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ON THE DERIVATION OF THE HARTREE EQUATION IN THE MEAN FIELD LIMIT: UNIFORMITY IN THE PLANCK CONSTANT

FRANÇOIS GOLSE, THIERRY PAUL, AND MARIO PULVIRENTI

ABSTRACT. In this paper the Hartree equation is derived from the N -body Schrödinger equation uniformly in the Planck constant in two different cases, specifically (a) for Töplitz initial data and Lipschitz interaction force, and (b) for analytic initial data and interaction potential, and over short time intervals, independent of the Planck constant. The convergence rates in these two cases are $1/\log \log N$ and $1/N$ respectively. The treatment of the second case is entirely self-contained and all the constants appearing in the final estimate are explicit. Moreover it provides a derivation of the Vlasov equation out of the N -body classical dynamics using hierarchies and not empirical measures.

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1. INTRODUCTION

We consider the evolution of a system of N quantum particles interacting through a (real-valued) two-body, even potential Φ , described by the Schrödinger equation

$$i\hbar\partial_t\psi = H_N\psi, \quad \psi|_{t=0} = \psi_{in} \in \mathfrak{H}_N := L^2(\mathbf{R}^d)^{\otimes N},$$

where

$$H_N = -\frac{1}{2}\hbar^2 \sum_{k=1}^N \Delta_{x_k} + \frac{1}{2N} \sum_{1 \leq k, l \leq N} \Phi(x_k - x_l)$$

is the N -body Hamiltonian. With the notation

$$X_N := (x_1, \dots, x_N) \in (\mathbf{R}^d)^N,$$

the N -body Hamiltonian is recast as

$$H_N = \frac{1}{2}\hbar^2 \Delta_{X_N} + V_N(X_N),$$

where V_N is the N -body potential in the mean field scaling, i.e. with $1/N$ coupling constant:

$$V_N(X_N) := \frac{1}{2N} \sum_{1 \leq k, l \leq N} \Phi(x_k - x_l).$$

Instead of the Schrödinger equation written in terms of wave functions, we shall rather consider the quantum evolution of density matrices. A N -body density matrix is an operator D_N such that

$$0 \leq D_N = D_N^* \in \mathcal{L}(\mathfrak{H}_N), \quad \text{trace}_{\mathfrak{H}_N}(D_N) = 1$$

(here $\mathcal{L}(\mathfrak{H}_N)$ denotes the set of bounded linear operators on \mathfrak{H}_N).

The evolution of the density matrix of a N -particle system is governed by the von Neumann equation

$$(1) \quad \partial_t D^N = \frac{1}{i\hbar} [H_N, D^N], \quad D_N|_{t=0} = D_{in}^N.$$

The density matrix D_N for a N -particle system described in terms of the N -particle wave function $\Psi_N \equiv \Psi_N(t, X_N)$ is the orthogonal projection in \mathfrak{H}_N on the one dimensional subspace $\mathbf{C}\Psi_N$. In other words, $D_N(t)$ is the integral operator on \mathfrak{H}_N with integral kernel $\Psi_N(t, X_N)\overline{\Psi_N(t, Y_N)}$. Up to multiplying the N -body wave function by a global phase factor, both formulations of the quantum dynamics of a N -particle system are equivalent.

If D_{in}^N is factorized, that is of the form

$$D_{in}^N = D_{in}^{\otimes N}$$

where D_{in} is a density matrix on $\mathfrak{H} := L^2(\mathbf{R}^d)$, then $D^N(t)$ is in general not factorized for $t > 0$. However, it is known that $D_N(t)$ has a ‘‘tendency to become factorized’’ for all $t > 0$ as $N \rightarrow \infty$, i.e. in the mean field limit, **for each** $\hbar > 0$.

The precise formulation of this ‘‘tendency to become factorized’’ involves the notion of marginal of a density operator.

For each $j = 1, \dots, N$, the j -particle marginal $D_j^N(t)$ of $D_N(t)$ is the unique operator on \mathfrak{H}_j such that, for all $A_1, \dots, A_j \in \mathcal{L}(\mathfrak{H})$, one has

$$\text{trace}_{\mathfrak{H}_N}[D^N(t)(A_1 \otimes \dots \otimes A_j \otimes I_{\mathfrak{H}_{N-j}})] = \text{trace}_{\mathfrak{H}_j}[D_j^N(t)(A_1 \otimes \dots \otimes A_j)].$$

In terms of this notion of j -particle marginal, the tendency of $D_N(t)$ to become factorized is expressed as follows: for each $\hbar > 0$ and each $t > 0$, one has

$$D_j^N(t) \rightarrow (D^H(t))^{\otimes j} \quad \text{for all } j \geq 1 \text{ in the limit as } N \rightarrow \infty,$$

(in some appropriate topology on the algebra of operators on \mathfrak{H}_j) where D^H is the solution of the Hartree equation

$$(2) \quad i\hbar\partial_t D^H(t) = \left[-\frac{1}{2}\hbar^2\Delta_{\mathbf{R}^d} + \Phi_{\rho^H(t)}, D^H(t) \right], \quad D^H(0) = D_{in}.$$

Here

$$\Phi_{\rho^H(t)} = \Phi \star \rho^H(t, \cdot),$$

where

$$\rho^H(t, x) := D^H(t, x, x)$$

abusing the notation $D^H(t, x, y)$ to designate the integral kernel of the operator $D^H(t)$ on $\mathfrak{H} := L^2(\mathbf{R}^d)$.

This program has been carried out in a sequence of papers: see [19, 1] for bounded interaction potentials Φ , and in [7, 16] for interaction potentials that have a singularity at the origin, such as the Coulomb potential (see also [2]). In all these results the convergence rate as $N \rightarrow \infty$ deteriorates as $\hbar \rightarrow 0$. See [3] for a more detailed discussion of this subject, supplemented with an extensive bibliography.

The analogous result in the classical setting, where (1) and (2) are replaced respectively by the Liouville and the Vlasov equations, have been known for a long time: see [14, 4, 6], where this limit has been established by different methods.

This suggests that the mean field limit in quantum dynamics holds uniformly in \hbar , at least for some appropriate class of solutions.

This problem has been addressed in [15] where the mean field limit is established by means of a semiclassical expansion for which the term by term convergence can be established rigorously. The limit of the N -body quantum dynamics as $N \rightarrow \infty$ and $\hbar \rightarrow 0$ jointly, leading to the Vlasov equation, has been discussed in [13] (in the case of fermions and assuming that $\hbar \sim N^{-1/3}$), and in [11]. (See also [8] for a uniform in \hbar estimate of some appropriate distance between the N -body and the Hartree dynamics, for velocity dependent interaction potentials.)

More recently, a new approach based on the quantization of the quadratic Monge-Kantorovich (or Wasserstein) distance, analogous to the one used in [6], has been introduced in [9, 10]. It provides an estimate of the convergence rate in the mean field limit ($N \rightarrow \infty$) of the N -body quantum dynamics that is uniform in \hbar as $\hbar \rightarrow 0$.

In the present paper, we complete the results recalled above on the mean field limit of the N -body quantum dynamics leading to the Hartree equation with two different theorems. Both statements estimate some distance between the solutions of (1) and of (2) as $N \rightarrow \infty$ uniformly in $\hbar \in [0, 1]$, without assuming that $\hbar \rightarrow 0$.

First, by some kind of interpolation between the convergence rate obtained in [9] and the “standard” convergence rate from [19, 1] for $\hbar > 0$ fixed, we establish a $O(1/\ln N)$ convergence rate for the mean field ($N \rightarrow \infty$) limit of the quantum N -body problem leading to the Hartree equation, uniformly in $\hbar \in [0, 1]$. This estimate is formulated in terms of a Monge-Kantorovich type distance analogous to Dobrushin’s in [6], and holds true for initial data which are Töplitz operators.

Our second result will establish the convergence in a much stronger topology using the trace norm together with the formalism of Wigner functions, a tool particularly well adapted to the transition from quantum to classical dynamics. Using this approach requires strong analytic assumptions on both the potential and the initial data. The advantage of this result over the previous one is a faster convergence rate, of order $O(1/N)$, much more satisfying than $O(1/\ln \ln N)$ from the physical point of view. Keeping in mind that the total number of nucleons in the universe is estimated to be of the order of 10^{80} , an $O(1/\ln \ln N)$ convergence rate may be satisfying from the mathematical point of view, but is of little practical interest.

2. QUANTUM HIERARCHIES, TÖPLITZ OPERATORS, AND WIGNER AND HUSIMI FUNCTIONS

First we recall the formalism of BBGKY hierarchies in the quantum context. Let us call \mathfrak{S}_N the group of permutations of the set of N elements. For each $\sigma \in \mathfrak{S}_N$ and each $X_N = (x_1, \dots, x_N) \in (\mathbf{R}^d)^N$, we denote

$$U_\sigma \Psi_N(X_N) := \Psi(\sigma \cdot X_N), \quad \text{with } \sigma \cdot X_N := (x_{\sigma(1)}, \dots, x_{\sigma(N)}).$$

Everywhere in this paper, it is assumed that the N particles under consideration are indistinguishable, meaning that, for each $t \geq 0$, one has

$$(3) \quad U_\sigma D^N(t) U_\sigma^* = D^N(t) \quad \text{for all } \sigma \in \mathfrak{S}_N.$$

A straightforward computation shows that this condition is verified provided that

$$U_\sigma D_{in}^N U_\sigma^* = D_{in}^N \quad \text{for all } \sigma \in \mathfrak{S}_N.$$

Multiplying both sides of (1) by $B_j \otimes I_{\mathfrak{H}_{N-j}}$, with $B_j \in \mathcal{L}(\mathfrak{H}_j)$ such that $[\Delta_{(\mathbf{R}^d)^j}, B_j] \in \mathcal{L}(\mathfrak{H}_j)$, one arrives at the following system of coupled equations satisfied by the sequence of marginals $D_j^N(t)$ of the N -particle density $D^N(t)$:

$$(4) \quad i\hbar \partial_t D_j^N = [-\frac{1}{2}\hbar^2 \Delta_{(\mathbf{R}^d)^j}, D_j^N] + \frac{1}{N} \mathcal{T}_j D_j^N + \frac{N-j}{N} \mathcal{C}_{j+1} D_{j+1}^N$$

where

$$(5) \quad \mathcal{T}_j D_j^N = \left[\frac{1}{2} \sum_{l \neq r=1}^j \Phi(x_l - x_r), D_j^N \right],$$

and

$$(6) \quad \mathcal{C}_{j+1} D_{j+1}^N = \left(\left[\sum_{l=1}^j \Phi(x_l - x_{j+1}), D_{j+1}^N \right] \right)_j,$$

where the subscript j is meant for taking the j th marginal as in Section 1 and where we have set

$$D_j^N = 0 \quad \text{for all } j > N.$$

In the limit $N \rightarrow \infty$ and for each j kept fixed, one expects that D_j^N converges in some sense to D_j satisfying the infinite sequence of equations

$$(7) \quad i\hbar \partial_t D_j = [-\frac{1}{2}\hbar^2 \Delta_{(\mathbf{R}^d)^j}, D_j] + \mathcal{C}_{j+1} D_{j+1}, \quad j \geq 1.$$

Since the linear map $F \mapsto [A, F]$ is a derivation of the subalgebra of $\mathcal{L}(\mathfrak{H})$ of the operators F satisfying $[A, F] \in \mathcal{L}(\mathfrak{H})$, one easily checks that $t \mapsto \{F(t)^{\otimes j}\}_{j=1 \dots \infty}$ is a solution of the infinite hierarchy (7) if $t \mapsto F(t)$ is a solution of (2).

