that arises from the fact that the operator $T_{N,j}^\varepsilon$ involved in the BBGKY hierarchy (3.2.6) is bounded in the norm appropriate to study the convergence (namely $\tilde{L}^1(\mathbb{R}^{3j} \times \mathbb{R}^{3j})$ or $L^1(\mathbb{R}^{3j} \times \mathbb{R}^{3j})$), but its norm is diverging when ε goes to zero (in particular it is $O(1/\varepsilon)$). This suggests to consider the semiclassical equations described in Sections 4.1 and 4.2. In this way, considering equations at each order in ε and analyzing the hierarchies associated with each of those equation, we have to deal with operators which are clearly independent of ε (e.g. $T_N^{(n)}$), , and we have to investigate only the limit $N \to \infty$ without any dependence on ε. The price we have to pay is that now those operators are unbounded, as it comes out for the classical mean-field limit we faced in Section 1.

Thus, if we want to prove that the coefficient of order ε^k of the expansion of the j-particle marginals $W^{\varepsilon}_{N,j}(t)$, namely:

$$W_{N,j}^{(k)}(X_j, V_j; t) = \int_{\mathbb{R}^{3(N-j)} \times \mathbb{R}^{3(N-j)}} \mathrm{d}X_{N-j} \mathrm{d}V_{N-j} W_N^{(k)}(X_j, X_{N-j}, V_j, V_{N-j}; t), \tag{4.3.5}$$

converges to the corresponding object $f_j^{(k)}(t)$ arising from the Hartree dynamics (i.e (4.3.4)), the use of the hierarchy solved by $W_{N,j}^{(k)}(t)$ does not seem a good idea. In fact, even at level zero, when we have to deal with the classical mean-field limit, the hierarchy is very difficult to handle with (see Section 1.4) because it involves derivation operators which are clearly unbounded, unless to make them act on analytic functions (see (1.4.3)-(1.4.5)). The obstacle which occurs in facing the higher order terms is precisely the same.

However, as we saw in Section 1, in the classical case we can treat the convergence in a more natural way, avoiding to use the hierarchy. Indeed we can control the j-particle marginals associated with the Liouville equation (1.1.5) in terms of the expectation of the j-fold product of empirical measures with respect to the initial N-particle probability distribution (see Section 1.4). Then, to use this strategy to establish the convergence of $W_{N,j}^{(0)}(t)$ to $(f^{(0)}(t))^{\otimes j}$, we have to choose the one-particle initial Wigner function f_0^{ε} in such a way that the zeroth order coefficient $f_0^{(0)}$ is a one-particle probability distribution. As a consequence, the (factorized) zeroth order coefficient $W_{N,0}^{(0)}$ (4.2.3) of the N-particle expansion is also a probability distribution (we will discuss this choice in Section 4.5). Then, we will follow a similar strategy in dealing with the convergence of the higher order terms of the expansion. More precisely, we will express $W_{N,j}^{(k)}(t)$ in terms of the expectation, with respect to $W_{N,0}^{(0)}$, of suitable (derivation) operators acting on empirical measures. The control of these objects will be obtained thanks to some estimates of the derivatives of the classical flow with respect to the initial data (see Proposition 4.4.1).

4.4 – Idea of the proof

As we already noticed in the previous section, the convergence of the j-particle marginal at zeroth order in ε is ensured by our assumption on the initial datum (to be specified in Section 4.5) and by the classical mean-field theory.

Thus, the first non-trivial term is that of order one in ε. By looking at (4.1.11) for $k = 1$, we realize that the first correction to the Vlasov equation in the Hartree dynamics satisfies

$$\begin{cases} (\partial_t + v \cdot \nabla_x) f^{(1)} = L(f^{(0)}) f^{(1)}, \\ f^{(1)}(x, v; t)\Big|_{t=0} = f_0^{(1)}(x, v), \end{cases} \tag{4.4.1}$$

(looking at the expression (4.1.13) for the source terms $\Theta^{(k)}$, we straightforward verify that $\Theta^{(1)} \equiv 0$). As we shall see in detail in the following section, our choice for the initial one-particle datum is a mixture of coherent states such that each coefficient of the expansion is given by suitable derivatives of the zeroth order term which, as we already observed, is a probability distribution. In particular, the explicit form for $f_0^{(1)}$ is:

$$f_0^{(1)}(x, v) = D_G^2 f_0^{(0)}(x, v), \tag{4.4.2}$$

where D_G^2 is a suitable second order derivation operator (see formula (4.5.8) below in the case $k = 2$) with respect to the variable $z \in \mathbb{R}^6$ (we recall the notation $z = (x, v) \in \mathbb{R}^3 \times \mathbb{R}^3$ introduced in Section 1).

As regard to the N-particle dynamics, looking at (4.2.4) in the case $k = 1$, we know that the initial datum for the coefficient of order one in ε is:

$$W_{N,0}^{(1)}(Z_N) = \sum_{j=1}^{N} f_0^{(1)}(z_j) \prod_{l \neq j}^{N} f_0^{(0)}(z_l) = \mathcal{D}^2 W_{N,0}^{(0)}(Z_N), \tag{4.4.3}$$

where

$$\mathcal{D}^2 = \sum_{j=1}^{N} D_{G,j}^2, \tag{4.4.4}$$

and $D_{G,j}^2$ is the operator D_G^2 acting on the variable $z_j \in \mathbb{R}^6$. Let us consider the time evolved empirical measure $\mu_N(t)$ (see Section 1.3) associated with the flow generated by the Newton equations (1.1.3) and let us define $\mathcal{D}^2 \mu_N(t)$ as the distribution acting on a test function u in the following way:

$$(u, \mathcal{D}^2 \mu_N(t)) = \mathcal{D}^2 \left(\frac{1}{N} \sum_{l=1}^{N} u(z_l(t)) \right) = \frac{1}{N} \sum_{l,j=1}^{N} D_{G,j}^2 u(z_l(t)). \tag{4.4.5}$$

We know that the operators $D_{G,j}^2$ involve derivatives with respect to the initial variables z_j, $j = 1, \dots, N$, thus, if at time $t = 0$ we have $\mu_N \to f_0^{(0)}$ when $N \to \infty$ in the weak sense of probability measures, it follows that:

$$\begin{aligned} \left(u, \mathcal{D}^2 \mu_N\right) = \mathcal{D}^2 \frac{1}{N} \sum_{l=1}^{N} u(z_l) = \frac{1}{N} \sum_{l,j=1}^{N} D_{G,j}^2 u(z_l) = \frac{1}{N} \sum_{j=1}^{N} D_{G,j}^2 u(z_j) = \\ = (D_G^2 u, \mu_N) \to (D_G^2 u, f_0^{(0)}) = (u, D_G^2 f_0^{(0)}) = (u, f_0^{(1)}) \end{aligned} \tag{4.4.6}$$

as $N \to \infty$.

By the Strong Law of Large Numbers (1.3.10) we know that the convergence (4.4.6) holds a.e with respect to the product measure $(f_0^{(0)})^{\otimes\infty}$, then, by (4.4.3) and (4.4.6), we can conclude that:

$$(u, W_{N,1}^{(1)}(t)|_{t=0}) = \left(u, \mathbb{E}_N\left[\mathcal{D}^2\mu_N\right]\right) \to (u, f_0^{(1)})\text{as } N \to \infty, \tag{4.4.7}$$

where $\mathbb{E}_N[cdot]$ denotes the expectation with respect to the N-particle probability distribution $W_{N,0}^{(0)} = (f_0^{(0)})^{\otimes N}$ (see (4.2.3)).

In the sequel, as in Section 1, we will say that a configuration Z_N is "typical" with respect to the probability measure $f_0^{(0)}$, if the corresponding empirical measure $\mu_N(z|Z_N)$ converges to $f_0^{(0)}$ in the weak topology of probability measures.

By equation (4.2.10) for $k = 1$, we have:

$$\begin{gathered}(\partial_t + V_N \cdot \nabla_{X_N})\, W_N^{(1)} = \nabla_{X_N} U \cdot \nabla_{V_N} W_N^{(1)},\\ W_N^{(1)}(Z_N;t)|_{t=0} = W_{N,0}^{(1)}(Z_N),\end{gathered} \tag{4.4.8}$$

namely, the classical Liouville equation (1.1.5), where, to simplify the notation, we omitted the superscript "*cl*". Therefore:

$$W_N^{(1)}(Z_N;t) = S_N(t) W_{N,0}^{(1)}(Z_N). \tag{4.4.9}$$

Finally, by virtue of (4.4.9) and (4.4.3), we obtain

$$\begin{aligned}(u, W_{N,1}^{(1)}(t)) &= \int_{\mathbb{R}^{3N}\times\mathbb{R}^{3N}} \mathrm{d}Z_N S_N(t) W_{N,0}^{(1)}(Z_N)(u,\mu_N) =\\ &= \int_{\mathbb{R}^{3N}\times\mathbb{R}^{3N}} \mathrm{d}Z_N W_{N,0}^{(1)}(Z_N)(u,\mu_N(t)) =\\ &= \int_{\mathbb{R}^{3N}\times\mathbb{R}^{3N}} \mathrm{d}Z_N \mathcal{D}^2 W_{N,0}^{(0)}(Z_N)(u,\mu_N(t)) =\\ &= \int_{\mathbb{R}^{3N}\times\mathbb{R}^{3N}} \mathrm{d}Z_N W_{N,0}^{(0)}(Z_N)(u,\mathcal{D}^2\mu_N(t)) =\\ &= \left(u, \mathbb{E}_N\left[\mathcal{D}^2\mu_N(t)\right]\right).\end{aligned} \tag{4.4.10}$$

Therefore, the behavior of $W_{N,1}^{(1)}(t)$ is determined by that of $\mathcal{D}^2\mu_N(t)$ for any initial configuration Z_N which is typical with respect to $f_0^{(0)}$. Finally, since $\mu_N(t)$ solves the Vlasov equation in the weak form (see Section 1):

$$\begin{cases}(\partial_t + v\cdot\nabla_x)\,\mu_N(t) = (\nabla\phi * \mu_N(t))\cdot\nabla_v\mu_N(t)\\ \mu_N(t)|_{t=0} = \mu_N,\end{cases} \tag{4.4.11}$$

applying $\mathcal{D}^2$, we get:

$$\begin{cases} (\partial_t + v\cdot\nabla_x)\,\mathcal{D}^2\mu_N(t) = L\left(\mu_N(t)\right)\mathcal{D}^2\mu_N(t) + R_N, \\ \mathcal{D}^2\mu_N(t)\big|_{t=0} = \mathcal{D}^2\mu_N, \end{cases} \tag{4.4.12}$$

where R_N is a term involving objects of the form $\sum_j (D_{G,j}\mu_N(t))(D_{G,j}\mu_N(t))$ which, as we shall see later, are of order $1/N$ when tested versus smooth functions. The equation (4.4.12) is similar to (4.4.1), except for the presence of the term R_N and for the fact that we have $L\left(\mu_N(t)\right)$ instead of $L\left(f^{(0)}\right)$. Therefore, the proof of the convergence of $W^{(1)}_{N,1}(t)$ to $f^{(1)}(t)$ reduces to that of a stability property for the solution of (4.4.1) with respect to suitable weak topologies. Proposition 4.5.1 in the forthcoming Section 4.5 will provide us such property.

The general case $k>1$ is only technically more complicated because of the presence of source terms, but the main ideas are those presented here.

Remark 4.4.1. By looking at the strategy of the proof for $k=1$ we realize that the basic idea is to apply the classical mean-field theory at suitable derivatives of the empirical measure. Therefore, if in the classical framework we have to deal with convergence with respect to the weak topology of probability measures, namely, with continuous and uniformly bounded test functions, now we need to deal with test functions whose derivatives are also continuous and uniformly bounded (e.g (4.4.6)). Therefore we can argue that we will establish the term by term convergence in a suitable distributional sense.

We conclude by establishing a Proposition controlling the size of the derivatives of the Hamilton flow associated with (1.1.3) with respect to the initial data.

From now on we shall denote by C a positive constant, independent of N, possibly changing from line to line.

Proposition 4.4.1. *Let $z_i(t) = (x_i(t), v_i(t))\,,\ i = 1,\dots,N$ be the solution of equations* (1.1.3) *with initial datum $z_i = (x_i, v_i)\,,\ i = 1,\dots,N$. Let $z_i^\beta\ \forall\,\beta = 1,\dots,6$ be the β-th component of $z_i \in \mathbb{R}^6$. If the pair interaction potential ϕ is assumed to satisfy Hypotheses H, then, for each $k\in\mathbb{N}$:*

$$\left|\frac{\partial^k z_i^\beta(t)}{\partial z_{j_1}^{\alpha_1}\dots\partial z_{j_k}^{\alpha_k}}\right| \le \frac{C}{N^{d_k^{(i)}}}, \tag{4.4.13}$$

where $I := (j_1,\dots,j_k)$ is any sequence of possibly repeated indices and $d_k^{(i)}$ is the number of different indices in I which are also different from i.

The physical significance of (4.4.13) is obvious. In the mean-field context, the quantity $z_i(t)$ depends weakly on z_j if $j \neq i$ for each $t > 0$. Actually $\frac{\partial z_i^\beta(t)}{\partial z_j^\alpha} = O\left(\frac{1}{N}\right)$ while $\frac{\partial z_i^\beta(t)}{\partial z_i^\alpha} = O(1)$ and these two estimates give rise to (4.4.13) in the case $k = 1$. Estimate (4.4.13) says that for each derivative of any order with respect to some z_j of $z_i(t)$, we gain a factor $1/N$. We have also the following corollary whose straightforward proof will be omitted.

Corollary 4.1.1. *Let $\mathcal{U} = \mathcal{U}(Z_N(t))$ be a function of the time evolved configuration $Z_N(t)$ of the form:*

$$\mathcal{U}(Z_N(t)) = \frac{1}{N}\sum_{i=1}^{N} u(z_i(t)),$$

where $u \in C_b^\infty(\mathbb{R}^3 \times \mathbb{R}^3)$. Then, if the pair interaction potential ϕ satisfies Hypotheses H, the following estimate holds:

$$\left|\frac{\partial^k \mathcal{U}(Z_N(t))}{\partial z_{j_1}^{\alpha_1} \dots \partial z_{j_k}^{\alpha_k}}\right| \leq \frac{C}{N^{d_k}}, \tag{4.4.14}$$

where d_k is the number of different indices in the sequence $I = (j_1, \dots, j_k)$.

The proof of Proposition 4.4.1 will be given in Appendix A.

