MEAN-FIELD APPROXIMATION OF QUANTUM SYSTEMS AND CLASSICAL LIMIT

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Abstract. We prove that, for a smooth two-body potentials, the quantum mean-field approximation to the nonlinear Schrödinger equation of the Hartree type is stable at the classical limit $h \to 0$, yielding the classical Vlasov equation.

Introduction

Consider a system of N identical classical particles of unit mass, evolving according to the dynamics generated by the following mean-field Hamiltonian

$$\mathcal{H} = \sum_{i=1}^{N} \frac{1}{2} v_i^2 + \frac{1}{N} \sum_{i<j} \varphi(x_i - x_j). \tag{1}$$

If the two-body interaction φ is sufficiently smooth, the behavior of the system for large N is well understood (Seee for instance Ref.s [1],[2],[3]). Namely, if the initial positions and velocities of the particles are independently and identically distributed according to the probability density $f = f(x, v)$, in the limit $N \to \infty$ each particle is distributed at time t according to the distribution $f = f(x, v, t)$, independently from the others. Here $f(x, v, t)$ is the solution of the Vlasov equation

$$(\partial_t + v \cdot \nabla_x + E \cdot \nabla_v) f(x, v, t) = 0, \tag{2}$$

where

$$E(x,t) = -\nabla\varphi * \rho(x,t) \tag{3}$$

and

$$\rho(x,t) = \int dv f(x,v,t). \tag{4}$$

The quantum analogue of this result has been proved in [4]. The framework is a system of N identical bosons interacting by a mean-field potential energy

$$U(x_1,\ldots,x_N) = \frac{1}{N}\sum_{i<j}\varphi(x_i - x_j). \tag{5}$$

Then, if the initial wave function factorizes in the limit $N \to \infty$, each particle evolves according to the following nonlinear Schrödinger equation of the Hartree type:

$$(i\hbar\partial_t + \frac{\hbar^2}{2}\Delta - \varphi * \rho)\psi(t) = 0 \tag{6}$$

where

$$\rho(x,t) = |\psi(x,t)|^2. \tag{7}$$

and $*$ denotes convolution. Further results concerning the Coulomb interaction (see [5], [6]) have been also proved.

In all these results, however, the convergence is strongly dependent on $\hbar$. This dependence prevents (see the case of the Kac potential below) all situations in which $N \to \infty$ entails $\hbar \to 0$ and the system is therefore asymptotically classical.

In the present paper we address precisely this problem and show that the Vlasov equation is indeed recovered in the limit $N \to \infty$ even when $\hbar \to 0$ according to an arbitrary law.

The problem has been approached and solved in Ref. [7], where the the result is obtained via compactness techniques, under the hypothesis that the Fourier transform of φ is compactly supported. Here we deal with C^2 potentials and compute the explicit rate of convergence by means of a constructive method.

Our technique is based on the WKB method applied to the N-particle system. In the same spirit of Ref. [8] where the classical limit for a class of nonlinear Schrödinger equation has been investigated, we choose the initial wave function in such a way that its phase fulfills the classical Hamilton-Jacobi equation. Consequently the equation for the amplitude, which in our context can be complex valued, satisfies an equation of hydrodynamical type. For it we deduce H^s estimates via the energy method. The regularity estimates we obtain are the key to prove the convergence of the Wigner transform of the solution in a rather straightforward way.

1. Problem and results

Consider an N- particle quantum system described by the following mean-field Hamiltonian:

$$H_N = -\frac{h^2}{2}\sum_{j=1}^{N}\Delta_j + \frac{1}{N}\sum_{i<j}\varphi(x_i - x_j), \quad x_k \in \mathbb{R}^d \tag{1.1}$$

where $\Delta_j = \sum_{\alpha=1}^{3}\frac{\partial^2}{\partial x_{j,\alpha}^2}$ and φ is a two-body smooth potential.

We are interested in the asymptotic behavior of the system at the limit when $N \to \infty$ and $h \to 0$ simultaneously.

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

$$V_\lambda(x) = \frac{1}{\lambda}\varphi\left(\frac{x}{\lambda}\right) \tag{1.2}$$

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

$$H_N = -\frac{\hbar^2}{2}\sum_{j=1}^{N}\Delta_j + \sum_{i<j}V_\lambda(x_i - x_j). \tag{1.3}$$

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

$$H_N = -\frac{1}{2}\left(\frac{\hbar}{\lambda}\right)^2 \sum_{j=1}^{N} \Delta_j + \lambda^{-1} \sum_{i<j} \varphi(q_i - q_j). \tag{1.4}$$

Setting $\lambda = N$, $h = \dfrac{\hbar}{\lambda} = \dfrac{\hbar}{N}$ we finally get:

$$H_N = -\frac{h^2}{2} \sum_{j=1}^{N} \Delta_j + \frac{1}{N} \sum_{i<j} \varphi(q_i - q_j). \tag{1.5}$$

The initial condition $\Psi_N = \psi^{\otimes N}$ is assumed to be factorized (and hence symmetric in the exchange of particles).

For the one-particle wave function we choose initially a WKB state:

$$\psi(x) = a(x) e^{i\frac{\sigma(x)}{h}} \tag{1.6}$$

where a and σ are smooth and independent of h. σ is real (more generally, one could also consider the case where $a \sim \sum_{j\geq 0} h^j a_j(x)$ is a semiclassical symbol).