To each trace class operator F defined on $\mathfrak{H}_N = L^2((\mathbf{R}^d)^N)$ with integral kernel $F(X_N, Y_N)$, we associate its Wigner function $W_\hbar[F]$ defined on the underlying phase space $(T^*\mathbf{R}^d)^N = (\mathbf{R}^d \times \mathbf{R}^d)^N$ by the formula

$$(8) \quad W_\hbar[F](X_N; \Xi_N) := \frac{1}{(2\pi)^{dN}} \int_{(\mathbf{R}^d)^N} F(X_N + \frac{1}{2}\hbar Y_N, X_N - \frac{1}{2}\hbar Y_N) e^{i\Xi_N \cdot Y_N} dY_N$$

Notice that $W_\hbar[F]$ exists for each trace class operator F and for each $\hbar > 0$, since

$$W_\hbar[F](X_N, \Xi_N) = \left(\frac{2}{\hbar}\right)^{Nd} \text{trace}[FM(X_N, \Xi_N)],$$

where $M(X_N, \Xi_N)$ is the unitary operator on $L^2((\mathbf{R}^d)^N)$ defined by

$$M(X_N, \Xi_N) : f(X) \mapsto f(2X_N - X) e^{-2i\Xi_N \cdot (X - X_N)/\hbar}.$$

By a straightforward computation

$$F(X_N, Y_N) = \int_{(\mathbf{R}^d)^N} W_\hbar[F]\left(\frac{1}{2}(X_N + Y_N); \Xi_N\right) e^{-i\Xi_N \cdot (X_N - Y_N)/\hbar} d\Xi_N.$$

In particular

$$F(X_N, X_N) = \int_{(\mathbf{R}^d)^N} W_\hbar[F](X_N; \Xi_N) d\Xi_N,$$

so that

$$\text{trace}[F] = \int_{(\mathbf{R}^d \times \mathbf{R}^d)^N} W_\hbar[F](X_N; \Xi_N) dX_N d\Xi_N.$$

More generally one easily shows that

$$\text{trace}(F_1 F_2) = (2\pi\hbar)^{dN} \int_{(\mathbf{R}^d \times \mathbf{R}^d)^N} W_\hbar[F_1](X_N; \Xi_N) W_\hbar[F_2](X_N; \Xi_N) dX_N d\Xi_N.$$

From this identity, writing $X_N = (x_1, \dots, x_N)$ and $\Xi_N = (\xi_1, \dots, \xi_N)$, one easily deduces that

$$\begin{aligned} W_\hbar[F_j](X_j, \Xi_j) &= \int_{(\mathbf{R}^d \times \mathbf{R}^d)^{N-j}} W_\hbar[F](X_N, \Xi_N) dx_{j+1} d\xi_{j+1} \dots dx_n d\xi_n \\ &= (W_\hbar[F])_j(X_j, \Xi_j) \end{aligned}$$

A straightforward computation shows that $t \mapsto D^N(t)$ is a solution of (1) if and only if $t \mapsto W_\hbar[D^N](t, \cdot, \cdot) = f^N(t)$ is a solution of the following equation, referred to as the ‘‘Wigner equation’’

$$(9) \quad \begin{aligned} & (\partial_t + \Xi_N \cdot \nabla_{X_N}) f^N(t, X_N, \Xi_N) \\ &= \int_{(\mathbf{R}^d)^N} \hat{V}_N(Z_N) e^{iZ_N \cdot X_N} \frac{f^N(t, X_N, \Xi_N - \frac{1}{2}\hbar Z_N) - f^N(t, X_N, \Xi_N + \frac{1}{2}\hbar Z_N)}{i\hbar} \frac{dZ_N}{(2\pi)^{dN}}, \end{aligned}$$

where \hat{V}_N designates the Fourier transform of V_N , normalized as follows

$$\hat{V}_N(\Xi_N) = \int_{(\mathbf{R}^d)^N} V_N(X_N) e^{-i\Xi_N \cdot X_N} dX_N.$$

In the limit as $\hbar \rightarrow 0$, the Wigner equation reduces formally to the Liouville equation, since

$$\begin{aligned} \int_{(\mathbf{R}^d)^N} \hat{V}_N(Z_N) e^{iZ_N \cdot X_N} \frac{f^N(t, X_N, \Xi_N - \frac{1}{2}\hbar Z_N) - f^N(t, X_N, \Xi_N + \frac{1}{2}\hbar Z_N)}{i\hbar} \frac{dZ_N}{(2\pi)^{dN}} \\ \rightarrow \int_{(\mathbf{R}^d)^N} \hat{V}_N(Z_N) e^{iZ_N \cdot X_N} iZ_N \cdot \nabla_{\Xi_N} f^N(t, X_N, \Xi_N) \frac{dZ_N}{(2\pi)^{dN}} \\ = \nabla V_N(X_N) \cdot \nabla_{\Xi_N} f^N(X_N, \Xi_N). \end{aligned}$$

See Proposition II.1 in [12] for a rigorous discussion on the argument.

The Husimi transform of a density matrix F on $\mathfrak{H} := L^2(\mathbf{R}^d)$ is defined as

$$\widetilde{W}_\hbar[F](q, p) := (2\pi\hbar)^{-d} \langle p, q | F | p, q \rangle \geq 0,$$

where

$$|p, q\rangle(x) := (\pi\hbar)^{-d/4} e^{-(x-q)^2/2\hbar} e^{ip \cdot x/\hbar}.$$

Here and in the sequel, we use the Dirac bra-ket notation whenever convenient. At variance with the Wigner function, there is no explicit ‘‘reconstruction’’ formula for F out of $\widetilde{W}_\hbar[F]$. Observe that the Husimi function captures only the diagonal part of the matrix elements of F on the (over)complete basis $\{|p, q\rangle \mid (p, q) \in \mathbf{R}^{2d}\}$. Yet $\widetilde{W}_\hbar[F]$ determines all the numbers $\langle p', q' | F | p, q \rangle$ as p, q, p', q' run through \mathbf{R}^d , and therefore F itself. Indeed, denoting $z := q + ip$ and $z' = q' + ip'$, a straightforward computation shows that

$$e^{(|q|^2 + |q'|^2)/2\hbar} \langle p', q' | F | p, q \rangle = f\left(\frac{1}{2}(z + z'), \frac{1}{2}i(z' - z)\right)$$

where f is an entire function on \mathbf{C}^{2d} . Knowing $\widetilde{W}_\hbar[F](q, p)$ for all $q, p \in \mathbf{R}^d$ is equivalent to knowing $f(\frac{1}{2}(z + z'), \frac{1}{2}i(z' - z))$ for $z = z'$, which is in turn equivalent to knowing the restriction of f to $\mathbf{R}^{2d} \subset \mathbf{C}^{2d}$. Since f is holomorphic on \mathbf{C}^{2d} , knowing the restriction of f to \mathbf{R}^{2d} determines f uniquely. Therefore, the knowledge of $\widetilde{W}_\hbar[F]$ determines F uniquely.

The Husimi function is sometime called a mollification of the Wigner function because of the following straightforward formula

$$\widetilde{W}_\hbar[F](x, \xi) = e^{\hbar\Delta_{x, \xi}} W_\hbar[F](x, \xi).$$

In particular, both the Wigner and the Husimi function of a \hbar -dependent family of density matrices have the same limit (if any) as $\hbar \rightarrow 0$ in the sense of distributions. Finally, we recall the definition of Töplitz operators used in [9]. For each positive Borel measure μ on $\mathbf{R}^d \times \mathbf{R}^d$, the Töplitz operator with symbol μ is

$$\text{OP}_\hbar^T[\mu] := \frac{1}{(2\pi\hbar)^d} \int_{(\mathbf{R}^d \times \mathbf{R}^d)} |p, q\rangle \langle p, q | \mu(dp dq).$$

For instance $\text{OP}_\hbar^T[1] = I_{\mathfrak{H}}$, where 1 designates the Lebesgue measure on $\mathbf{R}^d \times \mathbf{R}^d$. Elementary computations show that

$$W_\hbar[\text{OP}_\hbar^T[\mu]] = e^{\hbar\Delta_{p, q}/4} \mu, \quad \widetilde{W}_\hbar[\text{OP}_\hbar^T[\mu]] = e^{\hbar\Delta_{p, q}/2} \mu.$$

Therefore $\text{trace}(\text{OP}_\hbar^T[\mu]) = \int_{\mathbf{R}^{2d}} d\mu$ and probability measures give rise to physical states (positive operators of trace one) through Töplitz quantization.

The paper is organized as follows. The two main results of this article, Theorems 3.1 and 3.2, are presented in the next section. The proofs are essentially self-contained and given respectively in Part 2 and Part 1. We have chosen this order of presentation since part of the material if the proof of Theorem 3.2 is used in the proof of Theorem 3.1.

3. THE RESULTS

Our first uniform convergence result puts little regularity constraint on the interaction potential V . As a result, we obtain a convergence rate in some weak topology, which is most conveniently expressed in terms of a Monge-Kantorovich, or Wasserstein distance, associated to the cost function $(z, z') \mapsto \min(1, |z - z'|)$ on $(\mathbf{R}^d \times \mathbf{R}^d)^j$, for $j \geq 1$. Specifically, let μ, ν be Borel probability measures on $(\mathbf{R}^d \times \mathbf{R}^d)^j$, and let $\Pi(\mu, \nu)$ be the set of probability measures on $(\mathbf{R}^d \times \mathbf{R}^d)^j \times (\mathbf{R}^d \times \mathbf{R}^d)^j$ whose first and second marginals are μ and ν respectively. Define

$$(10) \quad \text{dist}_1(\mu, \nu) := \inf_{\pi \in \Pi(\mu, \nu)} \iint_{((\mathbf{R}^d \times \mathbf{R}^d)^j)^2} \min(1, |z - z'|) \pi(dz dz').$$

for each pair of Borel probability measures μ, ν on $(\mathbf{R}^d \times \mathbf{R}^d)^j$.

Theorem 3.1. *Assume that the interaction potential Φ is a real-valued, even differentiable function defined on \mathbf{R}^d with Lipschitz continuous gradient, and let $\Lambda := 3 + 4 \text{Lip}(\nabla \Phi)^2$. Let F^{in} be a Töplitz operator, and let F be the solution of the Hartree equation (2) with initial data F^{in} . On the other hand, for each $N \geq 1$, let F^N be the solution of (1) with initial data $(F^{in})^{\otimes N}$, and F_j^N its j -particle marginal for each $j = 1, \dots, N$. Then, for each fixed integer $j \geq 1$, and each $T > 0$, one has¹*

$$(11) \quad \text{dist}_1(\widetilde{W}_{F_j^N(t)}, \widetilde{W}_{F(t)^{\otimes j}})^2 \lesssim \frac{64(\log 2)dT\|\Phi\|_{L^\infty}(1 + je^{\Lambda T})}{\log \log N}$$

for all $t \in [0, T]$ and all $\hbar \in [0, 1]$ in the limit as $N \rightarrow \infty$.