4.5 – Results and technical preliminaries

We choose, as initial condition for the one-particle Wigner function, a mixture of coherent states. The Wigner function associated with a pure coherent state centered at the point (x_0, v_0) is given by:

$$w(x, v|x_0, v_0) = \frac{1}{(\pi\varepsilon)^3} e^{-\frac{(x-x_0)^2}{\varepsilon}} e^{-\frac{(v-v_0)^2}{\varepsilon}}. \tag{4.5.1}$$

Let now $g = g(x, v)$ be a smooth probability density on the one-particle phase space independent of ε (see Hypotheses H^1 below). Then we define:

$$f_0^\varepsilon(x, v) = \int_{\mathbb{R}^3\times\mathbb{R}^3} \mathrm{d}x_0 \mathrm{d}v_0 \; w(x, v|x_0, v_0) g(x_0, v_0). \tag{4.5.2}$$

Using the standard notation $z = (x, v)$ and $z_0 = (x_0, v_0)$, (4.5.2) is equivalent to:

$$f_0^\varepsilon(z) = \frac{1}{(\pi\varepsilon)^3} \int_{\mathbb{R}^6} \mathrm{d}z_0 \; e^{-\frac{(z-z_0)^2}{\varepsilon}} g(z_0) = \frac{1}{(\pi)^3} \int_{\mathbb{R}^6} \mathrm{d}\zeta e^{-\zeta^2} g(z - \sqrt{\varepsilon}\zeta). \tag{4.5.3}$$

Expanding

$$
(4.5.4)\qquad \begin{aligned} g(z-\sqrt{\varepsilon}\zeta) &= g(z) - (\zeta\cdot\nabla_z)\, g(z)\sqrt{\varepsilon} + (\zeta\cdot\nabla_z)^2\, g(z)\frac{(\sqrt{\varepsilon})^2}{2} + \\ &+ \cdots - (\zeta\cdot\nabla_z)^{2n-1}\, g(z)\frac{(\sqrt{\varepsilon})^{2n-1}}{(2n-1)!} + (\zeta\cdot\nabla_z)^{2n}\, g(z)\frac{(\sqrt{\varepsilon})^{2n}}{(2n)!} + \dots, \end{aligned}
$$

and performing the gaussian integrations (which cancels the terms with the odd powers of $\sqrt{\varepsilon}$), we readily arrive to the following expansion for the Wigner function f_0^ε:

$$
(4.5.5)\qquad f_0^\varepsilon = f_0^{(0)} + \varepsilon f_0^{(1)} + \cdots + \varepsilon^n f_0^{(n)} + \dots,
$$

where

$$
(4.5.6)\qquad f_0^{(0)} = g,
$$

$$
(4.5.7)\qquad f_0^{(n)} = D_G^{2n} f_0^{(0)} \quad \text{for } n \geq 1,
$$

and D_G^k (G stands for "Gaussian"), for each $k > 0$, is the following derivation operator with respect to the variable $z = (x, v)$:

$$
(4.5.8)\qquad D_G^k = \sum_{\substack{\alpha_1\dots\alpha_k:\\ \alpha_j=1,\dots,6}} C_G(\alpha_1\dots\alpha_k)\frac{\partial^k}{\partial z^{\alpha_1}\dots\partial z^{\alpha_k}},
$$

where

$$
(4.5.9)\qquad C_G(\alpha_1\dots\alpha_k) = \frac{1}{k!}\int_{\mathbb{R}^6} \mathrm{d}\zeta\, e^{-\zeta^2}\prod_{j=1}^{k}\zeta^{\alpha_j}.
$$

Therefore, $C_G(\alpha_1\dots\alpha_k)$ is equal to zero for each sequence $\alpha_1\dots\alpha_k$ in which at least one index appears an odd number of times.

Hypotheses $\mathbf{H}^1$:

We assume that $g = f_0^{(0)} \in \mathcal{S}(\mathbb{R}^3\times\mathbb{R}^3)$, thus (4.5.7) make sense for any $n \geq 1$ and, in particular, $f_0^{(n)} \in \mathcal{S}(\mathbb{R}^3\times\mathbb{R}^3)$ for any n. By the analysis done in Section 4.1, this allows to identify the time-evolved coefficients $f^{(n)}(t)$, $n \geq 1$, as the unique solutions of the initial value problems (4.1.11).

Remark 4.5.1. Here we consider a completely factorized N-particle initial state (see (4.2.1)), then property (3.2.4) is satisfied. Furthermore the one-particle state is a mixture and this automatically excludes the Bose statistics.

REMARK 4.5.2. We made the choice to expand fully the initial state f_0^ε according to equation (4.5.5). Another possibility is to assume the (ε dependent) state f_0^ε (which is a probability measure in the present case) as initial condition for the Vlasov problem and, consequently, $f_0^{(k)} = 0$ for the problems (4.1.11). Now the coefficients $f^{(k)}(t)$ are ε dependent but this does not change deeply our analysis because f_0^ε is smooth, uniformly in ε.

As we explained at the beginning of the present Section, our goal is to compare the j-particle semiclassical expansion associated with the N-particle flow, namely $W_{N,j}^{(k)}(t)$, $k = 0, 1, 2, \dots$, with the corresponding coefficients $f_j^{(k)}(t)$ of the expansion:

$$f_j^\varepsilon(t) = f_j^{(0)}(t) + \varepsilon f_j^{(1)}(t) + \cdots + \varepsilon^k f_j^{(k)}(t) + \dots, \tag{4.5.10}$$

where $f_j^{(k)}(t)$ is given by (4.3.4). The main result is the following.

THEOREM 4.5.1. *Let us consider the (Hartree) nonlinear Wigner-Liouville equation* (3.3.1) *as in* (4.5.2) *where the probability distribution g satisfies Hypotheses H^1. Moreover, let us consider the N-particle Wigner-Liouville equation* (3.2.1) *with factorized initial datum as in (4.2.1). If the pair interaction potential ϕ is assumed to verify Hypotheses H, for all $t > 0$, for any integers k and j, the following limit holds in $\mathcal{S}'(\mathbb{R}^{3j} \times \mathbb{R}^{3j})$:*

$$W_{N,j}^{(k)}(t) \to f_j^{(k)}(t). \tag{4.5.11}$$

as $N \to \infty$.

REMARK 4.5.3. As we shall see in the sequel, the convergence (4.5.11) is slightly stronger than the convergence in $\mathcal{S}'(\mathbb{R}^{3j} \times \mathbb{R}^{3j})$. Indeed, the sequence $W_{N,j}^{(k)}(t)$ converges also when it is tested on functions in $\mathcal{C}_b^\infty(\mathbb{R}^{3j} \times \mathbb{R}^{3j})$. Such kind of convergence, which is natural in the present context, will be called $\mathcal{C}_b^\infty$-weak convergence.

A crucial tool in proving Theorem 4.5.1 is provided by the following

PROPOSITION 4.5.1. *Let $\gamma_N(x, v; t)$ be a sequence in $\mathcal{S}'(\mathbb{R}^3 \times \mathbb{R}^3)$ (for each t) satisfying:*

$$\begin{cases} (\partial_t + v \cdot \nabla_x)\, \gamma_N = L(h_N)\gamma_N + \Theta_N, \\ \gamma_N(x, v; t)|_{t=0} = \gamma_{N,0}(x, v), \end{cases} \tag{4.5.12}$$

where $\gamma_{N,0}$, Θ_N are sequences in $\mathcal{S}'(\mathbb{R}^3 \times \mathbb{R}^3)$.

We assume that:

i) $h_N(x,v;t)$ *is a sequence of probability measures converging, as* $N\to\infty$, *to a measure* $h(t)\mathrm{d}x\mathrm{d}v$ *with a density* $h(t)\in\mathcal{C}_b^\infty(\mathbb{R}^3\times\mathbb{R}^3)$ *and such that* $|\nabla_v h|\in\mathcal{C}^0(L^1(\mathbb{R}^3\times\mathbb{R}^3),\mathbb{R}^+)$.

ii) *for all* u_1,u_2 *in* $\mathcal{C}_b^\infty(\mathbb{R}^3\times\mathbb{R}^3)$, *there exists a constant* $C=C(u_1,u_2)>0$, *not depending on* N, *such that:*

$$\|u_1*(u_2\gamma_N)\|_{L^\infty(\mathbb{R}^3\times\mathbb{R}^3)}<C<+\infty \quad \textit{for any } t. \tag{4.5.13}$$

iii) $\gamma_{N,0}\to\gamma_0$, *as* $N\to\infty$, $\mathcal{C}_b^\infty$*-weakly* , $\gamma_0=\gamma_0(x,v)$ *is a function belonging to* $L^1(\mathbb{R}^3\times\mathbb{R}^3)$.

iv) $\Theta_N\to\Theta$, *as* $N\to\infty$, $\mathcal{C}_b^\infty$*-weakly* , $\Theta=\Theta(x,v;t)$ *is a function belonging to* $\mathcal{C}^0(L^1(\mathbb{R}^3\times\mathbb{R}^3),\mathbb{R}^+)$.

Then:

$$\gamma_N\to\gamma, \textit{ as } \quad N\to\infty \quad \mathcal{C}_b^\infty\textit{-weakly}, \tag{4.5.14}$$

where γ *is the unique solution of the problem (4.1.14) in* $\mathcal{C}^0(L^1(\mathbb{R}^3\times\mathbb{R}^3),\mathbb{R}^+)$.

For the proof, see Appendix B.

4.6 – Convergence

This section is devoted to the proof of Theorem 4.5.1.

By (4.2.13) and (4.2.11), for $k\geq 0$ we have:

$$\begin{aligned} W_N^{(k)}(Z_N;t) = \sum_{n\geq 0}\sum_{r=0}^{k} \sum_{\substack{r_1\ldots r_n:\\ r_j>0\\ \sum r_j=k-r}} \int_0^t \mathrm{d}t_1\int_0^{t_1}\mathrm{d}t_2\cdots\int_0^{t_{n-1}}\mathrm{d}t_n\times\\ \times S_N(t-t_1)T_N^{(r_1)}S_N(t_1-t_2)\ldots T_N^{(r_n)}S_N(t_n)W_{N,0}^{(r)}(Z_N).\end{aligned} \tag{4.6.1}$$

It is useful to remind that, the only non-vanishing terms in (4.6.1) are those for which all $r_1,\ldots,r_n$ are even (because the odd terms in the expansion for the operator T_N^ε appearing in (3.2.1) are vanishing (see (4.2.7)).

According to (4.2.4) and (4.5.7),

$$W_{N,0}^{(r)}(Z_N) = \sum_{\substack{s_1\ldots s_N\\ 0\leq s_j\leq r\\ \sum_j s_j=r}} \prod_{j=1}^{N}\left(D_{G,j}^{2s_j}f_0^{(0)}(z_j)\right), \tag{4.6.2}$$

where $D^k_{G,j}$ is defined in (4.5.8) and the extra symbol j means that this operator acts on the variable z_j. Defining the operator $\mathcal{D}^{2r}$ as:

$$\mathcal{D}^0 = \mathbb{1},$$

$$\mathcal{D}^{2r} = \sum_{\substack{s_1\dots s_N:\\ 0\le s_j\le r\\ \sum_j s_j=r}} \prod_{j=1}^{N} D^{2s_j}_{G,j}, \quad r\ge 1, \tag{4.6.3}$$

we have:

$$W^{(r)}_{N,0}(Z_N) = \mathcal{D}^{2r} W^{(0)}_{N,0}(Z_N) \quad \forall\, r\ge 0. \tag{4.6.4}$$

In order to investigate the behavior of the j-particle functions $W^{(k)}_{N,j}(Z_j;t)$ when $N\to\infty$, we consider the following object, for a given configuration $Z'_j = (z'_1\dots z'_j)$:

$$\omega^{(k)}_{N,j}(Z'_j;t) = \int_{\mathbb{R}^{6N}} \mathrm{d}Z_N\, W^{(k)}_N(Z_N;t)\mu_N(z'_1|Z_N)\dots\mu_N(z'_j|Z_N). \tag{4.6.5}$$

In the end of the section, we will show that (4.6.5) is asymptotically equivalent to $W^{(k)}_{N,j}(Z'_j;t)$.

From (4.6.1), (4.6.4) and (4.6.5), it follows that:

$$\begin{aligned}\omega^{(k)}_{N,j}(Z'_j;t) = &\sum_{n\ge0}\sum_{r=0}^{k} \sum_{\substack{r_1\dots r_n:\\ r_j>0\\ \sum r_j=k-r}} \int_0^t \mathrm{d}t_1 \int_0^{t_1}\mathrm{d}t_2\cdots\int_0^{t_{n-1}}\mathrm{d}t_n\times\\ &\times\int_{\mathbb{R}^{6N}} \mathrm{d}Z_N \mu_{N,j}(Z'_j|Z_N) S_N(t-t_1) T^{(r_1)}_N S_N(t_1-t_2)\dots\\ &\dots T^{(r_n)}_N S_N(t_n)\mathcal{D}^{2r} W^{(0)}_{N,0}(Z_N),\end{aligned} \tag{4.6.6}$$

where

$$\mu_{N,j}(Z'_j|Z_N) = \mu_N(z'_1|Z_N)\dots\mu_N(z'_j|Z_N). \tag{4.6.7}$$

Integrating by parts, reminding that each r_j is even and that each $T^{(r_j)}_N$ involves derivatives of order r_j+1, we have:

$$\begin{aligned}\omega^{(k)}_{N,j}(Z'_j;t) = &\sum_{n\ge0}(-1)^n \sum_{r=0}^{k} \sum_{\substack{\underline{\mathbf{r}}_n:\ r_j>0\\ |\underline{\mathbf{r}}_n|=k-r}} \int_{ord}^{t} \mathrm{d}\underline{\mathbf{t}}_n\times\\ &\times \mathbb{E}_N\left[\mathcal{D}^{2r} T^{(r_n)}_N(t_n) T^{(r_{n-1})}_N(t_{n-1})\dots T^{(r_1)}_N(t_1)\mu_{N,j}(Z'_j|Z_N(t))\right],\end{aligned} \tag{4.6.8}$$

where $\underline{\mathbf{r}}_n$ is the sequence of positive integers $r_1, \dots, r_n$, $|\underline{\mathbf{r}}_n| = \sum_{j=1}^n r_j$ and $Z_N(t)$ is the Hamiltonian flow associated with (1.1.3). Moreover $\underline{\mathbf{t}}_n = t_1 \dots t_n$ and $\int_{ord}^t \mathrm{d}\underline{\mathbf{t}}_n$ denotes the integral over he simplex $0 < t_n < t_{n-1} < \dots < t_1 < t$. Finally, $\mathbb{E}_N$ stands for the expectation with respect to the N-particle density $W_{N,0}^{(0)}$ and

$$T_N^{(r)}(t) = S_N(-t) T_N^{(r)} S_N(t). \tag{4.6.9}$$

Therefore, the objects we have to investigate in the limit $N \to \infty$ are:

$$\nu_j^{(k)}(Z_j'; t) = \sum_{n \geq 0} (-1)^n \sum_{r=0}^k \sum_{\substack{\underline{\mathbf{r}}_n : r_j > 0 \\ |\underline{\mathbf{r}}_n| = k - r}} \int_{ord}^t \mathrm{d}\underline{\mathbf{t}}_n \eta_j(Z_j'; t, r, \underline{\mathbf{r}}_n, \underline{\mathbf{t}}_n, Z_N), \tag{4.6.10}$$

(for any configuration Z_N, typical with respect to $f_0^{(0)}$), where η_j is given by:

$$\begin{aligned} \eta_j(Z_j'; t, r, \underline{\mathbf{r}}_n, \underline{\mathbf{t}}_n, Z_N) = \mathcal{D}^{2r} T_N^{(r_n)}(t_n) T_N^{(r_{n-1})}(t_{n-1}) \dots \\ \dots T_N^{(r_1)}(t_1) \mu_{N,j}(Z_j' | Z_N(t)). \end{aligned} \tag{4.6.11}$$

Note that:

$$\nu_j^{(0)}(Z_j'; t) = \mu_{N,j}(Z_j' | Z_N(t)). \tag{4.6.12}$$

We start by analyzing the behavior of $\nu_j^{(k)}$ in the cases $j = 1, 2$, thus we are lead to consider:

$$\begin{aligned} \eta_1(z_1'; t, r, \underline{\mathbf{r}}_n, \underline{\mathbf{t}}_n, Z_N) = \mathcal{D}^{2r} T_N^{(r_n)}(t_n) T_N^{(r_{n-1})}(t_{n-1}) \dots \\ \dots T_N^{(r_1)}(t_1) \mu_N(z_1' | Z_N(t)), \end{aligned} \tag{4.6.13}$$

and

$$\begin{aligned} \eta_2(z_1', z_2'; t, r, \underline{\mathbf{r}}_n, \underline{\mathbf{t}}_n, Z_N) = \mathcal{D}^{2r} T_N^{(r_n)}(t_n) T_N^{(r_{n-1})}(t_{n-1}) \dots \\ \dots T_N^{(r_1)}(t_1) \mu_{N,2}(Z_2' | Z_N(t)). \end{aligned} \tag{4.6.14}$$

It is useful to stress that the operators $T_N^{(r_j)}(t_j)$ $(j = 1, \dots, n)$ and $\mathcal{D}^{2r}$ act as suitable distributional derivatives with respect to the variables Z_N. To evaluate η_1, let us first analyze the action of $T_N^{(r)}(\tau)$. By (4.6.9) and (4.2.14), for any function $G = G(Z_N)$, we have:

$$\begin{aligned} \left(T_N^{(r)}(\tau) G\right)(Z_N) &= S_N(-\tau)(\hat{T}_N^{(r)} + R_N^{(r)})(S_N(\tau) G)(Z_N) = \\ &= (-1)^{r/2} \frac{c_r}{N} \sum_{j,l} S_N(-\tau) D_x^{r+1} \phi(x_j - x_l) \cdot D_{v_j}^{r+1}(S_N(\tau) G)(Z_N) + \\ &+ \frac{1}{N} \sum_{l,j=1}^N \sum_{\substack{k_1, k_2 \in \mathbb{N}^3 \\ |k_1| + |k_2| = r+1}} C_{k_1,k_2} S_N(-\tau) \times \\ &\times \frac{\partial^{r+1}}{\partial_{x_l}^{|k_1|} \partial_{x_j}^{|k_2|}} \phi(x_l - x_j) \cdot \frac{\partial^{r+1}}{\partial_{v_l}^{|k_1|} \partial_{v_j}^{|k_2|}} (S_N(\tau) G)(Z_N). \end{aligned} \tag{4.6.15}$$

Note that the derivatives involved here are done with respect to the variables at time $t = 0$.