Setting $W_N = \dfrac{1}{N}\sum_{i<j} \varphi(x_i - x_j)$, we denote $\Psi_N(\cdot, t)$ the solution of the Schrödinger equation

$$(ih\partial_t + \frac{h^2}{2}\Delta_N - W_N)\Psi_N(t) = 0 \tag{1.7}$$

and introduce its Wigner transform:

$$f^N(X_N, V_N, t) :=$$
$$\left(\frac{1}{2\pi}\right)^{3N} \int dY_N e^{-iY_N \cdot V_N} \Psi_N(X_N + \frac{h}{2}Y_N, t)\bar{\Psi}_N(X_N - \frac{h}{2}Y_N, t). \tag{1.8}$$

Hereafter we use the shorthand notation $X_N = (x_1, \ldots, x_N)$, $Y_N = (y_1, \ldots, y_N)$, $V_N = (v_1, \ldots, v_N)$.

We also introduce the j-particle Wigner functions defined by:

$$f_j^N(X_j, V_j, t) = (1/2\pi)^{3(j-N)} \int dX_{N-j} \int dV_{N-j} f^N(X_N, V_N, t) =$$

$$(\frac{1}{2\pi})^{3j} \int dX_{N-j} \int dY_j e^{-iY_j \cdot V_j} \Psi_N(X_N + \frac{h}{2} Y_j, t) \bar{\Psi}_N(X_N - \frac{h}{2} Y_j, t) \tag{1.9}$$

where $X_{N-j} = (x_{j+1}, \dots, x_N), V_{N-j} = (v_{j+1}, \dots, v_N)$, $Y_j = (y_1, \dots, y_j)$ and $X_N + hY_j = (x_1 + hy_1, \dots, x_j + hy_j, x_{j+1}, \dots, x_N)$. Note that, at time $t = 0$, $f_j^N = f_0^{\otimes j}$ where f_0 is the Wigner transform of ψ. Hence

$$f_0 \to \rho(x)\delta(v - u(x)) \quad \text{in } \mathcal{D}' \text{ as } h \to 0 \tag{1.10}$$

where $\rho = |a|^2$ and $u = \nabla\sigma$ ($\rho = |a_0|^2$ in the case where $a \sim \sum_{j \geq 0} h^j a_j(x)$).

Remark. We remark that f_j^N is the Wigner transform of the reduced density matrices:

$$\rho(X_j, Z_j) = \int dX_{N-j} \bar{\Psi}(X_j, X_{N-j}) \Psi(Z_j, X_{N-j}).$$

The asymptotics of $f_j^N(t)$ is described by the following theorem:

Theorem 1.1. *Assume $\varphi \in C^2(\mathbb{R}^3)$, $\sigma \in C^2(\mathbb{R}^3)$, $\partial^\alpha \varphi$, $\partial^\alpha \sigma$ uniformly bounded for $|\alpha| \leq 2$, and $a \in C^2 \cap H^2(\mathbb{R}^3)$. Let $h = h(N) \to 0$ as $N \to \infty$. Then there exists $T > 0$, sufficiently small, such that for all $j \in \mathbb{N}$:*

$$f_j^N(t) \to f_j(t) \qquad \textit{in } \mathcal{D}'(\mathbb{R}^{3j} \times \mathbb{R}^{3j}), \quad t \in [0, T] \tag{1.11}$$

where $f_j(t) = f(t)^{\otimes j}$ and $f(t)$ is the unique (weak) solution of the classical Vlasov equation:

$$(\partial_t + v \cdot \nabla_x + E \cdot \nabla_v) f(x, v, t) = 0. \tag{1.12}$$

Here:

$$E(x, t) = -\nabla\varphi * \rho(x, t), \qquad \rho(x, t) = \int dv f(x, v, t). \tag{1.13}$$

Moreover, for $t \in [0,T]$:

$$f(x,v,t) = \rho(x,t)\delta(v-u(x,t)) \tag{1.14}$$

where the pair (ρ, u) fulfills the continuity and the momentum balance equations:

$$\partial_t \rho + div(u\rho) = 0; \quad \partial_t u + u \cdot \nabla u = -\nabla\phi * \rho. \tag{1.15a}$$

More precisely, for any test function $F \in \mathcal{D}(\mathbb{R}^{3j} \times \mathbb{R}^{3j})$, one has

$$\langle f_j^N(t) - f_j(t), F \rangle = \mathcal{O}(h + N^{-1}) \tag{1.15b}$$

for h small enough and N large enough.

We refer to this particular situation as hydrodynamic for obvious reasons. Theorem 1.1 is based on some regularity estimates to be established in the next section. We will write the solution of the Schrödinger equation (1.7) under the form

$$\Psi_N(X_N,t) = A^N(X_N,t)e^{i\frac{S^N(X_N,t)}{h}} \tag{1.16}$$

where S^N is the classical action satisfying the Hamilton-Jacobi equation:

$$\partial_t S^N + \frac{1}{2}|\nabla S^N|^2 + W_N = 0 \tag{1.17}$$

and, consequently, A_N is the solution of the "transport" equation:

$$\partial_t A^N + (P^N \cdot \nabla)A^N + \frac{1}{2}A^N \mathrm{div} P^N = -h\frac{i}{2}\Delta A^N. \tag{1.18}$$

Here $P^N := \nabla S^N$ satisfies:

$$\partial_t P^N + (P^N \cdot \nabla)P^N = -\nabla W. \tag{1.19}$$

As we shall show later on, the above representation holds for a short time $T > 0$ which may be chosen uniformly in N.