Note that dist_1 is the distance used by Dobrushin in [6]. For each $\phi \in C_b(\mathbf{R}^d)$, denote by $L_1(\phi)$ the Lipschitz constant of ϕ for the distance $(z, z') \mapsto \min(1, |z - z'|)$, i.e.

$$L_1(\phi) := \sup_{z \neq z'} \frac{|\phi(z) - \phi(z')|}{\min(1, |z - z'|)}.$$

By Monge-Kantorovich duality one has

$$\text{dist}_1(\mu, \nu) = \sup_{L_1(\phi) \leq 1} \left| \int \phi(z) \mu(dz) - \int \phi(z) \nu(dz) \right|.$$

Hence the distance dist_1 induces on the set of Borel probability measures on $\mathbf{R}^d \times \mathbf{R}^d$ a topology that is equivalent to the restriction of the Sobolev $W^{-1,1}(\mathbf{R}^d \times \mathbf{R}^d)$ metric. Since density matrices on $\mathfrak{H} := L^2(\mathbf{R}^d)$ are determined by their Husimi functions as recalled in the previous section, the expression

$$(D_1, D_2) \mapsto \text{dist}_1(\widetilde{W}_\hbar[D_1], \widetilde{W}_\hbar[D_2])$$

¹The statement $a_n \lesssim b_n$ means that $a_n \leq b_n(1 + \epsilon_n)$ with $\epsilon_n \rightarrow 0$ as $n \rightarrow \infty$.

defines a distance on the set of density matrices. This distance obviously depends on \hbar through the Husimi functions. However, if D_1^\hbar and D_2^\hbar are \hbar -dependent density matrices such that

$$\widetilde{W}_\hbar[D_1^\hbar] \rightarrow \mu_1 \text{ and } \widetilde{W}_\hbar[D_2^\hbar] \rightarrow \mu_2 \quad \text{in } \mathcal{S}'(\mathbf{R}^d \times \mathbf{R}^d)$$

in the limit as $\hbar \rightarrow 0$, then

$$\text{dist}_1(\widetilde{W}_\hbar[D_1^\hbar], \widetilde{W}_\hbar[D_2^\hbar]) \rightarrow \text{dist}_1(\mu_1, \mu_2).$$

For that reason (11) provides a convergence rate for the mean-field limit of the quantum N -body dynamics that is uniform in \hbar .

Our second uniform convergence is based on Cauchy-Kovalevskaja type estimates on the BBGKY hierarchy. It gives a better convergence rate, at the expense of much more stringent conditions on the interaction potential Φ and evolution over short time intervals, independent of the Planck constant. The convergence rate obtained in this second result is formulated in terms of the following family of norms. For each $\beta > 0$ and each $f \in L^1((\mathbf{R}^n \times \mathbf{R}^n)^2)$, we set

$$\|f\|_\rho := \sup_{\xi, \eta \in \mathbf{R}^n} |\widehat{f}(\xi, \eta)| e^{\rho(|\xi| + |\eta|)}$$

where \widehat{f} is the (twisted) Fourier transform of f

$$\widehat{f}(\xi, \eta) := \frac{1}{(2\pi)^{2n}} \int_{\mathbf{R}^n \times \mathbf{R}^n} e^{-i(q \cdot \xi - p \cdot \eta)} f(q, p) dq dp$$

By a slight abuse of notation, for each trace class operator F on $\mathfrak{H}_j := L^2(\mathbf{R}^{dj})$, we also denote

$$(12) \quad \|F\|_\rho := \|W_\hbar[F]\|_\rho.$$

Theorem 3.2. *Assume that, for some $\beta' > 0$, one has both*

$$\|F^{in}\|_{\beta'} < \infty \quad \text{and} \quad \int |h| |\widehat{\Phi}(h)| e^{\beta'|h|} dh < \infty.$$

Let $\alpha > \log \|F^{in}\|_{\beta'}$ and let β satisfy $0 < \beta < \beta'$; in addition, let $T = T(\beta', \beta, \alpha, \Phi)$ be defined by (24) below.

Let $F(t)$ be the solution of the Hartree equation with initial condition F^{in} , and let $F^N(t)$ be the solution of the N -body Schrödinger equation with initial condition $(F^{in})^{\otimes N}$.

Then for all t , $|t| < T$ and $j \in \mathbf{N}^*$, we have for $N \geq j$,

$$(13) \quad \|F_j^N(t) - F(t)^{\otimes j}\|_\beta \leq \frac{C(j, t)}{N} \frac{|t|}{T} \frac{\|F^{in}\|_{\beta'}}{1 - e^{-\alpha} \|F^{in}\|_{\beta'}}.$$

For all $t \in [0, T)$, the constant $C(j, t) > 0$ is defined by formula (35), is independent of N , and satisfies

$$C(j, t) \sim j \frac{e^{\alpha j} + e^{j \frac{|t|}{T} / e \log \frac{T}{|t|}}}{(1 - |t|/T)^2} \text{ as } j \rightarrow \infty$$

(see (35) for a more precise result).

A straightforward consequence of this theorem is the following statement.

Corollary 3.3. *Let $0 \leq |t|/T < 1$. Then, for all $\beta < \beta'$,*

$$\|F_j^N(t) - F(t)^{\otimes j}\|_\beta \rightarrow 0 \text{ as } N \rightarrow \infty,$$

uniformly in $j \leq C \log \left(\frac{N}{|t|/T} \right)$ for any $C < \left(\max \left(\alpha, \frac{|t|/T}{e \log T/|t|} \right) \right)^{-1}$.

Notice that estimate (13) implies that the N -particle system converges to the Hartree dynamics uniformly in $\hbar \in [0, 1]$ for a suitable class of relevant initial states, e.g. states for which $\|F\|_\beta$ is uniformly bounded for some $\beta > 0$. Examples of such initial data are superpositions of orthogonal projectors on coherent states with a positive density f with $\|f\|_{L^1(\mathbf{R}^d)} = 1$ and $\|f\|_\beta$ uniformly bounded for a some $\beta > 0$. Indeed consider

$$F = \int_{\mathbf{R}^{2d}} f(x, v) |x, v\rangle \langle x, v| dx dv.$$

Since

$$\widehat{W}_F(\xi, \eta) = e^{-\frac{\hbar}{4}(\xi^2 + \eta^2)} W_F(\xi, \eta)$$

we have

$$\|F\|_\beta = \|W_F\|_\beta \leq \|f\|_\beta.$$

Moreover

$$\begin{aligned} \|F_j^N(t) - F(t)^{\otimes j}\|_{\beta'} &= \|W_\hbar[F_j^N(t)] - W_\hbar[F(t)^{\otimes j}]\|_{\beta'} \\ &= \|W_\hbar[F^N(t)]_j - W_\hbar[F(t)]^{\otimes j}\|_{\beta'} \end{aligned}$$

and, by e.g. [12], $W_\hbar[F^N(t)] \rightarrow f^N(t)$ and $W_\hbar[F(t)] \rightarrow f(t)$ as $\hbar \rightarrow 0$, where $f(t)$ is the solution of the Vlasov equation with initial condition f^{in} , while $f^N(t)$ is the solution of the N -body Liouville equation with initial condition $(f^{in})^{\otimes N}$. Therefore taking the limit $\hbar \rightarrow 0$ in (13), we arrive at our last main result.

Corollary 3.4. *Assume that $\|f^{in}\|_{\beta'} < \infty$ and that*

$$\int |h| |\widehat{\Phi}(h)| e^{\beta'|h|} dh < \infty,$$

for some $\beta' > 0$. Let $\alpha > \log \|F\|_{\beta'}$, let $0 < \beta < \beta'$, and let T and $C(j, t)$ be given by the same prescription as in Theorem 3.2. Let $f(t)$ be the solution of the Vlasov equation with initial condition f^{in} and $f^N(t)$ the solution of the N -body Liouville equation with initial condition $(f^{in})^{\otimes N}$.

Then for all t satisfying $|t| < T$ and all $j \in \mathbf{N}^$*

$$\|f_j^N(t) - f(t)^{\otimes j}\|_\beta \leq \frac{C(j, t)}{N} \frac{|t|}{T} \frac{\|f^{in}\|_{\beta'}}{1 - e^{-\alpha} \|f^{in}\|_{\beta'}},$$

and $\|f_j^N(t) - f(t)^{\otimes j}\|_\beta \rightarrow 0$ as $N \rightarrow \infty$, uniformly in $j \leq C \log \left(\frac{N}{|t|/T} \right)$ for any $C < \left(\max \left(\alpha, \frac{|t|/T}{e \log T/|t|} \right) \right)^{-1}$.

Part 1. Results with analytic data

4. BOUNDS ON THE SOLUTIONS OF THE HIERARCHIES

Integrating the Wigner equation (9), with

$$V_N(x) = \frac{1}{2N} \sum_{l \neq r} \Phi(x_l - x_r)$$

over the $N - j$ last variables leads to the following finite hierarchy, henceforth referred to as the “Wigner hierarchy”, of course equivalent to (4),

$$(14) \quad \partial_t f_j^N + \sum_{i=1}^j v_i \cdot \nabla_{x_i} f_j^N = \frac{1}{N} T_j f_j^N + \frac{N-j}{N} C_{j+1} f_{j+1}^N,$$

where T_j and C_{j+1} are defined below by formulas (26)–(27), while

$$f_j^N(x_1, \dots, x_j; \xi_1, \dots, \xi_j) := \int f^N(x; \xi) dx_{j+1} d\xi_{j+1} \dots dx_N d\xi_N \text{ for } j \leq N,$$

$$f_j^N := 0 \text{ for } j > N.$$

Passing to the limit as $N \rightarrow \infty$, one arrives at the infinite hierarchy

$$\partial_t f_j + \sum_{i=1}^j v_i \cdot \nabla_{x_i} f_j = C_{j+1} f_{j+1}$$

henceforth referred to as the “Hartree hierarchy”. So far, this is a formal statement, and one of the goals in our study is to turn this formal statement into a precise convergence statement with an estimate of the convergence rate.

From now on, we regard both the Wigner and the Hartree hierarchies as governing the evolution of infinite sequences of Wigner distributions. It is therefore natural to seek controls on these hierarchies in appropriate functional spaces of sequences $\underline{f} = \{f_j\}_{j=1, \dots, \infty}$. These functional spaces are metrized by the following family of norms

$$\|\underline{f}\|_{\alpha, \beta} := \sum_{j=1}^{\infty} e^{-\alpha j} \|f_j\|_{\beta}, \quad \alpha, \beta > 0.$$

For $\beta > 0$ we set

$$C_{\Phi}^{\beta}(t) := \int |h| |\widehat{\Phi}(h)| e^{2\beta|h|(1+|t|)} dh, \quad C_{\Phi}^0 := \int |h| |\widehat{\Phi}(h)| dh.$$

Theorem 4.1. *Let $\underline{f}^N(t)$ be the solution of the N -body Wigner hierarchy with initial data $\underline{f}^{in} = \{f_j^{in}\}_{j=1, \dots, \infty}$ defined by*

$$f_j^{in} = (f^{in})^{\otimes j}, \quad j \leq N,$$

$$f_j^{in} = 0, \quad j > N,$$

and satisfying $\|f^{in}\|_{\beta'} < \infty$ for some $\beta' > 0$.

Then for each $\alpha \geq \log \|f^{in}\|_{\beta}$ and each β such that $0 < \beta < \beta'$, there exists $T \equiv T[\alpha, \beta, \beta'] > 0$ given by (24) below such that, for each $t \in [0, T)$

$$(15) \quad \|\underline{f}^N(t)\|_{\alpha, \beta} \leq \frac{\|\underline{f}^{in}\|_{\alpha, \beta'}}{1 - \frac{|t|}{T}}$$

Proof. Our proof of Theorem 3.2 based on the estimates in the next lemma, whose proof is deferred until the end of the present section.