Denoting by $D^r_{z_j}$ any derivative of order r with respect to a variable z_j at time $t = 0$, we observe that:

$$S_N(-t)D^r_{z_j}G(Z_N) = (D^r_{z_j}G)(Z_N(t)) = D^r_{z_j}(t)(S_N(-t)G)(Z_N), \tag{4.6.16}$$

where, by $D^r_{z_j}(t)$, we denote the same derivative of order r with respect to the variable $z_j(t)$. Then, by (4.6.16) and (4.6.15):

$$\begin{aligned}\left(T^{(r)}_N(\tau)G\right)(Z_N) &= S_N(-\tau)(\hat{T}^{(r)}_N + R^{(r)}_N)S_N(\tau)G(Z_N) = \\ &= (-1)^{r/2}\frac{c_r}{N}\sum_{j,l}(D^{r+1}_x\phi)(x_j(\tau) - x_l(\tau)) \cdot D^{r+1}_{v_j}(\tau)G(Z_N) + \\ &\quad + \frac{1}{N}\sum_{l,j=1}^{N}\sum_{\substack{k_1,k_2\in\mathbb{N}^3 \\ |k_1|+|k_2|=r+1}} C_{k_1,k_2}\times \\ &\quad \times\left(\frac{\partial^{r+1}}{\partial^{|k_1|}_{x_l}\partial^{|k_2|}_{x_j}}\phi\right)(x_l(\tau) - x_j(\tau)) \cdot \frac{\partial^{r+1}}{\partial^{|k_1|}_{v_l}\partial^{|k_2|}_{v_j}}(\tau)G(Z_N).\end{aligned} \tag{4.6.17}$$

Therefore, in computing the action of $T^{(r)}_N(\tau)$, we have to consider derivatives with respect to the variables at time τ. As a consequence, we have to deal with a complicated function of the configuration Z_N which, however, we do not need to make explicit, as we shall see in a moment.

On the basis of the previous considerations, we compute the time derivative of η_1 by applying the operators $\mathcal{D}^{2r}T^{(r_n)}_N(t_n)T^{(r_{n-1})}_N(t_{n-1})\dots T^{(r_1)}_N(t_1)$ to the Vlasov equation:

$$\left(\partial_t + v'_1 \cdot \nabla_{x'_1}\right)\mu_N(t) = (\nabla_{x'_1}\phi * \mu_N(t)) \cdot \nabla_{v'_1}\mu_N(t). \tag{4.6.18}$$

In doing this we have to compute

$$\mathcal{D}^{2r}T^{(r_n)}_N(t_n)T^{(r_{n-1})}_N(t_{n-1})\dots T^{(r_1)}_N(t_1)\mu_N(z'_1|Z_N(t))\mu_N(z'_2|Z_N(t)). \tag{4.6.19}$$

Now we select the contribution in which each $T^{(r_\ell)}_N(t_\ell)$ and $\mathcal{D}^{2r}$ apply either on $\mu_N(z'_1|Z_N(t))$ or to $\mu_N(z'_2|Z_N(t))$. The other contribution involves terms in which are present products of derivatives with respect to the same variable. By Proposition 4.4.1 and Corollary 4.4.1 we expect those terms to be negligible (in the $\mathcal{C}^\infty_b$-weak sense) in the limit $N \to \infty$. Therefore we obtain the following equation:

$$
\begin{aligned}
&\left(\partial_t + v_1' \cdot \nabla_{x_1'}\right) \eta_1(z_1', t, r, \underline{\mathbf{r}}_n, \underline{\mathbf{t}}_n, Z_N) = \\
&= L(\mu_N(t))\eta_1(z_1', t, r, \underline{\mathbf{r}}_n, \underline{\mathbf{t}}_n, Z_N) + \\
&+ \sum_{0\le \ell\le r} \sum_{0\le m\le n} \sum_{\substack{I\subset I_n: \\ |I|=m, \\ 0<|\underline{\mathbf{r}}_I|+\ell<k}} (\nabla_{x_1'}\phi * \eta_1(\cdot, t, \ell, \underline{\mathbf{r}}_I, \underline{\mathbf{t}}_I, Z_N))\cdot \\
&\cdot \nabla_{v_1'} \eta_1(z_1', t, r-\ell, \underline{\mathbf{r}}_{I_n\setminus I}, \underline{\mathbf{t}}_{I_n\setminus I}, Z_N) + E_N^1,
\end{aligned}
\tag{4.6.20}
$$

where E_N^1 is an error term which will be proven to be negligible in the limit $N \to \infty$ in Appendix C. In (4.6.20) we used the notations:

$$
I_n = \{1, 2, \dots, n\}, I \quad \text{is any subset of } I_n,\ \underline{\mathbf{r}}_I = \{r_j\}_{j\in I}, \underline{\mathbf{t}}_I = \{t_j\}_{j\in I}. \tag{4.6.21}
$$

Next, we compute the time derivative of $\nu_1^{(k)}$. We have:

$$
\begin{aligned}
&\left(\partial_t + v_1' \cdot \nabla_{x_1'}\right) \nu_1^{(k)} = \sum_{n\ge 0} (-1)^n \sum_{r=0}^{k} \sum_{\substack{|\underline{\mathbf{r}}_n|: \\ r_j>0 \\ |\underline{\mathbf{r}}_n|=k-r}} \times \\
&\times \int_0^t \mathrm{d}t_2 \int_0^{t_2} \mathrm{d}t_3 \cdots \int_0^{t_{n-1}} \mathrm{d}t_n \eta_1(z_1'; t, r, \underline{\mathbf{r}}_n, \underline{\mathbf{t}}_n, Z_N)|_{t_1=t} + \\
&+ \sum_{n\ge 0} (-1)^n \sum_{r=0}^{k} \sum_{\substack{|\underline{\mathbf{r}}_n|: \\ r_j>0 \\ |\underline{\mathbf{r}}_n|=k-r}} \int_{ord}^{t} \mathrm{d}\underline{\mathbf{t}}_n \times \\
&\times \left(\partial_t + v_1' \cdot \nabla_{x_1'}\right) \eta_1(z_1'; t, r, \underline{\mathbf{r}}_n, \underline{\mathbf{t}}_n, Z_N).
\end{aligned}
\tag{4.6.22}
$$

In evaluating the first term on the right hand side of (4.6.22), we are lead to consider η_1 evaluated in $t = t_1$. Thus, according to the expression of η_1 (see (4.6.13)), we have to deal with:

$$
T_N^{(r_1)}(t)\mu_N(z_1'|Z_N(t)) = S_N(-t)T_N^{(r_1)}\mu_N(z_1'|Z_N). \tag{4.6.23}
$$

Therefore:

$$
\begin{aligned}
&T_N^{(r_1)}(t)\mu_N(z_1'|Z_N(t)) = \\
&= (-1)^{r_1/2} c_{r_1} \times \left(D_{x_1'}^{r_1+1}\phi * \mu_N(t)\right)(x_1') \cdot D_{v_1'}^{r_1+1}\mu_N(z_1'|Z_N(t)) = \\
&= (-1)^{r_1/2} c_{r_1} \int \mathrm{d}x_2'\ \mathrm{d}v_2'\ D_{x_1'}^{r_1+1}\phi(x_1'-x_2')\cdot \\
&\cdot D_{v_1'}^{r_1+1}\mu_N(x_1', v_1'|Z_N(t))\mu_N(x_2', v_2'|Z_N(t)),
\end{aligned}
\tag{4.6.24}
$$

where the term involving off-diagonal derivatives, namely $R_N^{(r_1)}$ (see (4.2.16)), disappears because both the derivatives and the empirical distribution are evaluated at time t. Hence we compute η_1 in $t = t_1$ and, inserting it in the first term of the right hand side of (4.6.22), we obtain:

$$\begin{aligned}
&\sum_{n\geq 0}(-1)^n \sum_{r=0}^{k} \sum_{\substack{\underline{\mathbf{r}}_n:\ r_j>0 \\ |\underline{\mathbf{r}}_n|=k-r}} \int_0^t \mathrm{d}t_2 \int_0^{t_2} \mathrm{d}t_3 \mathrm{d}t_3 \cdots \int_0^{t_{n-1}} \times \\
&\times \mathrm{d}t_n \eta_1(z_1'; t, r, \underline{\mathbf{r}}_n, \underline{\mathbf{t}}_n, Z_N)|_{t_1=t} = \\
&= \sum_{\substack{0<r_1\leq k \\ r_1 \text{ even}}} (-1)^{r_1/2} c_{r_1} \int \mathrm{d}x_2'\ \mathrm{d}v_2'\ D_{x_1'}^{r_1+1}\phi(x_1'-x_2')\cdot \\
&\cdot D_{v_1'}^{r_1+1}\nu_2^{(k-r_1)}(x_1', v_1', x_2', v_2'; t).
\end{aligned} \tag{4.6.25}$$

Let us come back now to equation (4.6.22). It is useful to observe that:

$$\int_{ord}^{t} \mathrm{d}\underline{\mathbf{t}}_n \sum_{\substack{I\subset I_n: \\ |I|=m}} = \int_{ord}^{t} \mathrm{d}\underline{\mathbf{t}}_I \int_{ord}^{t} \mathrm{d}\underline{\mathbf{t}}_{I_n\setminus I}. \tag{4.6.26}$$

Then, putting together (4.6.22), (4.6.25), (4.6.20) and (4.6.26), we obtain the following equation for $\nu_1^{(k)}$:

$$\begin{aligned}
&\left(\partial_t + v_1' \cdot \nabla_{x_1'}\right) \nu_1^{(k)}(x_1', v_1'; t) = L(\mu_N(t))\nu_1^{(k)}(x_1', v_1'; t) \\
&+ \sum_{\substack{0<r_1\leq k \\ r_1 \text{ even}}} (-1)^{r_1/2} c_{r_1} \int \mathrm{d}x_2'\ \mathrm{d}v_2'\ D_{x_1'}^{r_1+1}\phi(x_1'-x_2')\cdot \\
&\quad \cdot D_{v_1'}^{r_1+1}\nu_2^{(k-r_1)}(x_1', v_1', x_2', v_2'; t) + \\
&+ \sum_{0<\ell<k} (\nabla_{x_1'}\phi * \nu_1^{(\ell)}(t)) \cdot \nabla_{v_1'}\nu_1^{(k-\ell)}(t) + E_N^2,
\end{aligned} \tag{4.6.27}$$

with initial datum given by:

$$\nu_1^{(k)}(x_1', v_1'; t)|_{t=0} = \eta_1((z_1'; 0, k, \underline{\mathbf{r}}_0, \underline{\mathbf{t}}_0, Z_N) = \mathcal{D}^{2k}\mu_N(z_1'|Z_N). \tag{4.6.28}$$

Here E_N^2 arises from E_N^1 (see (4.6.20)). Now, we want to prove that:

$$\nu_1^{(k)}(t) \to f^{(k)}(t), \quad \text{as} \quad N \to \infty, \quad \mathcal{C}_b^\infty - \text{weakly}, \tag{4.6.29}$$

and

$$\nu_2^{(k)}(t) \to f_2^{(k)}(t), \quad \text{as} \quad N \to \infty, \quad \mathcal{C}_b^\infty - \text{weakly}, \tag{4.6.30}$$

for any configuration Z_N such that $\mu_N \to f_0^{(0)}$ in the weak sense of probability measure (namely, for any Z_N typical with respect to $f_0^{(0)}$ (see Section 4.4)). As a consequence, reminding that $\nu_1^{(k)}(t)$ and $\nu_2^{(k)}(t)$ are equal to $\omega_{N,1}^{(k)}(t)$ and $\omega_{N,2}^{(k)}(t)$ respectively, a.e. with respect to $W_{N,0}^{(0)}$, (4.6.29) and (4.6.30) are equivalent to:

$$\omega_{N,1}^{(k)}(t) \to f^{(k)}(t), \quad \text{as} \quad N \to \infty, \quad \mathcal{C}_b^\infty - \text{weakly}, \tag{4.6.31}$$

and

$$\omega_{N,2}^{(k)}(t) \to f_2^{(k)}(t), \quad \text{as} \quad N \to \infty, \quad \mathcal{C}_b^\infty - \text{weakly}. \tag{4.6.32}$$

As we already remarked, the $\mathcal{C}_b^\infty$-weak convergence implies the convergence in $\mathcal{S}'$, therefore, (4.6.31) and (4.6.32) imply the convergence of $\omega_{N,1}^{(k)}(t)$ to $f^{(k)}(t)$ in $\mathcal{S}'(\mathbb{R}^3 \times \mathbb{R}^3)$ and of $\omega_{N,2}^{(k)}(t)$ to $f_2^{(k)}(t)$ in $\mathcal{S}'(\mathbb{R}^6 \times \mathbb{R}^6)$.

4.6.1 – One and two-particle convergence

In evaluating the behavior of $\nu_1^k(t)$ when $N \to \infty$, we note that it solves the initial value problem (4.6.27)-(4.6.28) for which we want to use Proposition 4.5.1. First, however, we have to verify the assumptions. The first one, namely **i)**, is verified as follows by our choice of the initial datum which ensures $f_0^{(0)}$ to be a smooth probability measure (see Section 4.5) and by the classical mean-field theory recalled in Section 1.