We then consider initial data which are not of hydrodynamical type. We restrict ourselves to classical data, namely those for which the Wigner transform is positive and normalized:

$$f^N(X_N, V_N) = f^{\otimes N}(X_N, V_N) \tag{1.20}$$

where f is a classical probability distribution on the one-particle phase space.

Consider now a one-particle superposition of particular WKB states, given by the following density matrix:

$$\rho(x, y) = \int dw \quad e^{i\frac{w}{h}\cdot(x-y)} a(x; w)\bar{a}(y, w). \tag{1.21}$$

The Wigner transform of the density matrix is:

$$f_\rho(x, v) = (\frac{1}{2\pi})^3 \int dw \int dz e^{iz\cdot(v-w)} a(x - \frac{h}{2}z; w)\bar{a}(x + \frac{h}{2}z, w) = |a(x, v)|^2 + O(h). \tag{1.22}$$

Setting $|a(x, v)| = \sqrt{f(x, v)}$ we see that f and f_ρ are asymptotically equivalent (in $\mathcal{D}'$)) in the limit $h \to 0$. Therefore we assume as initial condition

$$\rho^N(X_N, Y_N) = \prod_{i=1}^{N} \rho(x_i, y_i) \tag{1.23}$$

for the density matrix (1.21) with $a(x; w) = \sqrt{f(x, w)}$. We will prove

Theorem 1.2. *Assume $\varphi \in C^2(\mathbb{R}^3)$, $\sigma \in C^2(\mathbb{R}^3)$, $\partial^\alpha\varphi$, $\partial^\alpha\sigma$ uniformly bounded for $|\alpha| \leq 2$, a compactly supported in w and $a(\cdot, w) \in C^2 \cap H^2(\mathbb{R}^3)$ for all w. Let $h = h(N) \to 0$ as $N \to \infty$. Then for all $j \in \mathbb{N}$ and $t \geq 0$:*

$$f_j^N(t) \to f_j(t) \qquad in\ \mathcal{D}'(\mathbb{R}^{3j} \times \mathbb{R}^{3j}), \tag{1.24}$$

where $f_j(t) = f(t)^{\otimes j}$ *and* $f(t)$ *is the unique solution of the classical Vlasov equation:*

$$(\partial_t + v \cdot \nabla_x + E \cdot \nabla_v) f(x, v, t) = 0 \tag{1.25}$$

where

$$E(x,t) = -\nabla\varphi * \rho(x,t), \qquad \rho(x,t) = \int dv f(x,v,t), \tag{1.26}$$

with initial datum $f(x, v) = |a(x, v)|^2$.

Note that here the convergence result holds globally in time.

2. The classical system and its mean-field properties

Consider the associated Hamiltonian system:

$$\dot{X}_N(t) = V_N(t); \quad \dot{V}_N(t)_i = -\frac{1}{N} \sum_{j \neq i} \nabla\varphi(x_i(t) - x_j(t)) \tag{2.1}$$

where

$$X_N(t) = (x_1(t) \dots x_N(t)), \quad V_N(t) = (v_1(t) \dots v_N(t)).$$

Denote by $X_N(t, X_N, V_N)$, $V_N(t) = V_N(t, X_N, V_N)$ the solution of the Cauchy problem with initial conditions X_N, V_N. For a given initial datum (X_N, V_N), we consider the empirical distribution, that is a one-particle time depending measure, defined by:

$$\mu^N(dx, dv, t) := \frac{1}{N} \sum_{i=1}^{N} \delta(x - x_i(t)) \delta(v - v_i(t)) dx dv. \tag{2.2}$$

The following facts are well known (see e.g. [1],[2],[3]).

1) $\mu^N(dx, dv, t)$ is a weak solution of the Vlasov equation (1.12). Namely, for any test function $h = h(x, v)$, setting $\langle \mu^N(t), h \rangle = \int \mu^N(dx, dv, t) h(x, v)$, we have:

$$\frac{d}{dt} \langle \mu^N(t), h \rangle = \langle \mu^N(t), v \cdot \nabla_x h \rangle - \langle \mu^N(t), \nabla_x \varphi * \mu^N(t) \cdot \nabla_v h \rangle. \tag{2.3}$$

This follows by a direct computation.

2) Weak solutions to the Vlasov equation are continuous with respect to the initial datum in the topology of the weak convergence of the measures.

In particular 1) and 2) imply that if $\mu^N(0) \to f$ weakly, then $\mu^N(t) \to f(t)$weakly, where $f(t)$ is the unique solution to the Vlasov equation with initial datum f. If f is sufficiently regular then $f(t)$ hinerits such a regularity and the solution is classical.

3) Let $f^N(X_N, V_N, 0)$ be an initial symmetric N-particle distribution and let $f^N(X_N, V_N, t) = f^N(X_N(X_N, V_N, -t), V_N(X_N, V_N, -t))$ be the solution of the Liouville equation. Define the j-particle marginals by:

$$f_j^N(X_j, V_j, t) := \int dX_{N-j} \int dV_{N-j} f^N(X_N, V_N, t). \tag{2.4}$$

Then, if

$$f_j^N \to f^{\otimes j} \tag{2.5}$$

in the limit $N \to \infty$ and in the sense of the weak convergence of the measures, where $f = f(x, v)$ is a given 1-particle initial distribution, then

$$f_j^N(t) \to f^{\otimes j}(t) \tag{2.6}$$

weakly, where $f(t)$ solves the Vlasov equation with initial condition f. Property (2.6) is called propagation of chaos.