Lemma 4.2 (Propagation estimates). *Let $S_j(t)$ denote the group generated by the free transport operator in j variables*

$$- \sum_{k=1}^j \xi_k \cdot \nabla_{x_k}.$$

In other words,

$$S_j(t)f_j : (x_1, \dots, x_j, \xi_1, \dots, \xi_j) \mapsto f_j(x_1 - t\xi_1, \dots, x_j - t\xi_j, \xi_1, \dots, \xi_j)$$

is the value at time t of the solution of the Cauchy problem

$$\partial_t f_j^0 + \sum_{k=1}^j \xi_k \cdot \nabla_{x_k} f_j^0 = 0, \quad f_j^0|_{t=0} = f_j$$

Then,

$$(16) \quad \|S_j(t)f_j\|_\beta \leq \|f_j\|_{\beta'} \quad \text{provided that } \frac{\beta' - \beta}{\beta} \geq |t|,$$

while

$$(17) \quad \|S_j(-t)C_{j+1}S_j(t)f_{j+1}\|_\beta \leq \frac{(1+|t|)C_\Phi^0}{e^{(\beta' - \beta)}} \|f_{j+1}\|_{\beta'}$$

and

$$(18) \quad \|S_j(-t)T_jS_j(t)f_j\|_\beta \leq \frac{2j(1+|t|)C_\Phi^{\beta'}(t)}{e^{(\beta' - \beta)}} \|f_j\|_{\beta'}$$

whenever $\beta' > \beta$.

Define

$$(19) \quad T^N \underline{f} := \left\{ \frac{T_j}{N} f_j \right\}_{j=1 \dots \infty} \quad \text{and} \quad C^N \underline{f} := \left\{ \frac{N-j}{N} C_{j+1} f_{j+1} \right\}_{j=1 \dots \infty}$$

so that (14) reads

$$\partial_t \underline{f}^N + \sum_{i=1}^N v_i \cdot \nabla_{x_i} \underline{f}^N = (T^N + C^N) \underline{f}^N,$$

and let

$$S(t) \underline{f}^N := \{S_j(t)f_j^N\}_{j=1 \dots \infty}.$$

As a straightforward consequence of Lemma 4.2, we arrive at the following estimates.

Corollary 4.3. *Under the same hypothesis as in Lemma 4.2 and for $\beta' > \beta$, one has*

$$\|S(-t)C^N S(t) \underline{f}\|_{\alpha, \beta} \leq \frac{(1+|t|)C_\Phi^0 e^\alpha}{e^{(\beta' - \beta)}} \|\underline{f}\|_{\alpha, \beta'},$$

$$\|(S(-t)T^N S(t) \underline{f})_j\|_\beta \leq \frac{j}{N} e^{\alpha j} \frac{2(1+|t|)C_\Phi^{\beta'}(t)}{e^{(\beta' - \beta)}} \|\underline{f}\|_{\alpha, \beta'}$$

and

$$\|S(-t)T^N S(t) \underline{f}\|_{\alpha, \beta} \leq \frac{2(1+|t|)C_\Phi^{\beta'}(t)}{e^{(\beta' - \beta)}} \|\underline{f}\|_{\alpha, \beta'}.$$

We shall compute the norm of the solution of the Wigner hierarchy by using a Dyson expansion. For $0 \leq t_1 \leq t_2 \dots \leq t_n \leq t$, consider the string of distribution functions indexed by $n \geq 0$, and defined as follows: for $n > 0$,

$$(20) \quad g_n^N(t, t_1, \dots, t_n) := S(t)S(-t_n)(T^N + C^N)S(t_n) \dots S(-t_1)(T^N + C^N)S(t_1) \underline{f}^{in}$$

while

$$g_0^N(t) := S(t)\underline{f}^{in}$$

where $\underline{f}^{in} = \{f_j^{in}\}_{j=1\dots\infty}$ is the initial data.

For each $K \geq 1$, set

$$\underline{g}^{N,K}(t) := \sum_{n=0}^K \int_0^t dt_n \int_0^{t_n} dt_{n-1} \dots \int_0^{t_2} dt_1 g_n(t, t_1, \dots, t_n).$$

We see immediately that

$$\partial_t \underline{g}^{N,K} + \sum_{i=1}^N v_i \cdot \nabla_{x_i} \underline{g}^{N,K} = (T^N + C^N) \underline{g}^{N,K-1}, \quad \underline{g}^{N,K}(0) = \underline{f}^{in}.$$

The Dyson expansion is

$$\lim_{K \rightarrow \infty} \underline{g}^{N,K}(t) := \underline{g}^N(t)$$

and, if

$$\lim_{K \rightarrow \infty} (T^N + C^N) \underline{g}^{N,K-1} = (T^N + C^N) \underline{g}^N$$

then the Dyson expansion gives the solution \underline{f}^N of the N -body Wigner hierarchy with initial data \underline{f}^{in} . Uniqueness is obvious for finite N , since the last equation in the Wigner hierarchy is equivalent to the N -body quantum problem.

For $\beta < \beta_0 < \beta'$, defining $\beta_k := \beta_0 + k \frac{\beta' - \beta_0}{n}$ and applying Lemma 4.2 (16) and Corollary 4.3 with $|t| \leq \frac{\beta_0 - \beta}{\beta}$, we get

$$\begin{aligned} \|g_n(t, t_1, \dots, t_n)\|_{\alpha, \beta} &= \|S(t) \Sigma_N(t_n) \Sigma_N(t_{n-1}) \dots \Sigma_N(t_1) \underline{f}^{in}\|_{\alpha, \beta_0} \\ &\leq \|\Sigma_N(t_n) \Sigma_N(t_{n-1}) \dots \Sigma_N(t_1) \underline{f}^{in}\|_{\alpha, \beta_0} \\ &\leq \frac{3(1+|t|)C_{\Phi}^{\beta_1}(t)e^\alpha}{e^{(\beta_1 - \beta_0)}} \|\Sigma_N(t_{n-1}) \dots \Sigma_N(t_1) \underline{f}^{in}\|_{\alpha, \beta_1} \\ &\leq \frac{3(1+|t|)C_{\Phi}^{\beta'}(t)e^\alpha}{e^{(\beta' - \beta_0)}} n \|\Sigma_N(t_{n-1}) \dots \Sigma_N(t_1) \underline{f}^{in}\|_{\alpha, \beta_1} \\ (21) \quad &\leq \left(\frac{3(1+|t|)C_{\Phi}^{\beta'}(t)e^\alpha}{e^{(\beta' - \beta_0)}} n \right)^n \|\underline{f}^{in}\|_{\alpha, \beta'} \end{aligned}$$

where

$$\Sigma_N(t_k) := S(-t_k)(T^N + C^N)S(t_k).$$

Therefore

$$\begin{aligned} \sum_{n=0}^K \left\| \int_0^t dt_1 \int_0^{t_1} dt_2 \dots \int_0^{t_{n-1}} dt_n g_n(t, t_1, \dots, t_n) \right\|_{\alpha, \beta} \\ \leq \sum_{n=0}^K \left(\frac{3(1+|t|)C_{\Phi}^{\beta'}(t)e^\alpha}{e^{(\beta' - \beta_0)}} n \right)^n \|\underline{f}^{in}\|_{\alpha, \beta'} \frac{|t|^n}{n!} \\ (22) \quad \leq \sum_{n=0}^K \left(\frac{3(1+|t|)|t|C_{\Phi}^{\beta'}(t)e^\alpha}{(\beta' - \beta_0)} \right)^n \|\underline{f}^{in}\|_{\alpha, \beta'} \end{aligned}$$

where the inequality follows from Stirling's formula. Hence the Dyson expansion converges uniformly in N as soon as

$$|t| \leq \frac{\beta_0 - \beta}{\beta} \quad \text{and} \quad \frac{3(1 + |t|)|t|C_{\Phi}^{\beta'}(t)e^{\alpha}}{(\beta' - \beta_0)} < 1.$$

By construction, the function $t \mapsto C_{\Phi}^{\beta'}(t)$ is continuous and increasing on \mathbf{R}_+^* , so that there exists a unique $\beta_0 := \beta_0[\alpha, \beta, \beta']$ satisfying

$$(23) \quad \beta < \beta_0 < \beta' \quad \text{and} \quad 3\left(1 + \frac{\beta_0 - \beta}{\beta}\right) \frac{\beta_0 - \beta}{\beta} C_{\Phi}^{\beta'}\left(\frac{\beta_0 - \beta}{\beta}\right) e^{\alpha} = \beta' - \beta_0.$$

Defining

$$(24) \quad T[\alpha, \beta, \beta'] := \frac{\beta_0[\alpha, \beta, \beta'] - \beta}{\beta},$$

we see that

$$|t| < T[\alpha, \beta, \beta'] \Rightarrow |t| \leq \frac{\beta_0 - \beta}{\beta} \quad \text{and} \quad \frac{3(1 + |t|)|t|C_{\Phi}^{\beta'}(t)e^{\alpha}}{(\beta' - \beta_0)} < 1.$$

Hence the Dyson expansion converges uniformly in N for $|t| < T[\alpha, \beta, \beta']$.

Applying Corollary 4.3 with $t = 0$, and using the geometric series estimates in (22) shows that the term $(T^N + C^N)\underline{f}^{N, K-1}$ converges to $(T^N + C^N)\underline{f}^N$ as $K \rightarrow \infty$.

Therefore, $\underline{g}^{N, K}$ converges to \underline{f}^N as $K \rightarrow \infty$, and \underline{f}^N is given by the Dyson expansion. In particular, the estimate (15) follows from (22), after noticing that

$$(25) \quad \frac{3(1 + |t|)|t|C_{\Phi}^{\beta'}(t)e^{\alpha}}{(\beta' - \beta_0)} \leq \frac{|t|}{T} \times \frac{3(1 + T)TC_{\Phi}^{\beta'}(T)e^{\alpha}}{(\beta' - \beta_0)} \leq \frac{|t|}{T}$$

since $\frac{3(1+T)TC_{\Phi}^{\beta'}(T)e^{\alpha}}{(\beta' - \beta_0)} = 1$ by (24) and (23). \square

We conclude this section with the proof of Lemma 4.2.

Proof of Lemma 4.2. We shall write everything in Fourier variables, henceforth denoted $(\underline{\xi}_j; \underline{\eta}_j) := (\xi_1, \dots, \xi_j; \eta_1, \dots, \eta_j) \in \mathbf{R}^{2jd}$, together with $\underline{h}_r := (0_{r-1}, h, 0_{d-r})$ for $h \in \mathbf{R}^d$. In these definitions, we have used the notation $0_{r-1} := (0, \dots, 0) \in \mathbf{R}^{(r-1)d}$. In other words, ξ_j is the Fourier variable corresponding to x_j while η_j is the Fourier variable corresponding to v_j . With this, we get

$$(26) \quad \widehat{T_j f_j^N}(\underline{\xi}; \underline{\eta}) = \sum_{l \neq r} \int \frac{dh}{(2\pi)^d} \widehat{\Phi}(h) \frac{\sin \frac{\hbar}{2}(\eta_l - \eta_r) \cdot h}{\hbar} \widehat{f_j^N}(\underline{\xi}_j + \underline{h}_l - \underline{h}_r; \underline{\eta}_j)$$

$$(27) \quad \widehat{C_{j+1} f_{j+1}^N}(\underline{\xi}_j; \underline{\eta}_j) = \sum_{r=1}^j \int \frac{dh}{(2\pi)^d} \widehat{\Phi}(h) \frac{2 \sin(\frac{\hbar}{2} \eta_r \cdot h)}{\hbar} \widehat{f_{j+1}^N}(\underline{\xi}_j - \underline{h}_r, h; \underline{\eta}_j, 0)$$

Observe that one recovers the classical BBGKY hierarchy as the formal limit of the above as $\hbar \rightarrow 0$.