Now, we have to check that assumption **ii)** is satisfied, namely, we have to prove that

$$\begin{aligned}
&\forall u_1,\ u_2 \text{ in } \mathcal{C}_b^\infty(\mathbb{R}^3 \times \mathbb{R}^3),\\
&\text{there exists a constant} C = C(u_1, u_2) > 0,\\
&\text{independent of } N \text{, such that:}\\
&\left\| u_1 * (u_2\, \nu_1^{(k)}(t)) \right\|_{L^\infty(\mathbb{R}^3 \times \mathbb{R}^3)} < C \quad \text{for any } t.
\end{aligned} \tag{4.6.33}$$

We have:

$$\left\| u_1 * (u_2\ \nu_1^{(k)}(t)) \right\|_{L^\infty(\mathbb{R}^3\times\mathbb{R}^3)} =$$

$$= \sup_{x_1',v_1'} \left| \int \mathrm{d}y \mathrm{d}w\ u_1(x_1'-y, v_1'-w) u_2(y,w) \nu_1^{(k)}(y,w;t) \right| \leq$$

$$\leq \sum_{n\geq 0} \sum_{r=0}^{k} \sum_{\substack{\underline{\mathbf{r}}_n:\ r_j>0 \\ |\underline{\mathbf{r}}_n|=k-r}} \int_{ord}^{t} \mathrm{d}\underline{\mathbf{t}}_n$$

$$\sup_{x_1',v_1'} \left| \int \mathrm{d}y \mathrm{d}w\ u_1(x_1'-y, v_1'-w) u_2(y,w) \eta_1(y,w;t;r,\underline{\mathbf{r}}_n,\underline{\mathbf{t}}_n, Z_N) \right| =$$

$$= \sum_{n\geq 0} \sum_{r=0}^{k} \sum_{\substack{\underline{\mathbf{r}}_n:\ r_j>0 \\ |\underline{\mathbf{r}}_n|=k-r}} \int_{ord}^{t} \mathrm{d}\underline{\mathbf{t}}_n \tag{4.6.34}$$

$$\sup_{x_1',v_1'} \left| \int \mathrm{d}y \mathrm{d}w\ \left(u_1(x_1'-y, v_1'-w) u_2(y,w)\right) \mathcal{D}^{2r} T_N^{(r_n)}(t_n) \ldots \right.$$

$$\left. \ldots T_N^{(r_1)}(t_1) \mu_N(y,w|Z_N(t)) \right| = \sum_{n\geq 0} \sum_{r=0}^{k} \sum_{\substack{\underline{\mathbf{r}}_n:\ r_j>0 \\ |\underline{\mathbf{r}}_n|=k-r}} \int_{ord}^{t} \mathrm{d}\underline{\mathbf{t}}_n$$

$$\sup_{x_1',v_1'} \left| \int \mathrm{d}y \mathrm{d}w\ g(x_1',v_1',y,w) \mathcal{D}^{2r} T_N^{(r_n)}(t_n) \ldots T_N^{(r_1)}(t_1) \mu_N(y,w|Z_N(t)) \right|,$$

where we used the notation $g(x_1', v_1', y, w) := u_1(x_1'-y, v_1'-w)u_2(y,w)$ and, clearly, we have $g(x_1', v_1', \cdot, \cdot) \in \mathcal{C}_b^\infty(\mathbb{R}^3\times\mathbb{R}^3)$ for any x_1' and v_1' and $g(\cdot,\cdot,y,w) \in \mathcal{C}_b^\infty(\mathbb{R}^3\times\mathbb{R}^3)$ for any y and w. By some estimates which will be proven in Appendix C (see Lemma C.2), we are guaranteed that, applying the operator $\mathcal{D}^{2r} T_N^{(r_n)}(t_n) \ldots T_N^{(r_1)}(t_1)$ on the empirical measure $\mu_N(t)$ and integrating versus a function in $\mathcal{C}_b^\infty(\mathbb{R}^3\times\mathbb{R}^3)$ we obtain a quantity uniformly bounded in N. This feature, by virtue of the good properties of the function g ensures that (4.6.34) is finite.

Let us now look at the initial datum for $\nu_1^{(k)}(t)$, in order to verify assumption **iii)**.

From (4.6.28) we know that $\nu_1^{(k)}(0) = \mathcal{D}^{2k}\mu_N \in \mathcal{S}'(\mathbb{R}^3\times\mathbb{R}^3)$. As regard to its limiting behavior, we find that:

$$\nu_1^{(k)}(t)\Big|_{t=0} = \mathcal{D}^{2k}\mu_N = \sum_{n=1}^{N} \sum_{\substack{I\subset I_N \\ |I|=n}} \sum_{\substack{s_j: j\in I \\ 1\leq s_j\leq k \\ \sum_j s_j = k}} \prod_{j\in I} D_{G,j}^{2s_j} \mu_N, \tag{4.6.35}$$

where $I_N = \{1, \ldots, N\}$.

For our convenience, we have written the action of the operator $\mathcal{D}^{2k}$ in a equivalent and slightly different way from that we used in (4.6.3).

We realize that the only surviving term in the sum (4.6.35) is that with $n = 1$. Hence:

$$\nu_1^k(t)\big|_{t=0} = \sum_{j=1}^{N} D_{G,j}^{2k}\mu_N = \frac{1}{N}\sum_{j=1}^{N} D_{G,j}^{2k}\delta(z_1' - z_j) = D_G^{2k}\mu_N. \tag{4.6.36}$$

Therefore we can conclude, by using the mean-field limit:

$$\begin{aligned}\left(u, \nu_1^{(k)}(t)|_{t=0}\right) &= \left(u, D_G^{2k}\mu_N\right) = \\ &= \left(D_G^{2k}u, \mu_N\right) \to \left(D_G^{2k}u, f_0^{(0)}\right) = \\ &= \left(u, D_G^{2k}f_0^{(0)}\right) = \left(u, f_0^{(k)}\right), \text{ as } N \to \infty, \\ &\quad \forall u \text{ in } \mathcal{C}_b^\infty\left(\mathbb{R}^3 \times \mathbb{R}^3\right).\end{aligned} \tag{4.6.37}$$

Thus, $f_0^{(k)}$ plays the role of γ_0 in Proposition 4.5.1 and it is in $L^1(\mathbb{R}^3 \times \mathbb{R}^3)$ because $f_0^{(0)} \in \mathcal{S}(\mathbb{R}^3 \times \mathbb{R}^3)$.

We conclude the convergence proof (for the one and two-particle functions) by induction. For $k = 0$ we know that, for any configuration Z_N which is typical with respect to $f_0^{(0)}$, we have:

$$\nu_1^{(0)}(t) = \mu_N(t) \to f^{(0)}(t), \text{ as } N \to \infty \tag{4.6.38}$$

in the weak sense of probability measures (see (1.3.10) and (1.3.11)) and, as a consequence, the convergence holds $\mathcal{C}_b^\infty$ – weakly. Moreover

$$\nu_2^{(0)}(t) = \mu_N(t) \otimes \mu_N(t) \to f_2^{(0)}(t) = f^{(0)}(t) \otimes f^{(0)}(t), \text{ as } N \to \infty, \tag{4.6.39}$$

in the weak sense of probability measures and, as previously, the convergence holds $\mathcal{C}_b^\infty$ – weakly.

We make the following inductive assumptions for all $h < k$:

$$\nu_1^{(h)}(t) \to f^{(h)}(t), \text{ as } N \to \infty, \quad \mathcal{C}_b^\infty \text{ – weakly}, \tag{4.6.40}$$

for any configuration Z_N which is typical with respect to $f_0^{(0)}$, and

$$\nu_2^{(h)}(t) \to f_2^{(h)}(t) = \sum_{0 \le q \le h} f^{(q)}(t) f^{(h-q)}(t), \text{ as } N \to \infty, \quad \mathcal{C}_b^\infty\text{–weakly}, \tag{4.6.41}$$

for any configuration Z_N which is typical with respect to $f_0^{(0)}$.

Now we want to prove that (4.6.40) and (4.6.41) hold also for $h = k$.

Thanks to (4.6.40), we can affirm that:

$$\sum_{0<\ell<k} \left(\nabla_{x_1'}\phi * \nu_1^{(\ell)}\right) \cdot \nabla_{v_1'}\nu_1^{(k-\ell)} \to \sum_{0<\ell<k} \left(\nabla_{x_1'}\phi * f^{(\ell)}\right) \cdot \nabla_{v_1'} f^{(k-\ell)} = \\ = \sum_{0<\ell<k} T_\ell^{(0)} f^{(k-\ell)}, \quad \mathcal{C}_b^\infty - \text{weakly}, \tag{4.6.42}$$

and, thanks to (4.6.41), have:

$$\begin{aligned} &\sum_{\substack{0<r_1\le k\\ r_1 \text{ even}}} (-1)^{r_1/2} c_{r_1} \int \mathrm{d}x_2' \mathrm{d}v_2' D_{x_1'}^{r_1+1}\phi(x_1'-x_2')\cdot \\ &\cdot D_{v_1'}^{r_1+1}\nu_2^{(k-r_1)}(x_1',v_1',x_2',v_2';t) \\ &\downarrow \; \mathcal{C}_b^\infty - \text{weakly} \\ &\sum_{\substack{0<r_1\le k\\ r_1 \text{ even}}} (-1)^{r_1/2} c_{r_1} \int \mathrm{d}x_2' \mathrm{d}v_2' D_{x_1'}^{r_1+1}\phi(x_1'-x_2')\cdot \\ &\cdot D_{v_1'}^{r_1+1} f_2^{(k-r_1)}(x_1',v_1',x_2',v_2';t) = \\ &= \sum_{\substack{0<r_1\le k\\ r_1 \text{even}}} \sum_{0\le q\le k-r_1} (-1)^{r_1/2} c_{r_1} \int \mathrm{d}x_2' \mathrm{d}v_2' D_{x_1'}^{r_1+1} \times \\ &\times \phi(x_1'-x_2') f^{(k-r_1)}(x_2',v_2';t) \cdot D_{v_1'}^{r_1+1} f^{(q)}(x_1',v_1';t) = \\ &= \sum_{\substack{0<r_1\le k\\ r_1 \text{ even}}} \sum_{0\le q\le k-r_1} T_q^{(r_1)} f^{(k-r_1-q)}(t). \end{aligned} \tag{4.6.43}$$

At the end, putting together (4.6.42) and (4.6.43), we find that the sum of the source terms in equation (4.6.27) converges $\mathcal{C}_b^\infty$-weakly to:

$$\sum_{0<\ell<k} T_\ell^{(0)} f^{(k-\ell)} + \sum_{\substack{0<r_1\le k\\ 0\le q\le k-r_1}} T_q^{(r_1)} f^{(k-r_1-q)}, \tag{4.6.44}$$

which plays the role of Θ in Proposition 4.5.1 and it is easy to verify that it is in $\mathcal{C}^0(L^1(\mathbb{R}^3\times\mathbb{R}^3),\mathbb{R}^+)$. Therefore, we can apply Proposition 4.5.1 claiming that, for any typical configuration Z_N with respect to $f_0^{(0)}$, $\nu_1^{(k)}(t)$ converges $\mathcal{C}_b^\infty$-weakly to the solution of the problem (4.1.14). Looking at (4.1.11) and (4.1.13), we realize that we obtained the equation satisfied by $f^{(k)}(t)$.

In order to “close” the recurrence procedure, it remains to show the two-particle convergence at order k. It follows from the one-particle analysis and from the following computation (see (4.6.14)):

$$\begin{aligned}&\eta_2(z_1',z_2';t,r,\underline{\mathbf{r}}_n,\underline{\mathbf{t}}_n,Z_N)=\\&=\sum_{0\le\ell\le k}\sum_{0\le m\le n}\sum_{\substack{I:I\subseteq I_n\\|I|=m}}\times\\&\times\eta_1(z_1';t,\ell,\underline{\mathbf{r}}_I,\underline{\mathbf{t}}_I,Z_N)\eta_1(z_2';t,k-\ell,\underline{\mathbf{r}}_{I_n\setminus I},\underline{\mathbf{t}}_{I_n\setminus I},Z_N)+R_N^2,\end{aligned}\tag{4.6.45}$$

where R_N^2 is a remainder arising from the action of the operator $\mathcal{D}^{2r}T_N^{(r_n)}(t_n)\dots T_N^{(r_1)}(t_1)$ on a product of two empirical measures $\mu_N(t)$. In Appendix C we will see that it is vanishing in the limit. As a consequence, $\nu_2^{(k)}$ (see (4.6.10) for $j=2$) is such that:

$$\nu_2^{(k)}(t)=\sum_{0\le q\le k}\nu_1^{(q)}(t)\nu_1^{(k-q)}(t)+o(1),\tag{4.6.46}$$

in the limit $N\to\infty$. Therefore, from the inductive assumption (4.6.40) and from the one-particle convergence at order k, we conclude that:

$$\nu_2^{(k)}(t)\to\sum_{0\le q\le k}f^{(q)}(t)f^{(k-q)}(t)=f_2^{(k)}(t),\ \text{as } N\to\infty,\mathcal{C}_b^\infty-\text{weakly},\tag{4.6.47}$$

for any configuration Z_N which is typical with respect to $f_0^{(0)}$. Thus, we have just proven the convergence of $\omega_{N,j}^{(k)}$ in the cases $j=1$, $j=2$.

4.6.2 – j-particle convergence

As for $j=2$, the j-particle convergence can be reduced by the one-particle control. Indeed by (4.6.10) and (4.6.11) we have:

$$\begin{aligned}&\nu_j^{(k)}(t)=\sum_{\substack{s_1\dots s_j\\0\le s_m\le k\\\sum_m s_m=k}}\prod_{m=1}^{j}\nu_1^{(s_m)}(t)+R_N^j,\\&\text{with } R_N^j\to0 \text{ when } N\to\infty.\end{aligned}\tag{4.6.48}$$

Again the error term R_N^j arises from the presence of products of derivatives with respect to the same variable. In conclusion, the result we proved for $\nu_1^{(k)}(t)$, together with the estimates proven in Appendix C, is sufficient to guarantee the $\mathcal{C}_b^\infty$-weak convergence of $\nu_j^{(k)}(t)$ to $f_j^{(k)}(t)$ for any j (for any typical configuration

Z_N with respect to $f_0^{(0)}$), and, as a consequence, the $\mathcal{C}_b^\infty$-weak convergence of $\omega_{N,j}^{(k)}(t)$ is $f_j^{(k)}(t)$, for any j.

The final step is to realize that this convergence does imply that for the coefficients $W_{N,j}^{(k)}(t)$, namely what is established by Theorem 4.5.1.

First of all, we observe that, for any test function u we have:

$$
\begin{aligned}
(u, W_{N,1}^{(k)}(t) &= \int_{\mathbb{R}^6} \mathrm{d}z_1 W_{N,1}^{(k)}(z_1;t)u(z_1) = \\
&= \int_{\mathbb{R}^{3N}\times\mathbb{R}^{3N}} \mathrm{d}Z_N W_N^{(k)}(Z_N;t)u(z_1) = \\
&= \int_{\mathbb{R}^{3N}\times\mathbb{R}^{3N}} \mathrm{d}Z_N W_N^{(k)}(Z_N;t)\frac{1}{N}\sum_{l=1}^{N} u(z_l) = \\
&= \int_{\mathbb{R}^{3N}\times\mathbb{R}^{3N}} \mathrm{d}Z_N W_N^{(k)}(Z_N;t)(u,\mu_N) = (u, \omega_{N,1}^{(k)}(t)),
\end{aligned}
\tag{4.6.49}
$$

where we made use of the symmetry of the coefficient $W_N^{(k)}(Z_N;t)$ with respect to any permutation of the variables (the computation is the same we did in Section 4.4 for $W_{N,1}^{(1)}(t)$). From (4.6.49), we can see that $W_{N,1}^{(k)}(t)$ and $\omega_{N,1}^{(k)}(t)$ are equal as distributions in $\mathcal{S}'(\mathbb{R}^3\times\mathbb{R}^3)$ (in particular, we can choose test functions belonging to $\mathcal{C}_b^\infty(\mathbb{R}^3\times\mathbb{R}^3)$), then the convergence of $W_{N,1}^{(k)}(t)$ is proven. Moreover, for $j\geq 2$, a straightforward computation shows that, by fixing an index $\overline{j}$, we have

$$
(u_{\overline{j}}, \omega_{N,\overline{j}}^{(k)}(t)) = \frac{N(N-1)\dots(N-\overline{j}+1)}{N^{\overline{j}}}\left(u_{\overline{j}}, W_{N,\overline{j}}^{(k)}(t)\right) + \frac{C_{j<\overline{j}}}{N},
\tag{4.6.50}
$$

where $C_{j<\overline{j}} < \infty$ provided that $(u_j, W_{N,j}^{(k)}(t))$ is uniformly bounded for each $j < \overline{j}$. Then, to conclude the proof of Theorem 4.5.1, it is enough to use a recurrence argument.

5 – Outlooks and Perspectives

In this section we give an overview of possible developments of our research, both in the perspective of generalizing our result, and from the point of view of applications in other (somewhat related) fields.