We now specialize the above results to our hydrodynamical case. We suppose that initially:

$$f(x, v) = f(x, v, 0) = \rho(x)\delta(v - u(x)) \tag{2.7}$$

(in the sequel $u = \nabla\sigma$) and denote:

$$\Phi^t(X_N) := X_N(X_N, P^N(X_N), t) \tag{2.8}$$

where $P^N(X_N) := \{u(x_i)\}_{i=1}^N$. Then, for a given test function $F_j \in \mathcal{D}(\mathbb{R}^3 \times \mathbb{R}^3)$,

$$\int f_j^N(t) F_j dX_j dV_j =$$

$$\int dX_N dV_N f^{\otimes N}(X_N, V_N) F_j(X_N^j(X_N, V_N, t), V_N^j(X_N, V_N, t)) =$$

(by the Liouville theorem)

$$= \int dX_N \rho^{\otimes N}(X_N) F_j(\Phi^t(X_N)^j, \dot{\Phi}^t(X_N)^j) \rightarrow$$

$$\int dX_j dV_j f^{\otimes j}(X_j, V_j, t) F_j(X_j, V_j) \tag{2.9}$$

in the limit $N \to \infty$. Here we are using the notation X_N^j to indicate the vector $(x_1, \dots, x_j)$ if $X_N = (x_1, \dots, x_N)$. On the other hand, if $f(t)$ is the solution of the Vlasov equation, for a short time $t < T$ it has the form

$$f(x, v, t) = \rho(x, t)\delta(v - u(x, t)) \tag{2.10}$$

with ρ and u solution of eq.s (1.15) as follows by a direct computation. Indeed if the pair (ρ, a) solves Eq. (1.15), $f(x, v, t)$ given by (2.10) is a solution of the Vlasov equation and its uniqueness entails the assertion.

Moreover observe that the estimate:

$$0 < C_1 \leq |\nabla_{x_i} \Phi^t(X_N)| \leq C_2 < 1 \tag{2.11}$$

which holds for a short time $t < T$, with constants C_1 and C_2 independent of N due to the mean-field nature of the interaction, allows us to invert the mapping $X_N \to \Phi^t(X_N)$, so that S^N, P^N, A^N exist for such a time interval. The estimate (2.11) easily follows from the analysis developed in Section 4.

We conclude this section summarizing under the form of a Proposition some regularity estimates on the classical flow, established in Section 4 below, which will be used in the convergence proof.

Proposition 2.1. *Assume $\varphi \in C^2(\mathbb{R}^3)$, $\sigma \in C^2(\mathbb{R}^3)$, $\partial^\alpha \varphi$, $\partial^\alpha \sigma$ uniformly bounded for $|\alpha| \leq 2$, and $a \in C^2 \cap H^2(\mathbb{R}^3)$. Let $t \in [0,T]$ with T sufficiently small. Then, there exists $C_1 > 0$ independent of N such that for all N and all $j \in \{1, \dots, N\}$, one has,*

$$\|\nabla_{x_j} A^N(t)\|_{L^2} \leq C_1. \tag{2.12}$$

Moreover for $\tau \in [0,t]$, denoting by x_i^γ, $\gamma = 1, 2, 3$ the components of x_i

$$\left|\frac{\partial P_k^N(\Phi^{(t-\tau)}(X_N), t)}{\partial x_i^\gamma}\right| \leq C\left(\frac{1}{N} + \delta_{i,k}\right) \tag{2.13}$$

and

$$\left|\frac{\partial \Phi^{(t-\tau)}(X_N)_k}{\partial x_i^\gamma}\right| \leq C\left(\frac{1}{N} + \delta_{i,k}\right) \tag{2.14}$$

where the constant C is independent of N, k, and i.

We note that the estimates (2.13) and (2.14) express the weak dependence of the position and momentum of the k-th particle with respect to the position of the i-th particle at time 0, as it is expected in a mean-field theory.

3. Convergence

We are now in position to prove Theorem 1.1. We first observe that, for a time interval for which estimates (2.11), (2.12), (2.13) and (2.14) hold, we have classical solutions of eq.s (1.17), (1.19) and (1.18). Therefore we can express the j- particle Wigner function in terms of A^N, S^N and P^N. For $F_j \in \mathcal{D}(\mathbb{R}^{3j} \times \mathbb{R}^{3j})$, we have:

$$\int F_j(X_j, V_j) f_j^N(X_j, V_j, t) dX_j dV_j =$$

$$\left(\frac{1}{2\pi}\right)^{3j} \int dX_N \int dV_j \int dY_j e^{-iY_j \cdot V_j} F_j(X_j, V_j) \Psi_N(X_N + \frac{h}{2}Y_j, t) \bar{\Psi}_N(X_N - \frac{h}{2}Y_j, t)$$

$$= \left(\frac{1}{2\pi}\right)^{\frac{3}{2}j} \int dX_N \int dY_j \tilde{F}_j(X_j, Y_j) A^N(X_N + \frac{h}{2}Y_j, t) \bar{A}^N(X_N - \frac{h}{2}Y_j, t)$$

$$e^{\frac{i}{h}[S^N(X_N+\frac{h}{2}Y_j,t)-S^N(X_N-\frac{h}{2}Y_j,t)]}, \tag{3.1}$$