One also gets immediately

$$\widehat{S(t) f_j}(\underline{\xi}_j; \underline{\eta}_j) = \widehat{f_j}(\underline{\xi}_j; \underline{\eta}_j + t \underline{\xi}_j)$$

and by explicit computations

$$\begin{aligned} S(-t)\widehat{T_j}S(t)f_j^N(\underline{\xi}_j; \underline{\eta}_j) &= \sum_{l \neq r} \int \frac{dh}{(2\pi)^d} \widehat{\Phi}(h) \frac{\sin(\frac{h}{2}(\eta_l - \eta_r - t(\xi_l - \xi_r)) \cdot h)}{h} \\ &\quad \cdot \widehat{f_j^N}(\underline{\xi}_j + \underline{h}_l - \underline{h}_r; \underline{\eta}_j + t(\underline{h}_l - \underline{h}_r)) \\ S(-t)\widehat{C_{j+1}}S(t)f_{j+1}^N(\underline{\xi}_j; \underline{\eta}_j) &= \sum_{r=1}^j \int \frac{dh}{(2\pi)^d} \widehat{\Phi}(h) \frac{2 \sin(\frac{h}{2}(\eta_r + t\xi_r) \cdot h)}{h} \\ &\quad \cdot \widehat{f_{j+1}^N}(\underline{\xi}_j - \underline{h}_r, h; \underline{\eta}_j - t\underline{h}_r, -th) \end{aligned}$$

For $\beta' > \beta$ we have

$$\begin{aligned} \|S(t)f_j\|_\beta &\leq \|f_j\|_{\beta'} \sup_{\underline{\xi}_j, \underline{\eta}_j} \exp\left(-\beta' \sum_{i=1}^j (|\xi_i| + |\eta_i|) + \beta \sum_{i=1}^j (|\xi_i| + |\eta_i + t\xi_i|)\right) \\ &\leq \|f_j\|_{\beta'} \exp\left(-(\beta' - \beta) \sum_{i=1}^j (|\xi_i| + |\eta_i|) + \beta|t| \sum_{i=1}^j (|\xi_i|)\right) \leq \|f_j\|_{\beta'} \end{aligned}$$

provided $\frac{\beta' - \beta}{\beta} \geq |t|$, which proves (16).

Moreover, for $\beta' > \beta$,

$$\begin{aligned} \|S(-t)C_{j+1}S(t)f_{j+1}\|_\beta &\leq \|f_{j+1}\|_{\beta'} \sup_{\underline{\xi}_j, \underline{\eta}_j} e^{\beta \sum_{i=1}^j (|\xi_i| + |\eta_i|)} \\ &\times \sum_{r=1}^j \int dh |\widehat{\Phi}(h)| h (|\eta_r| + |t\xi_r|) e^{-\beta' \sum_{i=1}^j (|\xi_i - \delta_{r,i} h| + |\eta_i - t\delta_{r,i} h|)} e^{-\beta' (|h| + |th|)} \\ &\leq \|f_{j+1}\|_{\beta'} (1 + |t|) C_{\widehat{\Phi}}^0 \sup_{\underline{\xi}_j, \underline{\eta}_j} \sum_{k=1}^j (|\xi_k| + |\eta_k|) e^{(\beta - \beta') \sum_{i=1}^j (|\xi_i| + |\eta_i|)} \\ &\leq \|f_{j+1}\|_{\beta'} \frac{(1 + |t|) C_{\widehat{\Phi}}^0}{e^{(\beta' - \beta)}} \end{aligned}$$

where the second inequality above uses the triangle inequalities $|\eta_r + th| \geq |\eta_r| - |th|$ and $|\xi_r - h| \geq |\xi_r| - |h|$. This establishes (17).

To derive (18) we use the same type of argument:

$$\begin{aligned} \|S(-t)T_jS(t)f_j\|_\beta &\leq \|f_j\|_{\beta'} \sup_{\underline{\xi}_j, \underline{\eta}_j} e^{\beta \sum_{i=1}^j (|\xi_i| + |\eta_i|)} \sum_{1 \leq r < l \leq j} \int \frac{dh}{(2\pi)^d} |\widehat{\Phi}(h)| h \\ &\quad \times |\eta_l - \eta_r + t(\xi_l - \xi_r)| e^{-\beta' \sum_{i=1}^j (|\xi_i + \delta_{i,l} h - \delta_{i,r} h| + |\eta_i + t\delta_{i,l} h - t\delta_{i,r} h|)} \\ (28) \quad &\leq \|f_j\|_{\beta'} \sup_{\underline{\xi}_j, \underline{\eta}_j} e^{(\beta - \beta') \sum_{i=1}^j (|\xi_i| + |\eta_i|)} \\ &\quad \times (1 + |t|) \sum_{1 \leq r < l \leq j} (|\eta_r| + |\eta_l| + |\xi_r| + |\xi_l|) \int \frac{dh}{(2\pi)^d} |\widehat{\Phi}(h)| h e^{2\beta' |h| (1 + |t|)} \\ &\leq \|f_j\|_{\beta'} 2^j \frac{(1 + |t|) C_{\widehat{\Phi}}^{\beta'}(t)}{e^{(\beta' - \beta)}} \end{aligned}$$

□

5. COMPARISON WITH HARTREE

We want now to compare the solution of the N -body Wigner hierarchy to the solution of the infinite, Hartree hierarchy. The solution of the Hartree hierarchy, namely the sequence $\{f(t)^{\otimes j}\}_{j=1,\dots}$ can be also constructed exactly as in the previous section out of the string g_n given by the formula

$$\begin{cases} g_n(t, t_1, \dots, t_n) = S(t)S(-t_n)CS(t_n) \dots S(-t_1)CS(t_1)\underline{f}^{in}, & n > 0, \\ g_0(t) := S(t)\underline{f}^{in}, \end{cases}$$

where

$$C\underline{f} := \{C_{j+1}f_{j+1}\}_{j \geq 1}.$$

Let g_n^N be the string leading to the N -body Wigner hierarchy, that is

$$\begin{cases} g_n^N(t, t_1, \dots, t_n) := S(t)S(-t_n)(T^N + C^N)S(t_n) \dots S(-t_1)(T^N + C^N)S(t_1)\underline{f}^{in}, \\ g_0^N(t) := S(t)\underline{f}^{in}, \end{cases}$$

where we recall that T^N and C^N are given by (19). Finally we define g_n^{HHN} by

$$\begin{cases} g_n^{HHN}(t, t_1, \dots, t_n) = S(t)S(-t_n)C^N S(t_n) \dots S(-t_1)C^N S(t_1)\underline{f}^{in}, & n > 0, \\ g_0^{HHN}(t) := S(t)\underline{f}^{in}. \end{cases}$$

Notice that $g_0 = g_0^{HHN} = g_0^N$.

5.1. **Comparing g_n^N to g_n^{HHN} .** For $n_0 \geq 1$, one has

$$\begin{aligned} & \left\| \sum_{n=0}^{\infty} \int_0^t dt_n \int_0^{t_n} dt_{n-1} \dots \int_0^{t_2} dt_1 (g_n^N - g_n^{HHN})_j(t, t_1, \dots, t_n) \right\|_{\beta} \\ & \leq \left\| \sum_{n=1}^{n_0} \int_0^t dt_n \int_0^{t_n} dt_{n-1} \dots \int_0^{t_2} dt_1 (g_n^N - g_n^{HHN})_j(t, t_1, \dots, t_n) \right\|_{\beta} + R(n_0) \end{aligned}$$

where $R(n_0)$ is the sum of the two remainders of the (convergent) Dyson expansions of g_n^N and g_n^{HHN} . Using (25), one easily finds that

$$(29) \quad R(n_0) \leq \frac{2e^{\alpha j}}{1 - \frac{|t|}{T}} \left(\frac{|t|}{T} \right)^{n_0+1} \|\underline{f}\|_{\alpha, \beta'}.$$

In order to estimate the sum up to n_0 , we expand the string $g_n^N(t, t_1, \dots, t_n)$ as

$$(30) \quad g_n^N = \sum_{k=0}^n \sum_{\substack{\sigma_1, \dots, \sigma_n \in \{0,1\}, \\ \sum_{i=1}^n \sigma_i = n-k}} O_{\sigma_n}(t_n) \dots O_{\sigma_1}(t_1) \underline{f}^{in}$$

where

$$O_0(t) := S(-t)T^N S(t) \quad \text{and} \quad O_1(t) = S(-t)C^N S(t),$$

so that we detect the number of T^N s in the expansion.

Since the number k of shifts satisfies $k \leq n$ and $\|f_j\|_\beta \leq e^{\alpha j} \|\underline{f}\|_{\alpha, \beta}$, we deduce from Lemma 4.2 that

$$\begin{aligned} \|(g_n^N - g_n^{HHN})_j\|_\beta &\leq e^{\alpha(j+n)} (nc)^n \sum_{k=1}^n \left(\frac{j+n}{N}\right)^k \binom{n}{k} \|\underline{f}\|_{\alpha, \beta'} \\ &= e^{\alpha j} (nce)^n \left(\left(1 + \frac{j+n}{N}\right)^n - 1 \right) \|\underline{f}\|_{\alpha, \beta'} \end{aligned}$$

with

$$c = \frac{2(1+|t|)C_\Phi^{\beta'}(t)e^\alpha}{e^{(\beta' - \beta)}}$$

(notice that the term corresponding to $k = 0$ is precisely f_n^{HHN}).

For $n \leq n_0$, one has

$$\left(1 + \frac{j+n}{N}\right)^n - 1 \leq n \frac{j+n}{N} (1 + (j+n_0)/N)^{n_0-1};$$

besides

$$(1 + (j+n_0)/N)^{n_0-1} = e^{(n_0-1) \log 1 + (j+n_0)/N} \leq e^{(n_0-1)(j+n_0)/N} := c_{n_0},$$

with $c_{n_0} \rightarrow 1$ as $N \rightarrow \infty$ and $n_0 \ll \sqrt{N}$.