First we observe that the we can apply Theorem 4.5.1 even by considering as one-particle initial datum a suitable mixtures of WKB states. Indeed, let us consider the one-particle WKB state described by the wave function $\psi_{WKB}\in L^2(\mathbb{R}^3)$ given by:

$$
\psi_{WKB}(x|v_0) = a(x)e^{i\frac{v_0\cdot x}{\varepsilon}}, \qquad a\in\mathcal{S}(\mathbb{R}^3), a(x)\in\mathbb{R}\;\forall\, x,\; v_0 \text{ fixed in } \mathbb{R}^3,
\tag{5.1}
$$

where the amplitude a is assumed to verify

$$\int \mathrm{d}x\ a^2(x) = 1, \tag{5.2}$$

namely, $a^2(x)$ can be interpreted as a one-particle probability density in the position phase space $\mathbb{R}^3$. The Wigner function associated with (5.1), given by

$$\begin{aligned} f^{\varepsilon}_{WKB}(x,v|v_0) &= (2\pi)^{-3}\int_{\mathbb{R}^3} \mathrm{d}y e^{i\ v\cdot y}\times \\ &\quad \times \overline{\psi}_{WKB}\left(x+\frac{\varepsilon y}{2}|v_0\right)\psi_{WKB}\left(x-\frac{\varepsilon y}{2}|v_0\right) = \\ &= (2\pi)^{-3}\int_{\mathbb{R}^3} \mathrm{d}y e^{i\ y\cdot v} a\left(x+\frac{\varepsilon y}{2}\right) e^{-i\frac{v_0\cdot\left(x+\frac{\varepsilon y}{2}\right)}{\varepsilon}}\times \\ &\quad \times a\left(x-\frac{\varepsilon y}{2}\right) e^{i\frac{v_0\cdot\left(x-\frac{\varepsilon y}{2}\right)}{\varepsilon}} = \\ &= (2\pi)^{-3}\int_{\mathbb{R}^3} \mathrm{d}y e^{i\ y\cdot(v-v_0)} a\left(x+\frac{\varepsilon y}{2}\right) a\left(x-\frac{\varepsilon y}{2}\right), \end{aligned} \tag{5.3}$$

can be expanded as follows

$$f^{\varepsilon}_{WKB}(x,v|v_0) = f^{(0)}_{WKB}(x,v|v_0)+\varepsilon f^{(1)}_{WKB}(x,v|v_0)+\varepsilon^2 f^{(2)}_{WKB}(x,v|v_0)+\dots \tag{5.4}$$

where

$$f^{(0)}_{WKB}(x,v|v_0) = a^2(x)\delta(v-v_0), \tag{5.5}$$

$$f^{(2n+1)}_{WKB}(x,v|v_0) = 0 \qquad \forall\ n = 0,1,2,\dots, \tag{5.6}$$

$$\begin{aligned} f^{(2n)}_{WKB}(x,v|v_0) &= -\frac{1}{(2)^{2n}}\sum_{l=0}^{2n}\frac{1}{l!}\frac{1}{(2n-l)!}\times \\ &\times (-1)^l D^l a(x) D^{2n-l} a(x) D^{2n}_v \delta(v-v_0), \qquad \forall\ n = 1,2,\dots \end{aligned} \tag{5.7}$$

and $D^m_v\delta(v-v_0)$, for any $m>0$, is the distribution acting as

$$(u, D^m_v\delta(v-v_0)) = \int \mathrm{d}v\ u(v) D^m_v\delta(v-v_0) = \tag{5.8}$$

$$= (-1)^m\int \mathrm{d}v\ D^m_v u(v)\delta(v-v_0) = (-1)^m D^m_v u(v_0), \tag{5.9}$$

for any smooth test function u.

Then, we consider the Wigner function

$$f^{\varepsilon}_{W}(x,v) = \int \mathrm{d}v_0 \; g_W(v_0) f^{\varepsilon}_{WKB}(x,v|v_0), \qquad g_W \in \mathcal{S}(\mathbb{R}^3) \tag{5.10}$$

associated with the (continuum) mixed state (see paragraph "Mixed states" in Section 2.1) described by the density matrix (kernel)

$$\rho_W(x,v) = \int \mathrm{d}v_0 g_W(v_0) \overline{\psi}_{WKB}(x|v_0)\psi_{WKB}(y|v_0) \tag{5.11}$$

and we assume g_W to be a probability density with respect to the velocity variable, g_W not depending on ε (states similar to (5.9) have been considered in [24]). By (5.4), (5.5), (5.6) and (5.7) we obtain that (5.9) is expanded as:

$$f^{\varepsilon}_{W}(x,v) = f^{(0)}_{W}(x,v) + \varepsilon f^{(1)}_{W}(x,v) + \varepsilon^2 f^{(2)}_{W}(x,v) + \dots \tag{5.12}$$

where

$$f^{(0)}_{W}(x,v) = a^2(x) g_W(v), \tag{5.13}$$

$$f^{(2n+1)}_{W}(x,v) = 0 \qquad \forall\, n = 0,1,2,\dots, \tag{5.14}$$

$$f^{(2n)}_{W}(x,v) = -\frac{1}{(2)^{2n}} \sum_{l=0}^{2n} \frac{1}{l!} \frac{1}{(2n-l)!} (-1)^l D^l a(x) D^{2n-l} a(x) D^{2n}_v g_W(v). \qquad \forall\, n = 0,1,2,\dots \tag{5.15}$$

By virtue of our assumptions on a and g_W we find that $f^{(0)}_{W}$ defined by (5.13) is a one-particle probability density and $f^{(0)}_{W} \in \mathcal{S}(\mathbb{R}^3)$. Furthermore, we choose a in such a way that

$$D^m a(x) = \alpha^{(m)}(x) a(x),\ \forall\, m \geq 1 \quad \text{with} \quad \alpha^{(m)}(x) \in C^0(\mathbb{R}^3), \tag{5.16}$$

$C^0(\mathbb{R}^3)$ being the space of continuous functions. Therefore, by (5.15) we find

$$\begin{aligned} f^{(2n)}_{W}(x,v) &= -\frac{1}{(2)^{2n}} \sum_{l=0}^{2n} \frac{1}{l!} \frac{1}{(2n-l)!} (-1)^l D^l a(x) D^{2n-l} a(x) D^{2n}_v g_W(v) = \\ &= \beta^{(2n)}(x) a^2(x) D^{2n}_v g_W(v) = \\ &= \beta^{(2n)}(x) D^{2n}_v f^{(0)}_{W}(x,v) \quad \forall\, n = 0,1,2,\dots \end{aligned} \tag{5.17}$$

where $\beta^{(2n)}(x) = -\frac{1}{(2)^{2n}} \sum_{l=0}^{2n} \frac{1}{l!} \frac{1}{(2n-l)!} (-1)^l \alpha^{(l)}(x) \alpha^{(2n-l)}(x)$ for any $n \geq 1$ and in the last equality of (5.17) we used (5.13). By the smoothness of α (see (5.16)) it follows that $\beta^{(2n)}(x) \in C^0(\mathbb{R}^3)$ for all n, thus (2.17) together with the smoothness of $f_W^{(0)}$ implies that $f_W^{(2n)} \in \mathcal{S}(\mathbb{R}^3 \times \mathbb{R}^3)$ for all $n \geq 1$.

Therefore, we have

$$f_W^{(0)} \in \mathcal{S}(\mathbb{R}^3 \times \mathbb{R}^3) \tag{5.18}$$

$$f_W^{(2n+1)}(x, v) = 0 \qquad \forall\, n = 0, 1, 2, \ldots, \tag{5.19}$$

$$f_W^{(2n)} \in \mathcal{S}(\mathbb{R}^3 \times \mathbb{R}^3) \qquad \forall\, n = 1, 2, \ldots \tag{5.20}$$

and, by applying Proposition 4.1.1 as in Section 4.1, we can identify the time-evolved coefficients $f_W^{(k)}(t)$, for each $k \geq 0$, as the unique solutions of problems (4.1.10) and (4.1.11) in $L^1(\mathbb{R}^3 \times \mathbb{R}^3)$. Clearly, by (5.19) we find

$$f_W^{(2n+1)}(x, v; t) \equiv 0, \quad \text{for each } n \geq 0 \text{ and } \forall\, t, \tag{5.21}$$

while $f_W^{(2n)}(t) \in \mathcal{S}(\mathbb{R}^3 \times \mathbb{R}^3)$ for any $n \geq 0$. In particular, $f_W^{(0)}(t)$ is the unique solution of the Vlasov equation (1.1.8) with initial datum $f_W^{(0)}$, thus we are guaranteed that $f_W^{(0)}(t)$ is a one-particle probability density for all times.

Let us consider the following factorized initial datum for the N-particle Wigner-Liouville equation (3.2.1)

$$W_{N,W}^{\varepsilon}(X_N, V_N) = (f_W^{\varepsilon})^{\otimes N}(X_N, V_N). \tag{5.22}$$

Then we find

$$\begin{aligned} W_{N,W}^{\varepsilon}(X_N, V_N) = W_{N,W}^{(0)}(X_N, V_N) + \varepsilon W_{N,W}^{(1)}(X_N, V_N) + \\ + \varepsilon^2 W_{N,W}^{(2)}(X_N, V_N) + \ldots, \end{aligned} \tag{5.23}$$

where, by (5.12),

$$W_{N,W}^{(0)}(X_N, V_N) = (f_W^{(0)})^{\otimes N}(X_N, V_N) \tag{5.24}$$

$$W_{N,W}^{(n)}(X_N, V_N) = \sum_{\substack{s_1 \ldots s_N \\ 0 \leq s_j \leq n \\ \sum_j s_j = n}} \prod_{j=1}^{N} f_W^{(s_j)}(x_j, v_j) \quad \text{for } n \geq 1, \tag{5.25}$$

and we note that, as in the case we considered in Section 4, factorization holds only for the zero order coefficient which, furthermore, turns to be an N-particle probability density.

By (5.25), thanks to (5.14) and (2.17), we find

$$W^{(0)}_{N,W}(X_N,V_N) = (f^{(0)}_W)^{\otimes N}(X_N,V_N) \tag{5.26}$$

$$W^{(n)}_{N,W}(X_N,V_N) = \sum_{\substack{s_1\dots s_N \text{even}\\ 0\le s_j\le n\\ \sum_j s_j=n}} \prod_{j=1}^{N} \beta^{(s_j)} \times \tag{5.27}$$

$$\times\, (x_j) D^{s_j}_{v_j} W^{(0)}_{N,W}(X_j,V_j) \quad \text{for } n\ge 1.$$

Defining the operator $\hat{\mathcal{D}}^r$, for any r even, as:

$$\hat{\mathcal{D}}^0 = \mathtt{1},$$

$$\hat{\mathcal{D}}^r = \sum_{\substack{s_1\dots s_N \text{even:}\\ 0\le s_j\le k\\ \sum_j s_j=r}} \prod_{j=1}^{N} \beta^{(s_j)}(x_j) D^{s_j}_{v_j}, \quad r\ge 2, \tag{5.28}$$

we have:

$$W^{(2n+1)}_{N,W}(X_N,V_N) = 0, \qquad \text{for} n = 0,1,2,\dots \tag{5.29}$$

$$W^{(2n)}_{N,W}(X_N,V_N) = \hat{\mathcal{D}}^{2n} W^{(0)}_{N,W}(X_N,V_N) \qquad \text{for} n = 0,1,2,\dots. \tag{5.30}$$

Now, let us consider the factorized j-particle Wigner function $(f^\varepsilon_W(t))^{\otimes j}$, where $f^\varepsilon_W(t)$ is the solution of the (Hartree) nonlinear Wigner-Liouville equation (3.3.1) with initial datum f^ε_W given by (5.9). The product $(f^\varepsilon_W(t))^{\otimes j}$ can be expanded as

$$(f^\varepsilon_W(t))^{\otimes j} = f^{(0)}_{j,W}(t) + \varepsilon f^{(1)}_{j,W}(t) + \varepsilon^2 f^{(2)}_{j,W}(t) + \dots, \tag{5.31}$$

where, by the analysis done in Section 4.3 and thanks to (5.14), we have

$$f^{(0)}_{j,W}(t) = (f^{(0)}_W(t))^{\otimes j} \tag{5.32}$$

$$f^{(2n+1)}_{j,W}(t) = 0, \qquad \forall\, n\ge 0 \tag{5.33}$$

$$f^{(2n)}_{j,W}(t) = \sum_{\substack{s_1\dots s_j \text{even}\\ 0\le s_m\le 2n\\ \sum_m s_m=2n}} \prod_{m=1}^{j} f^{(s_m)}_W(t), \quad \forall\, n\ge 1, \tag{5.34}$$

$f^{(0)}_W(t)$ solving the Vlasov equation (1.1.8) with initial datum $f^{(0)}_W$ and $f^{(s_m)}_W(t)$, with $1\le s_m\le 2n$, obtained by (4.1.11).

By the analysis done in Section 4.2, we find that the N-particle zero order coefficient $W^{(0)}_{N,W}(t)$ solves

$$
\begin{cases} (\partial_t + V_N \cdot \nabla_{X_N})\, W^{(0)}_{N,W}(t) = T^{(0)}_N W^{(0)}_{N,W}(t), \\ W^{(0)}_{N,W}(X_N, V_N; t)\Big|_{t=0} = (f^{(0)}_W)^{\otimes N}(X_N, V_N) \end{cases} \tag{5.35}
$$

the odd coefficients $W^{(2n+1)}_{N,W}(t)$ are determined by

$$
\begin{cases} (\partial_t + V_N \cdot \nabla_{X_N})\, W^{(2n+1)}_{N,W}(t) = T^{(0)}_N W^{(2n+1)}_{N,W}(t), \\ W^{(2n+1)}_{N,W}(X_N, V_N; t)\Big|_{t=0} = 0, \qquad k = 0, 1, 2, \dots \end{cases} \tag{5.36}
$$

and the even terms $W^{(2n)}_{N,W}(t)$ solve

$$
\begin{cases} (\partial_t + V_N \cdot \nabla_{X_N})\, W^{(2n)}_{N,W}(t) = T^{(0)}_N W^{(2n)}_{N,W}(t) + \Theta^{(2n)}_{N,W}(t), \\ W^{(2n)}_{N,W}(X_N, V_N; t)\Big|_{t=0} = \hat{\mathcal{D}}^{2n} W^{(0)}_{N,W}(X_N, V_N), \qquad n = 1, 2, \dots \end{cases} \tag{5.37}
$$

where

$$
\Theta^{(2n)}_{N,W}(t) =_{0 \le l < 2n} T^{(2n-l)}_N W^{(l)}_{N,W}(t). \tag{5.38}
$$

We observe that the odd coefficients $W^{(2n+1)}_{N,W}(t)$ solve homogeneous Liouville equations with zero initial data, then $W^{(2n+1)}_{N,W}(t) \equiv 0$ for all $n \geq 0$. On the contrary, the zero order term $W^{(0)}_{N,W}(t)$ solve the Liouville problem (5.35), thus, denoting by $\{W^{(0)}_{j,W}(t)\}_{j=1}^N$ the corresponding j-particle marginals, by the classical mean-field theory we obtain

$$
W^{(0)}_{j,W}(t) \to (f^{(0)}_W(t))^{\otimes j}, \quad \text{as} \quad N \to \infty, \quad \text{for any fixed } j \tag{5.39}
$$

in the weak topology of probability measures and, in particular, in $\mathcal{S}'(\mathbb{R}^{3j} \times \mathbb{R}^{3j})$, where $(f^{(0)}_W(t))^{\otimes j}$ is given by (5.32).

As regard to the higher order terms, we can apply exactly the same strategy presented in Section 4, replacing the operator D^k_G defined in (4.5.8) with $\beta^{(k)}(x) D^k_v$ (see (5.17)) and the operator $\mathcal{D}^r$ (see Section 4.6) with $\hat{\mathcal{D}}^r$ (see (5.28)). In the end we prove that, for $k \geq 1$

$$
W^{(k)}_{j,W}(t) \to f^{(k)}_{W,j}(t), \quad \text{as} \quad N \to \infty, \quad \text{for any fixed } j \tag{5.40}
$$

in $\mathcal{S}'(\mathbb{R}^{3j} \times \mathbb{R}^{3j})$.

Clearly, (5.40) is trivially verified for $k = 2n+1$, because we have already noticed that

$$W_{j,W}^{(2n+1)}(t) \equiv f_{j,W}^{(2n+1)}(t) \equiv 0, \quad \forall\, n \geq 0. \tag{5.41}$$

As we observed in Remark 4.5.1, the assumption on the initial N-particle Wigner function to be a product of mixed states prevents the possibility of considering bosonic states. Indeed, factorized states could be compatible with the bosonic statistics if pure states were considered.