where $\tilde{F}_j$ is the Fourier transform of F_j in the second variable. Changing variable $X_N \to X_N - \frac{h}{2}Y_j$ and using the fact that

$$\int dY_j \sup_{X_j} |\tilde{F}_j(X_j, Y_j)||Y_j| + \int dY_j \sup_{X_j} |\nabla_{X_j}\tilde{F}_j(X_j, Y_j)| \leq Cj, \tag{3.2}$$

we obtain that (setting $X_j = X_N^j$):

$$(3.1) = (\frac{1}{2\pi})^{\frac{3j}{2}} \int dX_N \int dY_j \tilde{F}_j(X_j, Y_j) A^N(X_N + hY_j, t)\bar{A}^N(X_N, t)$$

$$e^{\frac{i}{h}[S^N(X_N+hY_j,t)-S^N(X_N,t)]} + O(h). \tag{3.3}$$

Now Lagrange's theorem yields:

$$A^N(X_N + hY_j, t) = A^N(X_N, t) + \int_0^h d\lambda \nabla_{X_j} A^N(X_N + \lambda Y_j, t) \cdot Y_j$$

Moreover, since

$$\|\nabla_{X_j} A^N\|_{L_2}^2 = \sum_{i=1}^{j} \|\nabla_{x_i} A^N\|_{L_2}^2 \leq Cj; \quad \|A^N(t)\|_{L_2} = \|A^N(0)\|_{L_2} = 1$$

by (3.2) and Proposition 2.1 we get the estimate

$$\int_0^h d\lambda \int dX_N \int dY_j |\tilde{F}_j(X_j, Y_j)||\nabla_{X_j} A^N(X_N + \lambda Y_j, t)||A^N(X_N, t)| \leq$$

$$h\|A^N\|_{L_2}\|\nabla_{X_j} A^N\|_{L_2} \int dY_j \sup_{X_j} |\tilde{F}_j(X_j, Y_j)||Y_j| \leq Ch\sqrt{j}. \tag{3.4}$$

Hence we can conclude that:

$$(3.1) = \left(\frac{1}{2\pi}\right)^{\frac{3j}{2}} \int dX_N \int dY_j \tilde{F}_j(X_j, Y_j)|A^N(X_N, t)|^2$$

$$e^{\frac{i}{h}[S^N(X_N+hY_j,t)-S^N(X_N,t)]}+O(h). \tag{3.5}$$

Note that $O(h)$ (as well $O(\frac{1}{N})$ later on) depends on j which however is fixed. Furthermore:

$$S^N(X_N+hY_j,t)-S^N(X_N,t)=\int_0^h d\lambda P^N(X_N+\lambda Y_j,t)^j\cdot Y_j=$$

$$hP^N(X_N,t)^j\cdot Y_j+O(h^2) \tag{3.6}$$

again by Proposition 2.1.

Here $P^N(X_N)^j$ denotes the projection on the j-particle subspace of the vector $P^N(X_N)$.

Hence

$$(3.1)=\left(\frac{1}{2\pi}\right)^{\frac{3j}{2}}\int dX_N\int dY_j\tilde{F}_j(X_j,Y_j)|A^N(X_N,t)|^2e^{-iP^N(X_N,t)^j\cdot Y_j}+O(h)=$$

$$\int dX_N F(X_j,P^N(X_N,t)^j)|A^N(X_N,t)|^2+O(h). \tag{3.7}$$

Setting $\Gamma^N=|A^N|^2$ we have by (1.18):

$$\partial_t\Gamma^N+\mathrm{div}\,(P^N\Gamma^N)=B^N \tag{3.8}$$

where

$$B^N=\frac{i}{2}h(\bar{A}^N\Delta A^N-A^N\Delta\bar{A}^N). \tag{3.9}$$

The solution of eq. (3.8) has the representation:

$$\Gamma^N(X_N,t)=\rho^{\otimes N}(\Phi^{-t}(X_N))J_N(X_N,t)+\int_0^t dsB^N(\Phi^{-(t-s)}(X_N))J_N(X_N,t-s), \tag{3.10}$$

where

$$J_N(X_N,t)=\det|\frac{\partial\Phi^{-t}(X_N))}{\partial X_N}|. \tag{3.11}$$

Therefore

$$\int dX_N F_j(X_j, P^N(X_N,t)^j)\Gamma^N(X_N,t) = \int dX_N \rho^{\otimes N}(X_N) F_j(\Phi^t(X_N)^j, \dot{\Phi}^t(X_N)^j)$$

$$+\int_0^t ds \int dX_N B^N(\Phi^{-(t-s)}(X_N),s) J(X_N,t-s) F_j(X_j, P^N(X_N,t)^j). \qquad (3.12)$$

The last term in the r.h.s. of (3.12) can be rewritten as:

$$\int_0^t ds \int dX_N B^N(X_N,s) F_j(\Phi^{(t-s)}(X_N)^j, P^N(\Phi^{(t-s)}(X_N)^j,t)) =$$

$$\frac{ih}{2}\int_0^t ds \int dX_N (\bar{A}^N \Delta A^N - A^N \Delta \bar{A}^N)(X_N,s)$$

$$F_j(\Phi^{(t-s)}(X_N)^j, P^N(\Phi^{(t-s)}(X_N)^j,t))$$

$$= \frac{ih}{2}\int_0^t ds \int dX_N (\bar{A}^N \nabla A^N \cdot \nabla F_j(\dots) - A^N \nabla \bar{A}^N \cdot \nabla F_j(\dots)), \qquad (3.13)$$

here we have integrated by parts and made use of a crucial cancellation.