Therefore

$$\begin{aligned} &\left\| \sum_{n=0}^{n_0} \int_0^t dt_n \int_0^{t_n} dt_{n-1} \dots \int_0^{t_2} dt_1 (g_n^N - g_n^{HHN})_j(t, t_1, \dots, t_n) \right\|_\beta \\ &\leq \left(c_{n_0} e^{\alpha j} \sum_{n=1}^{n_0} (tce)^n \frac{j+n}{N} n \right) \|\underline{f}^{in}\|_{\alpha, \beta'} \\ &\leq \left(c_{n_0} \frac{e^{\alpha j}}{N} \sum_{n=1}^{\infty} (tce)^n (j+n)n \right) \|\underline{f}^{in}\|_{\alpha, \beta'} = \frac{|t|}{T} \left(c_{n_0} \frac{c_1}{N} \right) \|\underline{f}^{in}\|_{\alpha, \beta'}, \end{aligned}$$

with

$$(31) \quad c_1 = e^{\alpha j} \frac{|t|}{T} \left(\frac{j}{(1 - \frac{|t|}{T})^2} + \frac{2}{(1 - \frac{|t|}{T})^3} \right) \text{ and } c_{n_0} = e^{(n_0-1)(j+n_0)/N}.$$

We finally get

$$(32) \quad \left\| \sum_{n=0}^{\infty} \int_0^t dt_n \int_0^{t_n} dt_{n-1} \dots \int_0^{t_2} dt_1 (g_n^N - g_n^{HHN})_j(t, t_1, \dots, t_n) \right\|_\beta \leq \frac{|t|}{T} \left(c_{n_0} \frac{c_1}{N} + \frac{2e^{\alpha j} (|t|/T)^{n_0}}{1 - \frac{|t|}{T}} \right) \|\underline{f}^{in}\|_{\alpha, \beta'}$$

5.2. Comparing g_n and g_n^{HHN} . We first remark that

$$\begin{aligned} &(g_n^{HHN}(t, t_1, \dots, t_n))_j \\ &= S(t)S(-t_1)C_{j+1}^N S(t_1)S(-t_2)C_{j+2}^N S(t_2) \dots S(-t_n)C_{j+n}^N S(t_n) f_{j+n}^{in}, \end{aligned}$$

and that the same holds for g_n :

$$\begin{aligned} &(g_n(t, t_1, \dots, t_n))_j \\ &= S(t)S(-t_1)C_{j+1} S(t_1)S(-t_2)C_{j+2} S(t_2) \dots S(-t_n)C_{j+n} S(t_n) f_{j+n}^{in}. \end{aligned}$$

Since $C_{j+1}^N = (1 - \frac{j}{N})C_{j+1}$, one has

$$(g_n^{HHN}(t, t_1, \dots, t_n) - g_n(t, t_1, \dots, t_n))_j = \left(\prod_{l=1}^n \left(1 - \frac{j+l}{N}\right) - 1 \right) (g_n(t, t_1, \dots, t_n))_j.$$

As before we truncate the summation at n_0 , and consider

$$\sum_{n=1}^{n_0} \int_0^t dt_n \int_0^{t_n} dt_{n-1} \dots \int_0^{t_2} dt_1 (g_n - g_n^{HHN})_j(t, t_1, \dots, t_n).$$

For $j + n_0 < N$ and $n \leq n_0$,

$$\left| \prod_{l=1}^n \left(1 - \frac{j+l}{N}\right) - 1 \right| \leq \left| \left(1 - \frac{j}{N}\right)^{n_0} - 1 \right| \leq c'_{n_0} n_0 \frac{j}{N},$$

with $c'_{n_0} = e^{j(n_0-1)/N} \rightarrow 1$ as $N \rightarrow \infty$ while $n_0 \ll N$ and j is kept fixed.

Therefore

$$\begin{aligned} & \left\| \sum_{n=1}^{n_0} \int_0^t dt_n \int_0^{t_n} dt_{n-1} \dots \int_0^{t_2} dt_1 (g_n - g_n^{HHN})_j(t, t_1, \dots, t_n) \right\|_{\beta} \\ & \leq c'_{n_0} \frac{\frac{(1+|t|)|t|C_{\Phi}^0 e^{\alpha}}{\beta' - \beta}}{\left(1 - \frac{(1+|t|)|t|C_{\Phi}^0 e^{\alpha}}{\beta' - \beta}\right)^2} \|f^{in}\|_{\alpha, \beta'} \leq \frac{|t|}{T} \left(c'_{n_0} \frac{c_3}{N}\right) \|f^{in}\|_{\alpha, \beta'}, \end{aligned}$$

where

$$(33) \quad c_3 = \frac{j}{\left(1 - \frac{|t|}{T}\right)^2} \quad \text{and} \quad c'_{n_0} = e^{j(n_0-1)/N}.$$

Here we have used the fact that

$$\frac{(1+|t|)|t|C_{\Phi}^0 e^{\alpha}}{\beta' - \beta} \leq \frac{|t|}{T}$$

following (25), since $C_{\Phi}^0 \leq C_{\Phi}^{\beta}(t)$ for all $\beta > 0$ and all t .

The same argument as for $g_n^N - g_n^{HHN}$ gives the estimate of the remainder. Recalling that

$$\frac{(1+|t|)|t|C_{\Phi}^0 e^{\alpha}}{\beta' - \beta} \leq \frac{|t|}{T},$$

we easily arrive at

$$(34) \quad \begin{aligned} & \left\| \sum_{n=0}^{\infty} \int_0^t dt_n \int_0^{t_n} dt_{n-1} \dots \int_0^{t_2} dt_1 (g_n - g_n^{HHN})_j(t, t_1, \dots, t_n) \right\|_{\beta} \\ & \leq \frac{|t|}{T} \left(c'_{n_0} \frac{c_3}{N} + \frac{2e^{\alpha j} (|t|/T)^{n_0}}{1 - \frac{|t|}{T}} \right) \|f^{in}\|_{\alpha, \beta'}. \end{aligned}$$

5.3. End of the proof of Theorem 3.2. Choosing now $n_0 = \log(N)/\log(T/|t|)$, we see that $(|t|/T)^{n_0} = 1/N$. Optimizing over N we find that

$$\begin{aligned} c_{n_0} &= e^{(n_0-1)(j+n_0)/N} \\ & \leq \exp \frac{x(j, t)^2 + (j-1) \log(T/|t|) x(j, t) - j(\log(T/|t|))^2}{(\log(T/|t|))^2 e^{x(j, t)}} =: \gamma(j, t) \end{aligned}$$

with

$$x(j, t) := \frac{1}{2} \log \frac{T}{|t|} \left(j - 1 + \frac{2}{\log \frac{T}{|t|}} + \sqrt{\left(j - 1 + \frac{2}{\log \frac{T}{|t|}} \right)^2 + 4 \left(\frac{j-1}{\log \frac{T}{|t|}} + j \right)} \right)$$

and

$$c'_{n_0} = e^{j(n_0-1)/N} \leq e^{j \frac{\frac{|t|}{T}}{e \log \frac{T}{|t|}}} =: \gamma'(j, t)$$

Observe that

$$\gamma(j, t) \rightarrow 1 \text{ and } \gamma'(j, t) \rightarrow 1 \text{ as } |t| \rightarrow 0, \quad \gamma(j, t) \leq 1 \text{ and } \gamma(j, t) \rightarrow 1 \text{ as } j \rightarrow \infty.$$

Adding (32) and (34) and applying the triangle inequality, we find that

$$\begin{aligned} & \left\| \sum_{n=0}^{\infty} \int_0^t dt_n \int_0^{t_n} dt_{n-1} \dots \int_0^{t_2} dt_1 (g_n^N - g_n)_j(t, t_1, \dots, t_n) \right\|_{\beta} \\ & \leq \frac{|t|}{T} \frac{1}{N} \left(c'_{n_0} c_3 + c_{n_0} c_1 + \frac{4e^{\alpha j}}{1 - \frac{|t|}{T}} \right) \| \underline{f}^{in} \|_{\alpha, \beta'} \end{aligned}$$

and therefore (recalling (12))

$$\begin{aligned} (35) \quad & \| F_j^N(t) - F(t)^{\otimes j} \|_{\beta} = \| f_j^N(t) - f(t)^{\otimes j} \|_{\beta} \\ & \leq \frac{1}{N} \frac{|t|}{T} \left(e^{\alpha j} \frac{|t|}{T} c_{n_0} \left(\frac{j}{(1 - \frac{|t|}{T})^2} + \frac{2}{(1 - \frac{|t|}{T})^3} \right) + c'_{n_0} \frac{j}{(1 - \frac{|t|}{T})^2} + \frac{4e^{\alpha j}}{1 - \frac{|t|}{T}} \right) \| \underline{f}^{in} \|_{\alpha, \beta'} \\ & \leq \frac{1}{N} \frac{|t|}{T} \left(e^{\alpha j} \frac{|t|}{T} \left(\frac{j\gamma(j, t)}{(1 - \frac{|t|}{T})^2} + \frac{2\gamma(j, t)}{(1 - \frac{|t|}{T})^3} \right) + \frac{j e^{j \frac{\frac{|t|}{T}}{e \log \frac{T}{|t|}}}}{(1 - \frac{|t|}{T})^2} + \frac{4e^{\alpha j}}{1 - \frac{|t|}{T}} \right) \frac{\| f^{in} \|_{\beta'}}{1 - e^{-\alpha} \| f^{in} \|_{\beta'}} \\ & =: \frac{C(j, |t|)}{N} \frac{|t|}{T} \frac{\| f^{in} \|_{\beta'}}{1 - e^{-\alpha} \| f^{in} \|_{\beta'}}, \end{aligned}$$

where $C(j, t)$ is defined by this last equality.

6. FINAL REMARKS

Our result, based on the Wigner formalism, holds for a short time only, provided that both the potential and initial data are smooth enough. However, this regularity assumption is used exclusively for obtaining estimates that are independent of \hbar .

If one is prepared to give up this requirement, a global in time convergence (under much less stringent assumptions) can indeed be recovered along the following lines, in the same spirit as in [20, 1, 16]. In terms of the L^1 norm of the Fourier transform of the Wigner function in the x variable only, it is easy to see that both operators T^N and C^N are bounded, with a norm that tends to ∞ as $\hbar \rightarrow 0$, while $S(t)$ is isometric. Proceeding as above, we prove the convergence in the mean-field limit, for a short time which depends only on the size of the norm of f^{in} .

However the procedure can be iterated because uniform bounds (in an arbitrary finite time interval) on the norm of the solutions can be obtained by means of H_s (with $s > d/2$) estimates on the Hartree dynamics.

Moreover, although not needed in the present paper, the following estimate improves on (15), and may be of independent interest:

$$(36) \quad \|\underline{f}^N(t) - \underline{f}^{in}\|_{\alpha,\beta} \leq |t| \left(\frac{\|\underline{f}^{in}\|_{\alpha,\beta'}}{\frac{\beta' - \beta}{3(1+|t|)C_{\Phi}^{\beta'}(t)e^{\alpha}} - |t|} + \frac{\sum_{l=1}^d \|v_l \underline{f}^{in}\|_{\alpha,\beta'}}{e(\beta' - \beta)} \right).$$

This bound is obtained in the following manner. First, an explicit computation based on the mean value theorem shows that

$$\|\underline{f}^{in} - S(t)\underline{f}^{in}\|_{\alpha,\beta} \leq \frac{|t|}{e(\beta' - \beta)} \sum_{l=1}^d \|v_l \underline{f}^{in}\|_{\alpha,\beta'}.$$

Notice that the second indices on the norms used in both sides of the inequality above are different and satisfy $\beta' > \beta$; observe indeed that

$$\|\partial_{x_j} \underline{\phi}\|_{\alpha,\beta} \leq \frac{\|\underline{\phi}\|_{\alpha,\beta'}}{e(\beta' - \beta)}, \quad j = 1, \dots, d,$$

this inequality is applied to $\underline{\phi} = v_j \underline{f}^{in}$. This account for the second term on the right hand side of (36). The first term on the right hand side of (36) is obtained by applying the geometric series estimate (22) to

$$\underline{g}^N(t) - S(t)\underline{f}^{in} = \sum_{n \geq 1} \int_0^t dt_n \int_0^{t_n} dt_{n-1} \dots \int_0^{t_2} dt_1 g_n(t, t_1, \dots, t_n).$$

At variance with (22), the summation here starts with $n = 1$; hence

$$\begin{aligned} \|\underline{f}^N(t) - S(t)\underline{f}^{in}\|_{\alpha,\beta} &\leq \sum_{n=1}^{\infty} \left(\frac{3(1+|t|)|t|C_{\Phi}^{\beta'}(t)e^{\alpha}}{(\beta' - \beta_0)} \right)^n \|\underline{f}^{in}\|_{\alpha,\beta'} \\ &= \|\underline{f}^{in}\|_{\alpha,\beta'} \frac{\frac{3(1+|t|)|t|C_{\Phi}^{\beta'}(t)e^{\alpha}}{(\beta' - \beta_0)}}{1 - \frac{3(1+|t|)|t|C_{\Phi}^{\beta'}(t)e^{\alpha}}{(\beta' - \beta_0)}}. \end{aligned}$$

Part 2. Interpolation

7. \hbar -DEPENDENT BOUND

In this section we give a proof of the convergence of the N -body density operator to the solution of the Hartree equation in trace norm. This result does not require any regularity condition on the two-body potential but the convergence is non uniform in the the Planck constant. Indeed, the estimate bearing on the interaction term will treats commutators as if they were anticommutators. In other words, we estimate both terms in the commutator separately and add the corresponding bounds, without taking into consideration any compensation that might come from the difference. This procedure is of course not original and there is a considerable amount of literature on this subject, starting with the seminal paper of Spohn [20].