It is easy to check that the classical limit is equivalent to the limit of heavy particles. In fact, if we set $\varepsilon = 1$ in the N-particle Hamiltonian (2.1.5) but we let the particle mass m (previously chosen equal to 1) become large, by imposing the condition that the kinetic energy per particle is independent of m, we find exactly the mean-field hamiltonian (2.1.5) where ε is replaced by the "effective Planck constant" $\varepsilon_m = 1/\sqrt{m}$ going to zero as $m \to \infty$. Then a possible application of our result would be that of studying the approximations of dynamics of this type, in which one looks at a particular scaling which corresponds to the semiclassical one, even if interpreted in a different sense.

– Appendix A

Proof of Proposition 4.4.1

To avoid inessential notational complications, we deal with the one-dimensional case. By the Newton equations, we have:

$$\frac{\partial x_i(t)}{\partial v_r} = \delta_{ir} t + \int_0^t \mathrm{d}s (t-s) \frac{1}{N} \sum_{j \neq i}^{N} \partial_x F\left(x_i(s) - x_j(s)\right) \left(\frac{\partial x_i(s)}{\partial v_r} - \frac{\partial x_j(s)}{\partial v_r} \right), \tag{A.1}$$

$$\frac{\partial v_i(t)}{\partial v_r} = \delta_{ir} + \int_0^t \mathrm{d}s \frac{1}{N} \sum_{j \neq i}^{N} \partial_x F\left(x_i(s) - x_j(s)\right) \left(\frac{\partial x_i(s)}{\partial v_r} - \frac{\partial x_j(s)}{\partial v_r} \right), \tag{A.2}$$

where:

$$F = -\nabla_x \phi, \tag{A.3}$$

is the force associated with the potential ϕ.

Let us analyze in detail the derivative of $x_i(t)$. From (A.1), we get:

$$\max_{\substack{i,r \\ t \leq T}} \left| \frac{\partial x_i(t)}{\partial v_r} \right| \leq C. \tag{A.4}$$

Inserting this estimate again in (A.1), we realize that we can obtain a better bound for $\frac{\partial v_i(t)}{\partial v_r}$ in the case $r \neq i$ (see [24]), namely:

$$\text{(A.5)}\qquad \left|\frac{\partial x_i(t)}{\partial v_r}\right| \le C\int_0^t \mathrm{d}s(t-s)\left|\frac{\partial x_i(s)}{\partial v_r}\right| + + C\int_0^t \mathrm{d}s(t-s)\frac{1}{N}\left|\frac{\partial x_r(s)}{\partial v_r}\right| +$$

$$\text{(A.6)}\qquad + C\int_0^t \mathrm{d}s(t-s)\frac{1}{N}\sum_{\substack{j\neq i\\ j\neq r}}^N \partial_x F\left(x_i(s)-x_j(s)\right)\left|\frac{\partial x_j(s)}{\partial v_r}\right|.$$

Hence, by virtue of the Gronwall lemma, we find:

$$\text{(A.7)}\qquad \max_{\substack{i\neq r\\ t\le T}}\left|\frac{\partial x_i(t)}{\partial v_r}\right| \le \frac{C}{N}.$$

By (A.2), we find that the same estimate holds for the derivative of $v_i(t)$ with respect to v_r. Analogous estimates hold for the derivatives with respect to the initial positions (see also [24]).

Therefore the claim of Proposition 4.4.1 is proven for derivatives of order one.

Now, let us consider a sequence $I := (j_1, \dots, j_k)$ of possibly repeated indices. We show that:

$$\text{(A.8)}\qquad \frac{1}{N}\sum_{i=1}^N \left|\frac{\partial^k x_i(t)}{\partial v_{j_1}\dots\partial v_{j_k}}\right| \le \frac{C}{N^{d_k}},$$

where d_k is the number of different indices in the sequence $j_1, \dots, j_k$. We know that (A.8) is verified for $k = 1$ (it follows directly by (A.4) and (A.7)), thus we prove (A.8) by induction on k. Denoting by:

$$\text{(A.9)}\qquad D(I) := \frac{\partial^k}{\partial v_{j_1}\dots\partial v_{j_k}},$$

estimate (A.8) can be rewritten as:

$$\text{(A.10)}\qquad \frac{1}{N}\sum_{i=1}^N |D(I)x_i(t)| \le \frac{C}{N^{d_k}}.$$

By (A.1) we derive the following estimate for $D(I)x_i(t)$:

$$\text{(A.11)}\qquad |D(I)x_i(t)| \le \int_0^t \mathrm{d}s(t-s)\frac{C}{N}\sum_{j\neq i}^N |D(I)\left(x_i(s)-x_j(s)\right)| + M_i(t),$$

where the term $M_i(t)$ can be computed from (A.1) according to the Leibniz rule. Let $\mathcal{P}_n := \{I_1, \ldots, I_n\}$ be a partition of the set I of cardinality n, with $2 \leq n \leq k$, then we have:

$$\begin{aligned} M_i(t) &\leq \int_0^t \mathrm{d}s(t-s)\frac{1}{N}\sum_{j\neq i}^{N}\sum_{n=2}^{k}\sum_{\mathcal{P}_n} C(\mathcal{P}_n)\left|\prod_{H\in\mathcal{P}_n}[D(H)(x_i(s)-x_j(s))]\right| \leq \\ &\leq \int_0^t \mathrm{d}s(t-s)\sum_{n=2}^{k}\sum_{\mathcal{P}_n} C(\mathcal{P}_n)\frac{1}{N}\sum_{j=1}^{N}\left|\prod_{H\in\mathcal{P}_n}[D(H)(x_i(s)-x_j(s))]\right|, \end{aligned} \tag{A.12}$$

where $D(H) := \prod_{h\in H}\frac{\partial}{\partial v_h}$ and $C(\mathcal{P}_n)$ are coefficients depending on the partition $\mathcal{P}_n$ and on suitable derivatives of F. By (A.11), it follows that:

$$\frac{1}{N}\sum_{i=1}^{N}|D(I)x_i(t)| \leq \int_0^t \mathrm{d}s(t-s)\frac{C}{N}\sum_{i=1}^{N}|D(I)x_i(s)| + M(t), \tag{A.13}$$

where $M(t) = \frac{1}{N}\sum_{i=1}^{N} M_i(t)$ and, by (A.12), we have:

$$M(t) \leq \int_0^t \mathrm{d}s(t-s)\sum_{n=2}^{k}\sum_{\mathcal{P}_n} C(\mathcal{P}_n)\frac{1}{N^2}\sum_{i=1}^{N}\sum_{j=1}^{N}\left|\prod_{H\in\mathcal{P}_n}[D(H)(x_i(s)-x_j(s))]\right|, \tag{A.14}$$

We observe that:

$$\begin{aligned} &\frac{1}{N^2}\sum_{i,j=1}^{N}\left|\prod_{H\in\mathcal{P}_n}[D(H)\,(x_i(s)-x_j(s))]\right| \leq \\ &\leq \frac{1}{N}\sum_{i=1}^{N}\prod_{H\in\mathcal{P}_n}|D(H)x_i(s)| + \frac{1}{N}\sum_{j=1}^{N}\prod_{H\in\mathcal{P}_n}|D(H)x_j(s)| + \\ &\quad + \sum_{\mathcal{Q}\subset\mathcal{P}_n} C(\mathcal{Q})\left(\frac{1}{N}\sum_{i=1}^{N}\prod_{Q\in\mathcal{Q}}|D(Q)x_i(s)|\right)\left(\frac{1}{N}\sum_{j=1}^{N}\prod_{J\in\mathcal{P}_n\setminus\mathcal{Q}}|D(J)x_j(s)|\right), \end{aligned} \tag{A.15}$$

where $\mathcal{Q}$ is any subpartition of $\mathcal{P}_n$ and $C(\mathcal{Q})$ are coefficients depending on $\mathcal{Q}$.

We assume that the estimate (A.10) holds for any $m \leq k-1$, namely:

$$\frac{1}{N}\sum_{i=1}^{N}|D(M)x_i(t)| \leq \frac{C}{N^{d_m}}, \quad \text{for any } M\subset I \text{ s.t. } |M| = m \leq k-1, \tag{A.16}$$

where d_m is the number of different indices in the sequence M.

Indeed, if we consider a partition $\mathcal{P}_n$ of cardinality $n \geq 2$, we are guaranteed that $|M| \leq k-1$ for each $M \in \mathcal{P}_n$. Then, by noting that:

$$\frac{1}{N}\sum_{i=1}^{N} \prod_{H\in\mathcal{H}} |D(H)x_i(t)| \leq \prod_{H\in\mathcal{H}} \frac{1}{N}\sum_{i=1}^{N} |D(H)x_i(t)|\,,\ \forall \text{ subpartition } \mathcal{H} \subseteq \mathcal{P}_n, \tag{A.17}$$

we can apply the inductive hypotheses (tag A.16) to estimate the derivatives of $x_i(s)$ and $x_j(s)$ appearing in (A.15). Thus, we obtain:

$$\begin{aligned} \frac{1}{N}\sum_{i=1}^{N} \prod_{H\in\mathcal{P}_n} |D(H)x_i(s)| &\leq \prod_{H\in\mathcal{P}_n} \frac{1}{N}\sum_{i=1}^{N} |D(H)x_i(s)| \leq \\ &\leq \prod_{H\in\mathcal{P}_n} \frac{C}{N^{d_h}} = \frac{C}{N^{\sum d_h}} \leq \frac{C}{N^{d_k}}, \end{aligned} \tag{A.18}$$

where d_h is the number of different indices in the sequence H and we used that $\sum_{H\in\mathcal{P}_n} d_h \geq d_k$.

In a similar way, we find

$$\frac{1}{N}\sum_{i=1}^{N} \prod_{Q\in\mathcal{Q}} |D(Q)x_i(s)| \leq \prod_{Q\in\mathcal{Q}} \frac{C}{N^{d_q}}, \tag{A.19}$$

where d_q is the number of different indices in the sequence Q.

Moreover, we have:

$$\frac{1}{N}\sum_{j=1}^{N} \prod_{H\in\mathcal{P}_n} |D(H)x_j(s)| \leq \prod_{H\in\mathcal{P}_n} \frac{C}{N^{d_h}} = \frac{C}{N^{\sum d_h}} \leq \frac{C}{N^{d_k}}, \tag{A.20}$$

and

$$\frac{1}{N}\sum_{j=1}^{N} \prod_{J\in\mathcal{P}_n\setminus\mathcal{Q}} |D(J)x_j(s)| \leq \prod_{J\in\mathcal{P}_n\setminus\mathcal{Q}} \frac{C}{N^{d_j}}, \tag{A.21}$$

where d_j is the number of different indices in the sequence J. Then, putting together (A.19) and (A.21), we find:

$$\begin{aligned} &\sum_{\mathcal{Q}\subset\mathcal{P}_n} C(\mathcal{Q}) \left(\frac{1}{N}\sum_{i=1}^{N} \prod_{Q\in\mathcal{Q}} |D(Q)x_i(s)|\right) \left(\frac{1}{N}\sum_{j=1}^{N} \prod_{J\in\mathcal{P}_n\setminus\mathcal{Q}} |D(J)x_j(s)|\right) \leq \\ &\leq \sum_{\mathcal{Q}\subset\mathcal{P}_n} C(\mathcal{Q}) \prod_{Q\in\mathcal{Q}} \prod_{J\in\mathcal{P}_n\setminus\mathcal{Q}} \frac{C}{N^{d_q+d_j}} \leq \sum_{\mathcal{Q}\subset\mathcal{P}_n} C(\mathcal{Q}) \prod_{Q\in\mathcal{Q}} \prod_{J\in\mathcal{P}_n\setminus\mathcal{Q}} \frac{C}{N^{d_k}} \leq \frac{C}{N^{d_k}}. \end{aligned} \tag{A.22}$$

In the end, we have just proven that each term in (A.15) is bounded by $\frac{C}{N^{d_k}}$. Therefore, by using this estimate in (A.14), we find:

$$M(t) \leq \frac{C}{N^{d_k}}. \tag{A.23}$$

By (A.23) and (A.13), it follows that:

$$\frac{1}{N}\sum_{i=1}^{N} |D(I)x_i(t)| \leq \int_0^t \mathrm{d}s(t-s)\frac{C}{N}\sum_{i=1}^{N} |D(I)x_i(s)| + \frac{C}{N^{d_k}}. \tag{A.24}$$

Therefore, by using the Gronwall lemma, we find:

$$\frac{1}{N}\sum_{i=1}^{N} |D(I)x_i(t)| \leq \frac{C}{N^{d_k}}. \tag{A.25}$$

As regard to the derivatives of $v_i(t)$ with respect to some initial velocities $v_{j_1}, \ldots,$ v_{j_k}, an analogous estimate holds and the proof works in the same way. Furthermore, this strategy leads to the same estimate for the derivatives of the function $\frac{1}{N}\sum_{i=1}^{N} z_i(t)$ with respect to some initial positions $x_{j_1}, \ldots, x_{j_k}$.

Now, thanks to the estimate we have just proven for the derivatives of the function $\frac{1}{N}\sum_{i=1}^{N} z_i(t)$, we are able to prove the claim of Proposition 4.4.1. In fact, we have:

$$\frac{1}{N}\sum_{i=1}^{N} |D(I)z_i(t)| = \frac{1}{N}\sum_{\substack{i=1\\ i\in D}}^{N} |D(I)z_i(t)| + \frac{1}{N}\sum_{\substack{i=1\\ i\notin D}}^{N} |D(I)z_i(t)| \leq \frac{C}{N^{d_k}}, \tag{A.26}$$

where $D \subset I$ contains the different indices appearing in the sequence I. Thus, according to our previous notation, $|D| = d_k$ and we denote the elements of D by $\tilde{j}_1, \ldots, \tilde{j}_{d_k}$. Then by (A.26) we find:

$$\begin{aligned} \frac{1}{N}\sum_{i=1}^{N} |D(I)z_i(t)| &= \frac{1}{N}\left|D(I)z_{\tilde{j}_1}(t)\right| + \cdots + \frac{1}{N}\left|D(I)z_{\tilde{j}_{d_k}}(t)\right| + \\ &\quad + \frac{1}{N}\sum_{\substack{i=1\\ i\notin D}}^{N} |D(I)z_i(t)| \leq \frac{C}{N^{d_k}}, \end{aligned} \tag{A.27}$$

which implies

$$|D(I)z_i(t)| \leq C\left(\frac{\sum_{\ell=1}^{d_k}\delta_{i\tilde{j}_\ell}}{N^{d_k-1}} + \frac{1}{N^{d_k}}\right), \tag{A.28}$$

or

$$|D(I)z_i(t)| \leq \frac{C}{N^{d_k^{(i)}}}, \tag{A.29}$$

where $d_k^{(i)}$ is the number of different indices in the sequence I which are also different from i.