We now observe that

$$\sum_{i=1}^N |\nabla_{x_i} F_j(\Phi^{(t-s)}(X_N)^j, P^N(\Phi^{(t-s)}(X_N)^j,t))| \qquad (3.14)$$

can be bounded by a constant dependent on j but not on N. Indeed:

$$\partial_{x_i^\alpha} F_j(\Phi^{(t-s)}(X_N)^j, P^N(\Phi^{(t-s)}(X_N)^j,t)) =$$

$$\sum_{k=1}^j [\nabla_{y_k} F_j(Y_j, P^N(\Phi^{(t-s)}(X_N)^j j,t))|_{Y_j=\Phi^{(t-s)}(X_N)^j} \cdot \frac{\partial \Phi^{(t-s)}(X_N)_k}{\partial x_i^\alpha} +$$

$$\nabla_{v_k} F_j(\Phi^{(t-s)}(X_N)_j, V_j, t))|_{V_j=P^N(\Phi^{(t-s)}(X_N)^j)} \cdot \frac{\partial P_k^N(\Phi^{(t-s)}(X_N),t)}{\partial x_i^\alpha}.$$

Then by Proposition 1.1 we have that:

$$\partial_{x_i^\alpha} F_j(\Phi^{(t-s)}(X_N)_j, P^N(\Phi^{(t-s)}(X_N)^j,t)) = O(1)$$

if $i = 1 \dots j$, while

$$\partial_{x_i^\alpha} F(\Phi^{(t-s)}(X_N)_j, P^N(\Phi^{(t-s)}(X_N)_j, t)) = O(\frac{1}{N})$$

if $i > j$. Hence, by (3.14):

$$|\int dX_N \bar{A}^N \nabla A^N \cdot \nabla F_j(\dots)| \leq \|A\|_{L_2} \sum_{i=1}^{N} |\nabla_{x_i} F_j(\dots)| \|\nabla_{x_i} A\|_{L_2} \leq Cj.$$

Therefore

$$(3.1) = \int dX_N \rho^{\otimes N}(X_N) F_j(\Phi^t(X_N)_j, \dot{\Phi}^t(X_N)_j) + O(h) + O(\frac{1}{N}). \tag{3.15}$$

Notice that the first term in the r.h.s. of (3.15) is purely classical so that we can apply the convergence result (2.9) to conclude the proof.

The proof of Theorem 1.2 follows along the same lines. Proceeding as as above the Wigner function is in this case:

$$f^N(X_N, V_N) = (\frac{1}{2\pi})^3 \int d\Omega_N \int dY_N e^{-iY_N \cdot V_N}$$

$$A^N(X_N - \frac{h}{2} Y_N, \Omega_N, t) \bar{A}^N(X_N + \frac{h}{2} Y_N, \Omega_N, t)$$

$$e^{\frac{i}{h}[S^N(X_N - \frac{h}{2}Y_N, \Omega_N, t) - S^N((X_N + \frac{h}{2}Y_N, \Omega_N, t)]} \tag{3.16}$$

where A^N and S^N are the amplitude and the action parametrized by the initial momenta Ω_N. S^N and A^N are the solution of eq.s (1.17) and (1.18) with initial conditions $S^N(X_N, \Omega_N) = \Omega_N \cdot X_N$ and $A^N(X_N, \Omega_N) = a^{\otimes N}(X_N, \Omega_N)$. Therefore for a test function F_j we have:

$$\int F_j(X_j, V_j) f_j^N(X_j, V_j, t) dX_j dV_j =$$

$$\left(\frac{1}{2\pi}\right)^{\frac{3}{2}j} \int d\Omega_N \int dX_N \int dY_j \tilde{F}_j(X_j, Y_j)$$

$$A^N(X_N+\frac{h}{2}Y_j,\Omega_N,t)\bar{A}^N(X_N-\frac{h}{2}Y_j,\Omega_N,t)e^{\frac{i}{h}[S^N(X_N+\frac{h}{2}Y_j,\Omega_N,t)-S^N(X_N-\frac{h}{2}Y_j,\Omega_N,t)]}. \tag{3.17}$$

Proceeding as in the proof of Theorem 1.1 we find:

$$(f_j^N,F)=\int d\Omega_N\int dX_N f^{\otimes N}(X_N,V_N)F(X_N(t,X_N,\Omega_N),\dot{X}_N(t,X_N,\Omega_N))$$

$$+O(h)+O(\frac{1}{N}). \tag{3.18}$$

Note that that a is assumed compactly supported in w to avoid complications with the integral in the initial momenta. However a sufficiently rapid decay of $a(\cdot,w)$, for large w, would yield the same result. Of course, once more, everything holds for a small time interval. However now the smallness of the time interval depends only on the smoothness of the potential φ (because of the particular form $\sigma(x)=w\cdot x$). Hence the convergence at time T allows us to extend the argument up to $2T$, using fact 2) of Section 2 and that $f(x,v,T)$ is still compactly supported in velocity. Therefore the convergence can be extended to arbitrary times and the proof of Theorem 1.2 is now completed.