The new feature in the analysis below is that we keep track of the dependence in \hbar of the rate of convergence so obtained in Theorem 7.1. Indeed, in the next section, the estimate in Theorem 7.1 is interpolated with the convergence rate obtained in [9] in order to obtain the uniform in \hbar bound stated in Theorem 3.1.

The explicit rate of convergence of the mean-field limit has been discussed in [18] and [5], among others. For $\hbar = 1$ and an initial condition in the form of a pure state with appropriate regularity, one can bound the error by Ce^{Ct}/N : see [5]. This result involves the formalism of quantum field theory in Fock space. Iterating the convergence rate obtained from estimating the BBGKY hierarchy for $\hbar = 1$ over short time intervals leads to a bound that is much less sharp. It is interesting to compare the result obtained in [21] with the bound obtained in the forthcoming Theorem 7.1 with $\hbar = 1$.

In our present context we need to track precisely the \hbar -dependence in the mean-field estimate, in view of the interpolation with the results in [9]. Therefore we discuss in detail the iteration procedure, similar to the one used in [17] for a different problem.

Since we seek a trace norm error estimate, it is more convenient to work directly on density operators rather than with their Wigner functions.

Consider the unitary flow $U_j(t)$ defined on $L^2(\mathbf{R}^{jd})$ by the formula

$$i\hbar\dot{U}_j(t) := -\hbar^2\Delta_{\mathbf{R}^{jd}}U_j(t), \quad U_j(0) = \text{Id}_{L^2(\mathbf{R}^{jd})}.$$

Consider the operator $\mathcal{S}_j(t)$ defined on density matrices by conjugation with $U_j(t)$:

$$\mathcal{S}_j(t)F = U_j(t)FU_j(-t).$$

Obviously, $\mathcal{S}_j(t)$ is a linear isometry on $\mathcal{L}^1(L^2(\mathbf{R}^{jd}))$, the space of trace class operators equipped with the trace norm.

We recall the definition of \mathcal{C}_j and \mathcal{T}_j given by (6) and (5). For notational convenience we also denote

$$(37) \quad \mathcal{C}_j^\hbar = \frac{\mathcal{C}}{i\hbar}; \quad \mathcal{T}_j^\hbar = \frac{\mathcal{T}_j}{i\hbar}$$

Henceforth we denote by $F_j^N(t)$ the solutions of the N -particle BBGKY hierarchy, and by $F(t)$ the solution of the Hartree equation. Thus $F_j(t) = F(t)^{\otimes j}$ is a solution of the Hartree hierarchy, and we arrive at the following estimate.

Theorem 7.1. *Let $\Phi \in L^\infty(\mathbf{R}^d)$. Then there exists $N_0(j)$ such that the following estimate holds true for $N \geq N_0(j)$ and $\log N \geq j2^{\frac{16\|\Phi\|_{L^\infty}t}{\hbar}+1}$*

$$\|F_j^N(t) - F(t)^{\otimes j}\|_{\mathcal{L}_1} \leq \frac{2^{j+\frac{16t\|\Phi\|_{L^\infty}}{\hbar}}}{N \left(2^{-\frac{16t\|\Phi\|_{L^\infty}}{\hbar} \log 2}\right)}$$

for all $t \geq 0$.

Proof. We first rephrase (4) and (7) in the following mild form

$$(38) \quad F_j^N(t) = \mathcal{S}(t)F_{0,j} + \int_0^t d\tau \left(\mathcal{S}(t-\tau) \frac{\mathcal{T}_j^\hbar}{N} F_j^N(\tau) + \frac{N-j}{N} \mathcal{S}(t-\tau) \mathcal{C}_{j+1}^\hbar F_{j+1}^N(\tau) \right)$$

and

$$(39) \quad F_j(t) = \mathcal{S}(t)F_{0,j} + \int_0^t d\tau \mathcal{S}(t-\tau) \mathcal{C}_{j+1}^\hbar F_{j+1}(\tau).$$

Here $\{F_{0,j}\}_{j=1}^\infty$ denotes the common initial datum for both sequences, assumed to be factorized, i.e. $F_{0,j} = f_0^{\otimes j}$. Using the group property $\mathcal{S}(t) = \mathcal{S}(t-t_1)\mathcal{S}(t_1)$

for all $0 \leq t_1 \leq t$, and splitting the integral into two parts, we see that

$$(40) \quad F_j^N(t) = S(t-t_1)F_j^N(t_1) + \int_{t_1}^t d\tau \left(S(t-\tau) \frac{\mathcal{T}_j^\hbar}{N} F_j^N(\tau) + \frac{N-j}{N} S(t-\tau) \mathcal{C}_{j+1}^\hbar F_{j+1}^N(\tau) \right)$$

and

$$(41) \quad F_j(t) = S(t-t_1)F_j(t_1) + \int_{t_1}^t d\tau S(t-\tau) \mathcal{C}_{j+1}^\hbar F_{j+1}(\tau).$$

We are interested in bounding the difference

$$(42) \quad \Delta_j(t) = F_j^N(t) - F_j(t),$$

which is recast as

$$(43) \quad \Delta_j(t) = \mathcal{R}_j(t) + \int_{t_1}^t dt_2 S(t-t_2) \mathcal{C}_{j+1}^\hbar \Delta_{j+1}(t_2),$$

where

$$(44) \quad \begin{aligned} \mathcal{R}_j(t) &= S(t-t_1) \Delta_j(t_1) \\ &+ \frac{1}{N} \int_{t_1}^t dt_2 S(t-t_2) \mathcal{T}_j^\hbar F_j^N(t_2) - \frac{j}{N} \int_{t_1}^t dt_2 S(t-t_2) \mathcal{C}_{j+1}^\hbar F_{j+1}^N(t_2). \end{aligned}$$

The following estimates rephrase Lemma 4.2 in the present context, and are obvious consequences of the definitions. For each $j > 0$,

$$(45) \quad \|\mathcal{S}_j(t)F_j\|_{\mathcal{L}^1} = \|F_j\|_{\mathcal{L}^1},$$

$$(46) \quad \|\mathcal{C}_{j+1}^\hbar F_{j+1}\|_{\mathcal{L}^1} \leq \frac{2j\|\Phi\|_{L^\infty}}{\hbar} \|F_{j+1}\|_{\mathcal{L}^1},$$

$$(47) \quad \|\mathcal{T}_j^\hbar \mathcal{S}_j(t)F_j\|_{\mathcal{L}^1} \leq \frac{j(j-1)\|\Phi\|_{L^\infty}}{\hbar} \|F_j\|_{\mathcal{L}^1}.$$

As a consequence

$$(48) \quad \|\mathcal{R}(t)\| \leq \|\Delta(t_1)\| + \frac{3|t-t_1|j^2\|\Phi\|_{L^\infty}}{N\hbar}.$$

Finally, we infer from (43) and (48) that

$$(49) \quad \|\Delta_j(t)\|_{\mathcal{L}^1} \leq \|\Delta_j(t_1)\|_{\mathcal{L}^1} + \frac{3j^2}{16N} + \frac{j}{8T_\hbar} \int_{t_1}^t dt_2 \|\Delta_{j+1}(t_2)\|_{\mathcal{L}^1}.$$

Here

$$T_\hbar = \frac{\hbar}{16\|\Phi\|_{L^\infty}} \text{ and } 0 \leq t-t_1 \leq T_\hbar.$$

Notice that, with this choice, the Dyson expansions associated to the two hierarchies are absolutely convergent (uniformly in N) for any $t \in (t_1, t_1 + T_\hbar)$. However, in contrast with the previous section, we will not consider the full Dyson expansion but only an its finite truncation.

Iterating n times (49) we obtain, for $t - t_1 \leq T_{\hbar}$,

$$(50) \quad \begin{aligned} \|\Delta_j(t)\|_{\mathcal{L}^1} &\leq \sum_{\ell=0}^n \frac{1}{8^\ell} \frac{j(j+1)\cdots(j+\ell-1)}{\ell!} \left(\sup_{t_1 \leq s \leq t} \|\Delta_{j+\ell}(s)\|_{\mathcal{L}^1} + \frac{3(j+\ell)^2}{16N} \right) \\ &\quad + \frac{1}{8^n} \frac{j(j+1)\cdots(j+n-1)}{n!} \\ &\leq 2^{j-1} \sum_{\ell=0}^n \frac{1}{4^\ell} \sup_{t_1 \leq s \leq t} \|\Delta_{j+\ell}(t_1)\|_{\mathcal{L}^1} + \frac{1}{4} 2^{j-1} \frac{(j+n)^2}{N} + \frac{1}{4^n} 2^{j-1}. \end{aligned}$$

Here we have used the obvious bound

$$\|\Delta_j^N(t)\|_{\mathcal{L}^1} \leq 2, \quad \text{for all } j \geq 1 \text{ and } t \geq 0,$$

together with the prescription

$$2 \frac{2\|\Phi\|_{L^\infty T}}{\hbar} = \frac{1}{8}$$

and the inequality

$$\frac{j(j+1)\cdots(j+\ell-1)}{\ell!} = \binom{j+\ell-1}{\ell} \leq 2^{j-1+\ell}.$$

At this point, we split the time interval $(0, t)$ into small intervals of length T_{\hbar} . Specifically, for $k = 1, \dots, [\frac{t}{T_{\hbar}}] + 1$, so that $t < kT_{\hbar}$, we set

$$A_j^k = \sup_{s \in ((k-1)T_{\hbar}, kT_{\hbar}]} \|\Delta_j(s)\|_{\mathcal{L}^1}.$$

Setting

$$(51) \quad \varphi(k, N) := 2^{-k} \log N,$$

we seek to prove that

$$(52) \quad A_j^k \leq 2^{j+k-\varphi(k, N)} \quad \text{for } j \leq \varphi(k, N),$$

which implies the thesis.

Setting $n = \varphi(k, N)$, the identity $\varphi(k, N) = \varphi(k-1, N) - \varphi(k, N)$ implies that $j + \ell \leq \varphi(k-1, N)$ for $j \leq \varphi(k, N)$, so that (50) becomes

$$(53) \quad A_j^k \leq 2^{j-1} \sum_{\ell=0}^n \frac{1}{4^\ell} A_{j+\ell}^{k-1} + \frac{1}{4} 2^{j-1} \frac{(j+n)^2}{N} + \frac{1}{4^n} 2^{j-1}.$$

We prove (52) by induction: for $k = 1$, the inequality (52) is obvious by (43).

Assuming now that the inequality (52) holds for $k-1$, we get

$$2^{j-1} \sum_{\ell=0}^n \frac{1}{4^\ell} A_{j+\ell}^{k-1} \leq 2 \cdot 2^{j-1} \cdot 2^{k-1-(\varphi(k-1, N)-\varphi(k, N))} \leq \frac{1}{2} \cdot 2^{j+k-\varphi(k, N)}.$$

Moreover

$$\frac{1}{4} \cdot 2^{j-1} \frac{(j+n)^2}{N} + \frac{1}{4^n} \cdot 2^{j-1} \leq \frac{1}{2} \cdot 2^{j+k-\varphi(k, N)}$$

for $n = \varphi(k, N)$ and $N > N_0$ with $N_0 = N_0(j)$ chosen so that (52) holds true.