– Appendix B

Proof of Proposition 4.1.1

Let $U_h(t,s)$ be the two parameters semigroup solution of the linear problem:

$$\begin{cases} (\partial_t + v\cdot\nabla_x)\, U_h(t,s)\gamma_0 = (\nabla\phi * h) * \nabla_v U_h(t,s)\gamma_0, \\ U_h(s,s)\gamma_0 = \gamma_0. \end{cases} \tag{B.1}$$

The solution of (B.1) is obtained by carrying the initial datum γ_0 along the characteristic flow

$$\begin{cases} \dot{x} = v, \\ \dot{v} = -\nabla\phi * h. \end{cases} \tag{B.2}$$

Next, we consider the problem

$$\begin{cases} (\partial_t + v\cdot\nabla_x)\,\tilde{\gamma} = L(h)\tilde{\gamma}, \\ \tilde{\gamma}|_{t=0} = \gamma_0. \end{cases} \tag{B.3}$$

which can be reformulated in integral form:

$$\tilde{\gamma}(t) = U_h(t,0)\gamma_0 + \int_0^t \mathrm{d}s\, U_h(t,s)\left[(\nabla\phi * \tilde{\gamma}(s))\cdot\nabla_v h(s)\right]. \tag{B.4}$$

The above formula can be iterated to yield the formal solution

$$\begin{aligned} &\tilde{\gamma}(x,v;t) = U_h(t,0)\gamma_0(x,v) + \\ &+\sum_{n\geq 1}\int_0^t \mathrm{d}t_1 \int_0^{t_1}\mathrm{d}t_2\cdots\int_0^{t_{n-1}}\mathrm{d}t_n \int \mathrm{d}x_1\int\mathrm{d}v_1\cdots\int\mathrm{d}x_n\int\mathrm{d}v_n \\ &U_h(t,t_1)\left[\nabla_v h(x,v;t_1)\cdot\nabla_x\phi(x-x_1)\right] \\ &U_h(t_1,t_2)\left[\nabla_{v_1} h(x_1,v_1;t_2)\cdot\nabla_{x_1}\phi(x_1-x_2)\right] \\ &\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots \\ &U_h(t_{n-1},t_n)\left[\nabla_{v_{n-1}} h(x_{n-1},v_{n-1};t_n)\cdot\nabla_{x_{n-1}}\phi(x_{n-1}-x_n)\right] \\ &U_h(t_n,0)\gamma_0(x_n,v_n). \end{aligned} \tag{B.5}$$

We remark that $U_h(t_k, t_{k+1})$ acts on the variables x_k, v_k with the convention that $(x_0, v_0) = (x, v)$ and, furthermore, U_h is multiplicative and preserves the $L^p(\mathbb{R}^3 \times \mathbb{R}^3)$ norms $(p = 1, 2, \dots, \infty)$.

Under the assumptions of Proposition 4.1.1, the above series is bounded in $L^1(\mathbb{R}^3 \times \mathbb{R}^3)$ by:

$$\sum_{n\geq 0} \frac{t^n}{n!} \left(\sup_{\tau\in[0,t]} \|\nabla_v h(\tau)\|_{L^1(\mathbb{R}^3\times\mathbb{R}^3)}\right)^n \|\nabla_x \phi\|^n_{L^\infty(\mathbb{R}^3)} \|\gamma_0\|_{L^1(\mathbb{R}^3\times\mathbb{R}^3)}, \tag{B.6}$$

which is converging for each t. Now, we denote by $\Sigma_h(t, s) : L^1(\mathbb{R}^3 \times \mathbb{R}^3) \to L^1(\mathbb{R}^3 \times \mathbb{R}^3)$, the two parameters semigroup given by the series (B.5). Then, the solution γ to the problem (4.1.14) is given by:

$$\gamma(t) = \Sigma_h(t, 0)\gamma_0 + \int_0^t \mathrm{d}s\ \Sigma_h(t, s)\Theta(s), \tag{B.7}$$

and, thanks to the assumption we made on Θ and to the fact that the above series (B.5) is converging for any t, we are guaranteed that $\gamma \in \mathcal{C}^0(L^1(\mathbb{R}^3 \times \mathbb{R}^3), \mathbb{R}^+)$.

The $\mathcal{C}^k$ regularity of $\tilde{\gamma}(t) = \Sigma_h(t, 0)\gamma_0$ follows by (B.5) and the fact that $U_h(t, t_1)$ propagates the $\mathcal{C}^k$ regularity. ∎

Proof of Proposition 4.5.1

The proof consists of two steps.

Step 1):

Let γ_N be as in Proposition 4.5.1. Then, we show that γ_N solves the problem:

$$\begin{cases} (\partial_t + v \cdot \nabla_x)\, \gamma_N = L(h)\gamma_N + \Theta'_N, \\ \gamma_N|_{t=0} = \gamma_{N,0}, \end{cases} \tag{B.8}$$

with

$$\Theta'_N = \Theta_N + R_N, \tag{B.9}$$

and R_N is such that:

$$R_N \to 0, \quad \mathcal{C}^\infty_b - \text{weakly}. \tag{B.10}$$

In proving (B.10), the assumption **ii)** on γ_N is crucial.

Step 2):

By virtue of Step 1), the hypotheses we made on $\nabla_v h$ and Proposition 4.1.1, we find that:

$$\gamma_N(t) = \Sigma_h(t, 0)\gamma_{N,0} + \int_0^t \mathrm{d}s\ \Sigma_h(t, s)\Theta'_N(s). \tag{B.11}$$

Then, reminding that:

- $h(t) \in \mathcal{C}_b^\infty(\mathbb{R}^3 \times \mathbb{R}^3)$ for any t,
- the flow Σ_h propagates the $\mathcal{C}^k$ regularity,
- $R_N \to 0, \quad \mathcal{C}_b^\infty$ – weakly,

and by virtue of the assumptions on $\gamma_{N,0}$ and Θ_N, we can easily show that:

(B.12) $$\gamma_N \to \gamma, \quad \text{as} \quad N \to \infty, \quad \mathcal{C}_b^\infty - \text{weakly},$$

where

(B.13) $$\gamma(t) = \Sigma_h(t,0)\gamma_0 + \int_0^t \mathrm{d}s\, \Sigma_h(t,s)\Theta(s).$$

Therefore, we recognize that γ solves the problem (4.1.14) and, by virtue of Proposition 4.1.1, it is uniquely determined by (B.13) and hence it is in $\mathcal{C}^0(L^1(\mathbb{R}^3 \times \mathbb{R}^3), \mathbb{R}^+)$.

Proof of Step 1):

We have:

(B.14) $$\begin{cases} (\partial_t + v \cdot \nabla_x)\,\gamma_N = L(h)\gamma_N + \Theta_N + L(h_N - h)\gamma_N \\ \gamma_N(x,v;t)\big|_{t=0} = \gamma_{N,0}(x,v), \end{cases}$$

where

(B.15) $$R_N = R_N(x,v;t) := L(h_N - h)\gamma_N.$$

We want to show that $R_N \to 0$, $\mathcal{C}_b^\infty$-weakly. According to the definition of the operator L, we have:

(B.16) $$R_N = (\nabla_x\phi * (h_N - h))\nabla_v\gamma_N + (\nabla_x\phi * \gamma_N)\nabla_v(h_N - h),$$

thus, we have to show that

(B.17) $$(u, (\nabla_x\phi * (h_N - h))\nabla_v\gamma_N) \to 0, \quad \text{as} \quad N \to \infty, \quad \forall\, u \in \mathcal{C}_b^\infty(\mathbb{R}^3 \times \mathbb{R}^3),$$

and

(B.18) $$(u, (\nabla_x\phi * \gamma_N)\nabla_v(h_N - h)) \to 0, \quad \text{as} \quad N \to \infty, \quad \forall\, u \in \mathcal{C}_b^\infty(\mathbb{R}^3 \times \mathbb{R}^3).$$

We show only (B.18) in detail because (B.17) will follow the same line. We have:

(B.19) $$\begin{aligned} &(u, (\nabla_x\phi * \gamma_N)\nabla_v(h_N - h)) = \\ &= \int \mathrm{d}x\mathrm{d}v \int \mathrm{d}y\mathrm{d}w\, u(x,v)\nabla_x\phi(x-y)\gamma_N(y,w;t)\nabla_v(h_N(x,v;t) - h(x,v;t)) = \\ &= -\int \mathrm{d}x\mathrm{d}v \int \mathrm{d}y\mathrm{d}w \nabla_v u(x,v)\nabla_x\phi(x-y)\gamma_N(y,w;t)(h_N(x,v;t) - h(x,v;t)) = \\ &= \int \mathrm{d}x\mathrm{d}v \int \mathrm{d}y\mathrm{d}w\, \nabla_v u(x,v)(\nabla_x\phi * \gamma_N)(x,v;t)(h - h_N)(x,v;t). \end{aligned}$$

Setting

$$\zeta_N(x,v) := \nabla_v u(x,v) \int \mathrm{d}y\mathrm{d}w \nabla_x \phi(x-y)\gamma_N(y,w;t), \tag{B.20}$$

we can write (B.19) as:

$$\begin{aligned}(u, (\nabla_x\phi * \gamma_N)\nabla_v(h_N - h)) &= \int \mathrm{d}x\mathrm{d}v\, \zeta_N(x,v)(h(x,v;t) - h_N(x,v;t)) = \\ &= \int \mathrm{d}x\mathrm{d}v \int \mathrm{d}x'\mathrm{d}v'\, (\zeta_N(x,v) - \zeta_N(x',v'))\, P_N(x,v;x',v';t),\end{aligned} \tag{B.21}$$

where P_N is a coupling of h and h_N, namely a probability density in $\mathbb{R}^6 \times \mathbb{R}^6$ with marginals given by h and h_N. Now we observe that:

$$\nabla_{x,v}\zeta_N(x,v) := \int \mathrm{d}y\mathrm{d}w \nabla_{x,v} \left[\nabla_v u(x,v)\nabla_x\phi(x-y)\right] \gamma_N(y,w;t), \tag{B.22}$$

and, thanks to the assumption **ii)** we made on γ_N, we know that there exists a constant $C = C(u,\phi) > 0$ such that:

$$\sup_{x,v} |\nabla_{x,v}\zeta_N(x,v)| = \|\nabla\zeta_N\|_{L^\infty(\mathbb{R}^3\times\mathbb{R}^3)} < C < +\infty. \tag{B.23}$$

Therefore, coming back to (B.21), we find:

$$\begin{aligned}|(u, (\nabla_x\phi * \gamma_N)\nabla_v(h_N - h))| &\leq \int \mathrm{d}z \int \mathrm{d}z'\, |\zeta_N(z) - \zeta_N(z')|\, P_N(z;z';t) \\ &\leq \int \mathrm{d}z \int \mathrm{d}z' C\, |z - z'|\, P_N(z;z';t).\end{aligned} \tag{B.24}$$

where we used the standard notation $z = (x,v)$ and $z' = (x',v')$. Then, taking in (B.24) the infimum over all couplings between h and h_N, we obtain that:

$$|(u, (\nabla_x\phi * \gamma_N)\nabla_v(h_N - h))| \leq C\mathcal{W}(h_N, h), \tag{B.25}$$

where, as in Section 1.2, $\mathcal{W}$ denotes the Wasserstein distance. But we know that the right hand side of (B.25) goes to zero because of the assumption **i)**, then we have just proven that:

$$|(u, (\nabla_x\phi * \gamma_N)\nabla_v(h_N - h))| \to 0, \quad \forall\, u \in \mathcal{C}_b^\infty(\mathbb{R}^3 \times \mathbb{R}^3). \tag{B.26}$$

Analogously, we can prove that

$$|(u, (\nabla_x\phi * (h_N - h))\nabla_v\gamma_N)| \to 0, \quad \forall\, u \in \mathcal{C}_b^\infty(\mathbb{R}^3 \times \mathbb{R}^3). \tag{B.27}$$

Therefore we have just proven that R_N goes to zero in the $\mathcal{C}_b^\infty$-weak sense and the proof of Step 1) is done.

Proof of Step 2).

Thanks to Step 1) and to the assumption on $\nabla_v h$, we know that $\gamma_N(t)$ can be written as in (B.11). Then, for any function u in $\mathcal{C}_b^\infty(\mathbb{R}^3 \times \mathbb{R}^3)$, we have that:

$$(u, \gamma_N(t)) = (u, \Sigma_h(t,0)\gamma_{N,0}) + \int_0^t \mathrm{d}s\; (u, \Sigma_h(t,s)\Theta'_N(s)), \tag{B.28}$$

namely

$$(u, \gamma_N(t)) = \left((\Sigma_h(t,0))^* u, \gamma_{N,0}\right) + \int_0^t \mathrm{d}s\; \left((\Sigma_h(t,s))^* u, \Theta'_N(s)\right), \tag{B.29}$$

where Σ_h^* is the adjoint of Σ_h. We remind that the two-parameters semigroup $\Sigma_h(t,s)$ propagates the $\mathcal{C}^k$ regularity, provided that $\nabla_v h \in \mathcal{C}^k(\mathbb{R}^3 \times \mathbb{R}^3)$. In particular, if Σ_h acts on a function u which is in $\mathcal{C}_b^\infty(\mathbb{R}^3 \times \mathbb{R}^3)$ and the function $h(t)$ is supposed to be in $\mathcal{C}_b^\infty(\mathbb{R}^3 \times \mathbb{R}^3)$ for any t, as it is in the assumptions of Proposition 4.5.1, we are clearly guaranteed that $\nabla_v h(t)$ is in $\mathcal{C}_b^\infty(\mathbb{R}^3 \times \mathbb{R}^3)$ for any t, and then, $u(t) := \Sigma_h(t,0)u(x,v)$ is also in $\mathcal{C}_b^\infty(\mathbb{R}^3 \times \mathbb{R}^3)$ for any t. Obviously, the same holds for Σ_h^*. Thus, the functions $(\Sigma_h(t,0))^* u$ and $(\Sigma_h(t,s))^* u$ appearing in (B.29) are in $\mathcal{C}_b^\infty(\mathbb{R}^3 \times \mathbb{R}^3)$ for any t. Therefore, thanks to the assumptions we made on $\gamma_{N,0}$ and Θ_N, and of what we know about R_N, we find that:

$$\begin{aligned} &\left((\Sigma_h(t,0))^* u, \gamma_{N,0}\right) + \int_0^t \mathrm{d}s\; ((\Sigma_h(t,s))^* u, \Theta'_N(s)) \\ &\qquad \downarrow \qquad N \to \infty \\ &\left((\Sigma_h(t,0))^* u, \gamma_0\right) + \int_0^t \mathrm{d}s\; ((\Sigma_h(t,s))^* u, \Theta(s)) = \\ &= (u, \Sigma_h(t,0)\gamma_0) + \int_0^t \mathrm{d}s\; (u, \Sigma_h(t,s)\Theta(s)). \end{aligned} \tag{B.30}$$

Finally, by Proposition 4.1.1, we know that the expression (B.30) identifies properly the unique solution of the problem (4.1.14) in $\mathcal{C}^0(L^1(\mathbb{R}^3 \times \mathbb{R}^3), \mathbb{R}^+)$ and Proposition 4.5.1 is proven. ∎

– Appendix C

Lemma C.1. *For each time $\tau > 0$, let us define the operator $\hat{T}_N^{(n)}(\tau)$ as follows:*

$$\hat{T}_N^{(n)}(\tau) := S_N(-\tau)\hat{T}_N^{(n)} S_N(\tau).$$

Then, for each $m \geq 0$ and for each $u \in \mathcal{C}_b^\infty(\mathbb{R}^3 \times \mathbb{R}^3)$, there exists a constant $C > 0$, not depending on N, such that:

$$\text{(C.1)} \qquad \textbf{i)} \left|\left(u, \hat{T}_N^{(r_m)}(t_m)\dots\hat{T}_N^{(r_1)}(t_1)\mu_N(t)\right)\right| < C.$$

Moreover, we have:

$$\text{(C.2)} \qquad \begin{aligned} &\textbf{ii)} \left|\left(u, T_N^{(r_m)}(t_m)\dots T_N^{(r_1)}(t_1)\mu_N(t)\right)\right| \leq \\ &\leq \left|\left(u, \hat{T}_N^{(r_m)}(t_m)\dots\hat{T}_N^{(r_1)}(t_1)\mu_N(t)\right)\right| + O\left(\frac{1}{N}\right). \end{aligned}$$

Proof. We observe that:

$$\text{(C.3)} \qquad \begin{aligned} &\left(u, \hat{T}_N^{(r_m)}(t_m)\dots\hat{T}_N^{(r_1)}(t_1)\mu_N(t)\right) = \\ &= \hat{T}_N^{(r_m)}(t_m)\hat{T}_N^{(r_{m-1})}(t_{m-1})\dots\hat{T}_N^{(r_1)}(t_1)\mathcal{U}(Z_N(t)), \end{aligned}$$

where:

$$\text{(C.4)} \qquad \mathcal{U}(Z_N(t)) := (u, \mu_N(t)) = \frac{1}{N}\sum_{\ell=1}^{N} u(z_\ell(t)).$$

We assume $m > 0$ being the case $m = 0$ obvious.