4. Regularity estimates

In this section we prove Proposition 2.1. We start by considering

$$\partial_t P^N+(P^N\cdot\nabla)P^N=-\nabla W. \tag{4.1}$$

which is independent of

$$\partial_t A^N+(P^N\cdot\nabla)A^N+\frac{1}{2}A^N\mathrm{div}P^N=-h\frac{i}{2}\Delta A^N. \tag{4.2}$$

to be considered later on.

Notice that, for $s \in [0,t]$,

$$P_i^N(\phi^{(t-s)}(X_N),t) = \dot{\Phi}^t(Y_N(s))_i, \quad \text{where} \quad Y_N(s) = \Phi^{-s}(X_N), \quad i = 1 \dots N. \tag{4.3}$$

Using now the short-hand notation $x_i(t) = \Phi^t(X_N)_i$, $p_i(t) = \dot{\Phi}^t(X_N)_i$ and denoting $x_i^\alpha(t)$ and $p_i^\alpha(t)$ the α-th components, $\alpha = 1,2,3$, we have:

$$x_i(t) = x_i + \int_0^t p_i(s)ds$$

$$p_i(t) = \nabla\sigma(x_i) - \int_0^t \frac{1}{N}\sum_{k\neq i}\nabla\varphi(x_i(s)-x_k(s))ds. \tag{4.4}$$

where $X_N = (x_1 \dots x_N)$.

Introducing the force $F^\alpha = -\partial_{x^\alpha}\varphi$, we have:

$$\frac{\partial x_i^\beta(t)}{\partial x_j^\gamma} = \delta_{i,j}\delta_{\beta,\gamma} + \int_0^t ds \frac{\partial p_i^\beta(s)}{\partial x_j^\gamma} \tag{4.5}$$

$$\frac{\partial p_i^\beta(t)}{\partial x_j^\gamma} = \frac{\partial^2\sigma}{\partial x_j^\gamma \partial x_i^\beta}\delta_{i,j} + \int_0^t ds \frac{1}{N}\sum_{k\neq i}\sum_\alpha \partial_{x^\alpha}F^\beta(x_i(s)-x_k(s))\left(\frac{\partial x_i^\alpha(s)}{\partial x_j^\gamma} - \frac{\partial x_k^\alpha(s)}{\partial x_j^\gamma}\right). \tag{4.6}$$

Hence:

$$\frac{\partial p_i^\beta(t)}{\partial x_j^\gamma} = \frac{\partial^2\sigma}{\partial x_j^\gamma \partial x_i^\beta}\delta_{i,j} + \int_0^t ds \frac{1}{N}\sum_{k\neq i}\sum_\alpha \partial_{x^\alpha}F^\beta(x_i(s)-x_k(s))(\delta_{i,j}-\delta_{k,j})\delta_{\alpha,\gamma} +$$

$$\int_0^t ds \int_0^s d\tau \frac{1}{N}\sum_{k\neq i}\sum_\alpha \partial_{x^\alpha}F^\beta(x_i(s)-x_k(s))\left(\frac{\partial p_i^\alpha(\tau)}{\partial x_j^\beta} - \frac{\partial p_k^\alpha(t)}{\partial x_j^\beta}\right). \tag{4.7}$$

We now observe that, if $i \neq j$, the first two terms in the r.h.s. of (4.7) are $O(\frac{1}{N})$ and hence (taking $t \in [0,T]$ with T small enough):

$$\left|\frac{\partial x_i^\beta(t)}{\partial x_j^\gamma}\right| + \left|\frac{\partial p_i^\beta(t)}{\partial x_j^\gamma}\right| \leq C\left(\frac{1}{N} + \delta_{i,j}\right), \tag{4.8}$$

with C independent of N.

Remark. Higher derivatives could be handled in the same way to obtain:

$$\left|\frac{\partial^s x_i^\beta(t)}{\partial x_{j_1}^{\gamma_1}\ldots\partial x_{j_s}^{\gamma_s}}\right| + \left|\frac{\partial^s p_i^\beta(t)}{\partial x_{j_1}^{\gamma_1}\ldots\partial x_{j_s}^{\gamma_s}}\right| \leq C\left(\frac{1}{N}+\prod_{r=1}^{s}\delta_{i,j_r}\right), \tag{4.9}$$

assuming a stronger regularity.

Furthermore, setting $Y_N(s) = (y_1(s),\ldots,y_N(s))$,

$$\frac{\partial P_i^\alpha(Y_N,t)}{\partial x_j^\gamma} = \sum_k\sum_\beta \frac{\partial\dot{\Phi}^t(Y_N)_i^\alpha}{\partial y_k^\beta}|_{Y_N=Y_N(s)}\frac{\partial y_k^\beta(s)}{\partial x_j^\gamma}. \tag{4.10}$$

We note that the terms in the sum with $k \neq i$ and $k \neq j$ are $O(\frac{1}{N^2})$, while the term with $k = i$ or $k = j$ are $O(\frac{1}{N})$. Therefore, if $i \neq j$, the full sum is $O(\frac{1}{N})$. If $i = j$ the sum is $O(1)$ because of the term $k = i = j$ which is indeed $O(1)$. Summarizing:

$$\left|\frac{\partial P_i^\alpha(\Phi^{(t-s)}(X_N),t)}{\partial x_j^\gamma}\right| \leq C\left(\frac{1}{N}+\delta_{i,j}\right). \tag{4.11}$$