This concludes the proof of Theorem 7.1. \square

8. PROOF OF THEOREM 3.1

We begin with the following elementary observation.

Lemma 8.1. *For each trace-class operator ρ , one has*

$$\|\widetilde{W}_\rho\|_{L^1} \leq \|\rho\|_{\mathcal{L}^1}.$$

Proof. For $z = (q, p)$, one has

$$\widetilde{W}_\rho(z) = (2\pi\hbar)^{-d} \langle z | \rho | z \rangle = (2\pi\hbar)^{-d} \text{trace}(\rho |z\rangle \langle z|)$$

so that

$$(2\pi\hbar)^d |\widetilde{W}_\rho(z)| \leq \text{trace} |\rho |z\rangle \langle z| = \text{trace} |\rho| |z\rangle \langle z|$$

because $|z\rangle \langle z| \geq 0$. Therefore

$$\|\widetilde{W}_\rho\|_{L^1} \leq \text{trace} \left(|\rho| (2\pi\hbar)^{-d} \int |z\rangle \langle z| dz \right) = \|\rho\|_{\mathcal{L}^1}$$

since

$$(2\pi\hbar)^{-d} \int |z\rangle \langle z| dz = I.$$

□

Therefore, applying Theorem 7.1 implies that, for all $T > 0$ and for $|t| < T$,

$$\|\widetilde{W}_{F_j^N(t)} - \widetilde{W}_{F(t) \otimes j}\|_{L^1} \leq \frac{2^{j + \frac{16t\|\Phi\|_{L^\infty}}{\hbar}}}{N \left(2^{-\frac{16t\|\Phi\|_{L^\infty}}{\hbar} \log 2} \right)}.$$

Assume that F^{in} is a Töplitz operator in the sense of [9]. Then one knows from [9] that

$$\text{dist}_{\text{MK},2}(\widetilde{W}_{F_j^N(t)} - \widetilde{W}_{F(t) \otimes j})^2 \leq j \left(2d\hbar + \frac{C}{N} \right) e^{\Lambda t} + 2d\hbar,$$

where

$$\Lambda := 3 + 4 \text{Lip}(\nabla V)^2 \quad \text{and} \quad C := 8j \|\nabla \Phi\|_{L^\infty} / \Lambda$$

while $\text{dist}_{\text{MK},2}$ is the Wasserstein distance of exponent 2. We recall that, for each pair of Borel probability measures on \mathbf{R}^d with finite second order moments,

$$(54) \quad \text{dist}_{\text{MK},2}(\mu, \nu) := \inf_{\pi \in \Pi(\mu, \nu)} \sqrt{\iint_{((\mathbf{R}^d \times \mathbf{R}^d)^j)^2} |z - z'|^2 \pi(dz dz')},$$

where $\Pi(\mu, \nu)$ is the set of couplings of μ and ν defined before (10) — see chapter 7 in [22].

Then, we deduce from Theorem 7.1 that

- for $\varphi([\frac{t}{T\hbar}], N) < j$ or $N < N_0(j)$

$$\begin{aligned}
& \inf \left(\|\widetilde{W}_{F_j^N(t)} - \widetilde{W}_{F(t)\otimes j}\|_{L^1}^2, \text{dist}_{\text{MK},2}(\widetilde{W}_{F_j^N(t)} - \widetilde{W}_{F(t)\otimes j})^2 \right) \\
& \leq \inf \left(2, j \left(2d\hbar + \frac{C}{N} \right) e^{\Lambda t} + 2d\hbar \right) \\
& \leq j \left(2d\hbar + \frac{C}{N} \right) e^{\Lambda t} + 2d\hbar \Big|_{\varphi([\frac{t}{T\hbar}], N) < j} \\
& \leq j \left(2d\hbar + \frac{C}{N} \right) e^{\Lambda t} + 2d\hbar \Big|_{\hbar \leq \frac{16\|\Phi\|_{L^\infty}}{\log \log N - \log j}} \\
& \leq \frac{32dT\|\Phi\|_{L^\infty}(1 + je^{\Lambda T})}{\log \log N - \log j} + \frac{C}{N} e^{\Lambda T}.
\end{aligned}$$

If $N \rightarrow \infty$ (in which case obviously $N \geq N_0(j)$), one has

$$\frac{32dT\|\Phi\|_{L^\infty}(1 + je^{\Lambda T})}{\log \log N - \log j} + \frac{C}{N} e^{\Lambda T} \sim \frac{32dT\|\Phi\|_{L^\infty}(1 + je^{\Lambda T})}{\log \log N}.$$

- for $j \leq \varphi([\frac{t}{T\hbar}], N)$ and $N \geq N_0(j)$

$$\begin{aligned}
& \inf \left(\|\widetilde{W}_{F_j^N(t)} - \widetilde{W}_{F(t)\otimes j}\|_{L^1}^2, \text{dist}_{\text{MK},2}(\widetilde{W}_{F_j^N(t)} - \widetilde{W}_{F(t)\otimes j})^2 \right) \\
& \leq \inf \left(\frac{2^{2j + \frac{32t\|\Phi\|_{L^\infty}}{\hbar}}}{N \left(2^{-\frac{32t\|\Phi\|_{L^\infty}}{\hbar} \log 2} \right)}, j \left(2d\hbar + \frac{C}{N} \right) e^{\Lambda t} + 2d\hbar \right) \\
& \leq \inf \left(\frac{2^{2j + \frac{32t\|\Phi\|_{L^\infty}}{\hbar}}}{N \left(2^{-\frac{32t\|\Phi\|_{L^\infty}}{\hbar} \log 2} \right)}, 2d\hbar(1 + je^{\Lambda t}) \right) + \frac{jC}{N} e^{\Lambda t} \\
& \leq 2d\hbar(1 + je^{\Lambda t}) \Big|_{\frac{2^{2j + \frac{32t\|\Phi\|_{L^\infty}}{\hbar}}}{N \left(2^{-\frac{32t\|\Phi\|_{L^\infty}}{\hbar} \log 2} \right)} = 2d\hbar(1 + je^{\Lambda t})} + \frac{jC}{N} e^{\Lambda t},
\end{aligned}$$

the two arguments of the *inf* being respectively decreasing and increasing functions of \hbar .

Observe that

$$\begin{aligned}
\frac{2^{2j + \frac{32t\|\Phi\|_{L^\infty}}{\hbar}}}{N \left(2^{-\frac{32t\|\Phi\|_{L^\infty}}{\hbar} \log 2} \right)} = 2d\hbar(1 + je^{\Lambda t}) & \Leftrightarrow \frac{2^{2j + \frac{32t\|\Phi\|_{L^\infty}}{\hbar}}}{2d\hbar(1 + je^{\Lambda t})} = N \left(2^{-\frac{32t\|\Phi\|_{L^\infty}}{\hbar} \log 2} \right) \\
& \Leftrightarrow \left(\frac{2^{2j + \frac{32t\|\Phi\|_{L^\infty}}{\hbar}}}{2d\hbar(1 + je^{\Lambda t})} \right)^{2^{\frac{32t\|\Phi\|_{L^\infty}}{\hbar} / \log 2}} = N
\end{aligned}$$

is an equation for \hbar in terms of N with only one solution $\hbar(N)$, since the left hand side of the last equality is a continuous function of \hbar decreasing from $+\infty$ to 0.

We find that

$$\log N = \frac{2^{\frac{32t\|\Phi\|_{L^\infty}}{\hbar(N)}}}{\log 2} \left(\left(2j + \frac{32t\|\Phi\|_{L^\infty}}{\hbar(N)} \right) \log 2 - \log(2d\hbar(N)(1 + je^{\Lambda t})) \right)$$

and therefore

$$\begin{aligned} \log \log N &= \frac{32t\|\Phi\|_{L^\infty}}{\hbar(N)} \log 2 - \log \log 2 \\ &\quad + \log \left(\left(2j + \frac{32t\|\Phi\|_{L^\infty}}{\hbar(N)} \right) \log 2 - \log (2d\hbar(N)(1 + je^{\Lambda t})) \right), \end{aligned}$$

so that, as $N \rightarrow \infty$ with j kept fixed,

$$\hbar(N) \sim \frac{32T\|\Phi\|_{L^\infty} \log 2}{\log \log N}.$$

Finally

$$\begin{aligned} &\inf \left(\|\widetilde{W}_{F_j^N(t)} - \widetilde{W}_{F(t) \otimes j}\|_{L^1}^2, \text{dist}_{\text{MK},2}(\widetilde{W}_{F_j^N(t)} - \widetilde{W}_{F(t) \otimes j})^2 \right) \\ &\leq 2d\hbar(N)(1 + je^{\Lambda T}) + j \frac{C}{N} e^{\Lambda T} \\ &\sim 64(\log 2) \frac{dT\|\Phi\|_{L^\infty}}{\log \log N} (1 + je^{\Lambda T}) \quad \text{as } N \rightarrow \infty \text{ with } \frac{\log j}{\log \log N} = o(1). \end{aligned}$$

Theorem 3.1 is then proven by our last result:

Lemma 8.2. *Let μ and ν be two Borel probability measures absolutely continuous with respect to the Lebesgue measure. Then*

$$\text{dist}_1(\mu, \nu) \leq \inf (\|\mu - \nu\|_{L^1}, \text{dist}_{\text{MK},2}(\mu, \nu)).$$

Proof. Let $D_1(z, z') = \min(|z - z'|, 1)$. Obviously $D_1(z, z')^2 \leq |z - z'|^2$ so that, for each Borel probability measure π ,

$$\begin{aligned} \left(\iint \pi(dz, dz') D_1(z, z') \right)^2 &\leq \iint \pi(dz, dz') \iint \pi(dz, dz') |z - z'|^2 \\ &= \iint \pi(dz, dz') |z - z'|^2. \end{aligned}$$

In particular

$$\text{dist}_1(\mu, \nu) \leq \text{dist}_{\text{MK},2}(\mu, \nu).$$

Consider now the particular coupling π defined as follows:

$$\pi(\mu, \nu) := \begin{cases} \mu(z)\delta(z - z') & \text{if } \mu = \nu, \\ \lambda(z)\delta(z - z') + \frac{(\mu(z) - \lambda(z))(\nu(z') - \lambda(z'))}{1 - \int \lambda(dz'')} & \text{if } \mu \neq \nu, \end{cases}$$

where $\lambda = \min(\mu, \nu)$. Then

$$\text{dist}_1(\mu, \nu) \leq \int \pi(dz, dz') \min(|z - z'|, 1) \leq 1 - \int \lambda(dz) \leq \|\mu - \nu\|_{L^1}$$

and this completes the proof. \square

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(F.G.) CMLS, ECOLE POLYTECHNIQUE, CNRS, UNIVERSITÉ PARIS-SACLAY, 91128 PALAISEAU
CEDEX, FRANCE

E-mail address: `francois.golse@polytechnique.edu`

(T.P.) CMLS, ECOLE POLYTECHNIQUE, CNRS, UNIVERSITÉ PARIS-SACLAY, 91128 PALAISEAU
CEDEX, FRANCE

E-mail address: `thierry.paul@polytechnique.edu`

(M.P.) SAPIENZA UNIVERSITÀ DI ROMA, DIPARTIMENTO DI MATEMATICA, PIAZZALE ALDO MORO
5, 00185 ROMA

E-mail address: `pulvirenti@mat.uniroma1.it`