By using the notations:

$$\text{(C.5)} \qquad S(\underline{\mathbf{r}}_m, \underline{\mathbf{t}}_m) := T_N^{(r_m)}(t_m)\dots T_N^{(r_1)}(t_1)$$

and

$$\text{(C.6)} \qquad \hat{S}(\underline{\mathbf{r}}_m, \underline{\mathbf{t}}_m) := \hat{T}_N^{(r_m)}(t_m)\dots\hat{T}_N^{(r_1)}(t_1),$$

we have (see the first term in the right hand side of (4.6.15)):

$$\text{(C.7)} \qquad \begin{aligned} &\hat{S}(\underline{\mathbf{r}}_m, \underline{\mathbf{t}}_m)\mathcal{U}(Z_N(t)) = \\ &= \frac{C}{N^m}\sum_{j_1\dots j_m}\sum_{l_1\dots l_m} D_x^{r_m+1}\phi(x_{j_m}(t_m) - x_{l_m}(t_m)) \cdot D_{v_{j_m}}^{r_m+1}(t_m) \\ &D_x^{r_{m-1}+1}\phi(x_{j_{m-1}}(t_{m-1}) - x_{l_{m-1}}(t_{m-1}))D_{v_{j_{m-1}}}^{r_{m-1}+1}(t_{m-1}) \\ &\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots \\ &D_x^{r_1+1}\phi(x_{j_1}(t_1) - x_{l_1}(t_1)) \cdot D_{v_{j_1}}^{r_1+1}(t_1)U(Z_N(t)), \end{aligned}$$

C depending on $\underline{\mathbf{r}}_m$.

By setting:

$$\Phi_{j_n}(Z_N(t_n)) := \frac{1}{N}\sum_{l_n=1}^{N} D_x^{r_n+1}\phi(x_{j_n}(t_n) - x_{l_n}(t_n)) \qquad \forall\, n = 1, 2, \dots, m \tag{C.8}$$

(C.7) can be rewritten as

$$\begin{aligned}\hat{S}(\underline{\mathbf{r}}_m, \underline{\mathbf{t}}_m)\mathcal{U}(Z_N(t)) = C \sum_{j_1\cdots j_m} &\Phi_{j_m}(Z_N(t_m)) \cdot D_{v_{j_m}}^{r_m+1}(t_m)\\ &\times \Phi_{j_{m-1}}(Z_N(t_{m-1})) \cdot D_{v_{j_{m-1}}}^{r_{m-1}+1}(t_{m-1}) \dots\\ &\dots \Phi_{j_1}(Z_N(t_1)) \cdot D_{v_{j_1}}^{r_1+1}(t_1) U(Z_N(t)).\end{aligned} \tag{C.9}$$

We observe that, thanks to the smoothness of the potential ϕ, Φ_{j_n} (for each n) is a uniformly bounded function of the configuration Z_N, together with its derivatives.

Performing the derivatives in (C.9), we realize that $\hat{S}(\underline{\mathbf{r}}_m, \underline{\mathbf{t}}_m)\mathcal{U}(Z_N(t))$ is a linear combination of terms of the following type:

$$\begin{aligned}&\sum_{j_1\cdots j_m} \Phi_{j_m}(Z_N(t_m)) \cdot D_{v_{j_m}}^{a_{m,1}}(t_m) \dots D_{v_{j_2}}^{a_{2,1}}(t_2) D_{v_{j_1}}^{a_{1,1}}(t_1) U(Z_N(t))\\ &D_{v_{j_m}}^{a_{m,2}}(t_m) \dots D_{v_{j_2}}^{a_{2,2}}(t_2)\Phi_{j_1}(Z_N(t_1))\\ &\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\dots\\ &D_{v_{j_m}}^{a_{m,m-1}}(t_m) D_{v_{j_{m-1}}}^{a_{m-1,m-1}}(t_{m-1})\Phi_{j_{m-2}}(Z_N(t_{m-2})\\ &D_{v_{j_m}}^{a_{m,m}}(t_m)\Phi_{j_{m-1}}(Z_N(t_{m-1})),\end{aligned} \tag{C.10}$$

with the constraint

$$\begin{cases} a_{1,1} = r_1 + 1\\ a_{2,1} + a_{2,2} = r_2 + 1\\ \dots\\ a_{m,1} + a_{m,2} + \dots + a_{m,m} = r_m + 1. \end{cases} \tag{C.11}$$

For a fixed sequence $a_{\ell,s}$, we have to compensate the divergence arising from the sum $\sum_{j_1\cdots j_m}$, which is $O(N^m)$, by the decay of the derivatives as given by Proposition 4.4.1 and Corollary 4.4.1. Indeed we have:

$$\left| D_{v_{j_m}}^{a_{m,1}}(t_m) \dots D_{v_{j_2}}^{a_{2,1}}(t_2) D_{v_{j_1}}^{a_{1,1}}(t_1)\mathcal{U}(Z_N(t))\right| \le \frac{C}{N^d}, \tag{C.12}$$

where d is the number of different indices in the sequence $j_1, j_2, \dots, j_m$ for which $a_{m,1}, \dots, a_{2,1}, a_{1,1}$ are strictly positive. Note that the fact that the derivatives are not computed at time $t = 0$ but at different times $t_1, t_2, \dots, t_m$, does not change the estimate in an essential way.

An analogous estimate holds when we replace $\mathcal{U}$ by some Φ_{j_s}, namely

$$\left| D^{a_{m,k}}_{v_{j_m}}(t_m) D^{a_{m-1,k}}_{v_{j_{m-1}}}(t_{m-1}) \dots D^{a_{k,k}}_{v_{j_k}}(t_k) \Phi_{j_{k-1}}(Z_N(t_{k-1})) \right| \le \frac{C}{N^{d_{k-1}}}, \tag{C.13}$$

where d_{k-1} is the number of different indices in the sequence $j_k, \dots, j_m$ which are also different from j_{k-1} and from which $a_{m,k}, \dots, a_{k,k}$ are strictly positive.

As regard to the term in the sum $\sum_{j_1 \dots j_m}$ in which all the indices are different (which is the only one of size $O(N^m)$), the constraints (C.11) together with estimates (C.12) and (C.13) ensure that the product of derivatives on the right hand side of (C.10) is bounded by $1/N^m$. Thus this term is of order one. Now for each $s = 1, \dots, m-1$ consider the $\frac{m!}{s!(m-s)!}$ terms in the sum $\sum_{j_1 \dots j_m}$ in which s indices are equal. The sum is bounded by N^{m-s}. On the other hand, the constraints (C.11) together with (C.12) and (C.13) ensure that the product of derivatives on the right hand side of (C.10) is bounded by $1/N^{m-s}$. Thus even these terms are of size one and **i)** is proven.

To prove **ii)** we observe that:

$$S(\underline{\mathbf{r}}_m, \underline{\mathbf{t}}_m)\mathcal{U}(Z_N(t)) - \hat{S}(\underline{\mathbf{r}}_m, \underline{\mathbf{t}}_m)\mathcal{U}(Z_N(t)) \tag{C.14}$$

can be expanded as in (C.7) and (C.10). However now we have an extra derivative, arising from the definition of $R_N^{(n)}$ (see (4.2.16)), which yields an additional $1/N$. We omit the details of the proof which follows the same line of **i)**. □

In the same way we can also prove the following

Lemma C.2. *For each $m \ge 0$, $k > 0$ and $u \in \mathcal{C}_b^\infty(\mathbb{R}^3 \times \mathbb{R}^3)$, there exists a constant $C > 0$, not depending on N, such that:*

$$\left| \mathcal{D}^{2k} S(\underline{\mathbf{r}}_m, \underline{\mathbf{t}}_m)\mathcal{U}(Z_N(t)) \right| < C.$$

where $\mathcal{U}(Z_N(t))$ is defined as in (C.4).

Proof. First we look at the case $m > 0$. Reminding the structure of the operator $\mathcal{D}^{2k}$ (see (4.6.3)), we are led to consider the term $D^{2s_j}_{G,j}\hat{S}(\underline{\mathbf{r}}_m, \underline{\mathbf{t}}_m)\mathcal{U}(Z_N(t))$. We remind that $D^{2s_j}_{G,j}$ is a derivation operator with respect to the variable z_j that acts as specified by (4.5.8). By the expansion (C.10) we readily arrive to the bound:

$$\left| D^{2s_j}_{G,j}\hat{S}(\underline{\mathbf{r}}_m, \underline{\mathbf{t}}_m)\mathcal{U}(Z_N(t)) \right| \le \frac{C}{N}. \tag{C.16}$$

Indeed by applying $D^{2s_j}_{G,j}$ to (C.10) either $j \notin (j_1 \dots j_m)$ so that we gain $1/N$ by the extra derivative, or $j \in (j_1 \dots j_m)$ so that we reduce the sum $\sum_{j_1 \dots j_m}$ by a factor $1/N$. More generally, by the same argument we find:

$$\left| \prod_{j \in I} D^{2s_j}_{G,j} \hat{S}(\underline{\mathbf{r}}_m, \underline{\mathbf{t}}_m) \mathcal{U}(Z_N(t)) \right| \leq \frac{C}{N^n}, \tag{C.17}$$

where $n = |I|$.

Finally by writing the action of the operator $\mathcal{D}^{2k}$ as in (4.6.35), we obtain

$$\begin{aligned} \left| \mathcal{D}^{2k} \hat{S}(\underline{\mathbf{r}}_m, \underline{\mathbf{t}}_m) \mathcal{U}(Z_N(t)) \right| &\leq \sum_{n=1}^{N} \frac{N!}{n!(N-n)!} \sum_{\substack{s_1 \dots s_n \\ 1 \leq s_j \leq k \\ \sum_j s_j = k}} \frac{C}{N^n} \leq \\ &\leq B^k \sum_{n=1}^{N} \frac{N!}{n!(N-n)!} \frac{C^n}{N^n} \leq B^k \left(1 + \frac{C}{N}\right)^N \leq C, \end{aligned} \tag{C.18}$$

B, C being positive constants not depending on N. Again $\mathcal{D}^{2k} \hat{S}(\underline{\mathbf{r}}_m, \underline{\mathbf{t}}_m) \mathcal{U}(Z_N (t))$ is the leading term of $\mathcal{D}^{2k} S(\underline{\mathbf{r}}_m, \underline{\mathbf{t}}_m) \mathcal{U}(Z_N(t))$ for the same reasons we discussed in Lemma C.1.

If $m = 0$, the estimates (C.16) and (C.17) follow directly by Proposition 5.2. Thus, even in this case, the proof is concluded by (C.18). ∎

The fact that the error term E^1_N (see (4.6.20)) and hence E^2_N (see (4.6.27)) are $\mathcal{C}^\infty_b$-weakly vanishing when $N \to \infty$ is an immediate consequence of the following

Lemma C.3. *Let $\underline{\mathbf{r}}_J$ and $\underline{\mathbf{t}}_J$ be defined as in Section 7, for any $J \subset I_n$ with $I_n = \{1, 2, \dots, n\}$. For any $r \geq 0$ we have:*

$$\begin{aligned} &\mathcal{D}^{2r} S(\underline{\mathbf{r}}_n, \underline{\mathbf{t}}_n) \mu_N(z'_1 | Z_N(t)) \mu_N(z'_2 | Z_N(t)) = \\ &= \sum_{0 \leq \ell \leq r} \sum_{0 \leq m \leq n} \sum_{\substack{I \subset I_n \\ |I| = m}} \left(\mathcal{D}^{2\ell} S(\underline{\mathbf{r}}_I, \underline{\mathbf{t}}_I) \mu_N(z'_1 | Z_N(t)) \right) \times \\ &\times \left(\mathcal{D}^{2(r-\ell)} S(\underline{\mathbf{r}}_{I_n \setminus I}, \underline{\mathbf{t}}_{I_n \setminus I}) \mu_N(z'_2 | Z_N(t)) \right) + e_{r,N} \end{aligned} \tag{C.19}$$

where

$$e_{r,N} \to 0 \text{ as } N \to \infty \quad \mathcal{C}^\infty_b - \text{weakly}. \tag{C.20}$$

PROOF.

It is enough to prove (C.19) and (C.20) replacing each streak S with the corresponding $\hat{S}$, being the difference $S - \hat{S}$ negligible in the limit.

We start by assuming $r = 0$. In that case, testing the left hand side of (C.19) against a product of two test functions u_1, u_2, we are led to consider:

$$\hat{S}(\underline{\mathbf{r}}_n, \underline{\mathbf{t}}_n)\mathcal{U}_1(Z_N(t))\mathcal{U}_2(Z_N(t)) \tag{C.21}$$

for which we can apply the expansion (C.7).

Proceeding as in the proof of Lemma C.1 (see (C.10)), we have to consider:

$$D^{a_{m,1}}_{v_{j_m}}(t_m)\dots D^{a_{2,1}}_{v_{j_2}}(t_2)D^{a_{1,1}}_{v_{j_1}}(t_1)\mathcal{U}_1(Z_N(t))\mathcal{U}_2(Z_N(t)), \tag{C.22}$$

where $a_{1,1} = r_1 + 1 > 0$. Now any contribution of the form

$$D^{\alpha}_{v_{j_1}}(t_1)\mathcal{U}_1(Z_N(t))D^{\beta}_{v_{j_1}}(t_1)\mathcal{U}_2(Z_N(t)), \tag{C.23}$$

with $\alpha > 0$, $\beta > 0$, $\alpha + \beta = a_{1,1}$ is $O\left(\frac{1}{N^2}\right)$, therefore it is negligible in the limit. The same argument applies to $D^{a_{k,1}}_{v_{j_k}}(t_k)$ whenever $a_{k,1} > 0$. This means that each derivative appearing in $\hat{S}$ either applies to $\mu_N(z_1'|Z_N(t))$ or to $\mu_N(z_2'|Z_N(t))$ up to an error $e_{0,N}$ vanishing in the limit. This is exactly what (C.19) and (C.20) say for $r = 0$.

For $r > 0$ we have to apply $\mathcal{D}^{2r}$ to (C.19) (replacing S by $\hat{S}$) with $r = 0$. Clearly $\mathcal{D}^{2r}e_{0,N}$ vanishes in the limit. Moreover:

$$\begin{aligned} &D^{2s_j}_{G,j}\left[\hat{S}(\underline{\mathbf{r}}_I, \underline{\mathbf{t}}_I)\mathcal{U}_1(Z_N(t))\hat{S}(\underline{\mathbf{r}}_{I_n\setminus I}, \underline{\mathbf{t}}_{I_n\setminus I})\mathcal{U}_2(Z_N(t))\right] = \\ &= \left(D^{2s_j}_{G,j}\hat{S}(\underline{\mathbf{r}}_I, \underline{\mathbf{t}}_I)\mathcal{U}_1(Z_N(t))\right)\hat{S}(\underline{\mathbf{r}}_{I_n\setminus I}, \underline{\mathbf{t}}_{I_n\setminus I})\mathcal{U}_2(Z_N(t)) + \\ &+ \hat{S}(\underline{\mathbf{r}}_I, \underline{\mathbf{t}}_I)\mathcal{U}_1(Z_N(t))\left(D^{2s_j}_{G,j}\hat{S}(\underline{\mathbf{r}}_{I_n\setminus I}, \underline{\mathbf{t}}_{I_n\setminus I})\mathcal{U}_2(Z_N(t))\right) + O\left(\frac{1}{N^2}\right) \end{aligned} \tag{C.24}$$

By simple algebraic manipulation we finally arrive to (C.19) and (C.20).

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Indirizzo dell'Autore:

Federica Pezzotti – Departamento de Matemáticas – Facultad de Ciencias y Tecnología – Universidad del Pais Vasco – Barrio Sarriena s/n – 48940 Lejona (Vizcaya) – Spain
E-mail: federica.pezzotti@ehu.es