Remark. A similar analysis on the higher derivatives yields:

$$\left|\frac{\partial^s P_i^\beta(\Phi^{(t-s)}(X_N),t)}{\partial x_{j_1}^{\gamma_1}\ldots\partial x_{j_s}^{\gamma_s}}\right| \leq C\left(\frac{1}{N}+\prod_{r=1}^{s}\delta_{i,j_r}\right). \tag{4.12}$$

We now proceed to analyze eq. (4.2) to obtain estimate of the solution in H^1. Applying the operator ∇_{x_j} to the equation, we obtain:

$$\partial_t\nabla_{x_j}A^N + (\nabla_{x_j}P^N\cdot\nabla)A^N + (P^N\cdot\nabla)\nabla_{x_j}A^N + \frac{1}{2}\nabla_{x_j}A^N\mathrm{div}P^N =$$
$$-\frac{1}{2}A^N\mathrm{div}\nabla_{x_j}P^N - h\frac{i}{2}\Delta\nabla_{x_j}A^N. \tag{4.14}$$

In computing

$$\frac{d}{dt}(\nabla_{x_j}A^N,\nabla_{x_j}A^N) = (\partial_t\nabla_{x_j}A^N,\nabla_{x_j}A^N) + (\nabla_{x_j}A^N,\partial_t\nabla_{x_j}A^N) \tag{4.15}$$

we realize that, due to the symmetry of Δ, the last term does not give any contribution. Also, the sum of the terms non involving $\nabla_{x_j} P^N$ vanishes:

$$(\nabla_{x_j} A^N, P^N \cdot \nabla\nabla_{x_j} A^N) + (P^N \cdot \nabla\nabla_{x_j} A^N, \nabla_{x_j} A^N) +$$
$$\frac{1}{2}(\nabla_{x_j} A^N, \nabla_{x_j} A^N \mathrm{div} P^N) + \frac{1}{2}(\mathrm{div} P^N \nabla_{x_j} A^N, \nabla_{x_j} A^N) = 0. \tag{4.16}$$

Here we use the reality of P^N and the identity:

$$\int P^N \cdot \nabla |\nabla_{x_j} A^N|^2 = -\int \mathrm{div} P^N |\nabla_{x_j} A^N|^2 \tag{4.17}$$

We finally observe that, by eq. (4.11),

$$(\nabla_{x_j} P^N \cdot \nabla) A^N = (\nabla_{x_j} P_j^N \cdot \nabla_{x_j}) A^N + \mathcal{O}(N^{-1} \sum_{k \neq j} \|\nabla_{x_k} A^N\|_{L_2}) \tag{4.18}$$

and thus, denoting $\|A^N\|_1 := (\sum_k \|\nabla_{x_k} A^N\|_{L_2}^2)^{1/2}$ (so that $\sum_{k\neq j} \|\nabla_{x_k} A^N\|_{L_2} \leq \sqrt{N}\|A^N\|_1$), we arrive to the inequality:

$$\frac{d}{dt}\|\nabla_{x_j} A^N(t)\|_{L_2}^2 \leq C\{\|\nabla_{x_j} A^N(t)\|_{L_2}^2 + N^{-1/2}\|A^N\|_1 \|\nabla_{x_j} A^N(t)\|_{L_2}\} \tag{4.19}$$

with C independent of N and j. In particular, taking the sum over all j, we obtain,

$$\frac{d}{dt}\|A^N(t)\|_1^2 \leq 2C\|A^N(t)\|_1^2. \tag{4.20}$$

Since at time zero $\|A^N\|_1^2$ is $\mathcal{O}(N)$ the same conclusion holds on any time interval. Going back to Eq. (4.19), we obtain

$$\frac{d}{dt}\|\nabla_{x_j} A^N(t)\|_{L_2}^2 \leq C\|\nabla_{x_j} A^N(t)\|_{L_2}^2 \tag{4.21}$$

with a new constant C independent of N and j. Then the result follow by observing that $\|\nabla_{x_j} A^N(0)\|_{L_2}$ is uniformly bounded.

References

[1] W. Braun, K. Hepp, *The Vlasov dynamics and its fluctuations in the 1/N limit of interacting classical particles*, Comm.Math.Phys **56** (1977), 101-120.

[2] R. L. Dobrushin, *Vlasov equations*, Sov.J.Funct.An. **13** (1979), 115-119.

[3] H. Neunzert, *in Kinetic Theory and Boltzmann equation*, C. Cercignani ed. Springer lect notes n. 207 (1984), 60-110.

[4] H. Spohn, *Kinetic equations from Hamiltonian dynamics: Markovian limits*, Rev.Mod.Phys. **53** (1980), 569-615.

[5] C. Bardos, F. Golse, N. Mauser, *Weak coupling limit of the N-particle Schrdinger equation.*, Methods Appl.Anal. **n. 2** (2000), 275–293.

[6] C. Bardos, L. Erds, F. Golse, N. Mauser and H-T Yau, *Derivation of the Schrödinger-Poisson equation from the quantum N-body problem*, C.R. Acad. Sci. Paris **334 no. 6,** (2002), 515–520.

[7] H. Narnhofer, G. Sewell, *Vlasov hydrodynamics of a quantum mechanical model*, Comm.-Math.Phys **79** (1981), 9-24.

[8] E. Grenier, *Semiclassical limit of the nonlinear Schrödinger equation in small time*, Proc.-Amer.Math.Soc. **126, n.2** (1998), 523-530.