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ON THE MEAN-FIELD AND CLASSICAL LIMITS OF QUANTUM MECHANICS

FRANÇOIS GOLSE, CLÉMENT MOUHOT, AND THIERRY PAUL

ABSTRACT. The main result in this paper is a new inequality bearing on solutions of the N -body linear Schrödinger equation and of the mean field Hartree equations. This inequality implies that the mean field limit of the quantum mechanics of N identical particles is uniform in the classical limit and provides a quantitative estimate of the quality of the approximation. This result applies to the case of $C^{1,1}$ interaction potentials. The quantity measuring the approximation of the N -body quantum dynamics by its mean field limit is analogous to the Monge-Kantorovich (or Wasserstein) distance with exponent 2. The inequality satisfied by this quantity is reminiscent of the work of Dobrushin on the mean field limit in classical mechanics [Func. Anal. Appl. **13** (1979), 115–123]. Our approach of this problem is based on a direct analysis of the N -particle Liouville equation, and avoids using techniques based on the BBGKY hierarchy or on second quantization.

1. STATEMENT OF THE PROBLEM

In nonrelativistic quantum mechanics, the dynamics of N identical particles of mass m in \mathbf{R}^d is described by the linear Schrödinger equation

$$i\hbar\partial_t\Psi = -\frac{\hbar^2}{2m}\sum_{k=1}^N\Delta_{x_k}\Psi + \sum_{k,l=1}^NV(x_k-x_l)\Psi,$$

where the unknown is $\Psi \equiv \Psi(t, x_1, \dots, x_N) \in \mathbf{C}$, the N -particle wave function, while x_1, x_2, \dots, x_N designate the positions of the 1st, 2nd, \dots , N th particle. The interaction between the k th and l th particles is given by the potential V , a real-valued measurable function defined a.e. on \mathbf{R}^d , such that

$$(1) \quad V(z) = V(-z), \quad \text{for a.e. } z \in \mathbf{R}^d.$$

Denoting the macroscopic length scale by $L > 0$, we define a time scale $T > 0$ such that the total interaction energy of the typical particle with the $N-1$ other particles is of the order of $m(L/T)^2$. With the dimensionless space and time variables defined as

$$\hat{x} := x/L, \quad \hat{t} := t/T,$$

the interaction potential is scaled as

$$\hat{V}(\hat{z}) := \frac{NT^2}{mL^2}V(z).$$

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In terms of the dimensionless parameter

$$\epsilon := \hbar T / m L^2$$

and the new unknown

$$\hat{\Psi}(t, \hat{x}_1, \dots, \hat{x}_N) := \Psi(t, x_1, \dots, x_N),$$

the Schrödinger equation becomes

$$i\partial_t \hat{\Psi} = -\frac{1}{2}\epsilon \sum_{k=1}^N \Delta_{\hat{x}_k} \hat{\Psi} + \frac{1}{N\epsilon} \sum_{k,l=1}^N \hat{V}(\hat{x}_k - \hat{x}_l) \hat{\Psi}.$$

In the present paper, we obtain a new estimate for solutions of this Schrödinger equation which is of particular interest in the asymptotic regime where

$$\epsilon \ll 1 \text{ (classical limit)} \quad \text{and} \quad N \gg 1 \text{ (mean field limit)}.$$

Henceforth we drop all hats on rescaled quantities in the Schrödinger equation and consider the Cauchy problem

$$(2) \quad \begin{cases} i\partial_t \Psi = -\frac{1}{2}\epsilon \sum_{k=1}^N \Delta_{x_k} \Psi + \frac{1}{N\epsilon} \sum_{k,l=1}^N V(x_k - x_l) \Psi, \\ \Psi|_{t=0} = \Psi^{in}. \end{cases}$$

While the discussion above applies to all types of particles, from now on we restrict our attention to the case of bosons, i.e. to the case where the wave function Ψ is a symmetric function of the space variables x_1, \dots, x_N .

1.1. The mean field limit. The mean field limit is the asymptotic regime where $N \rightarrow \infty$, with $\epsilon > 0$ fixed. Set the initial data in (2) to be

$$\Psi_N^{in}(x_1, \dots, x_N) := \prod_{k=1}^N \psi^{in}(x_k) \quad \text{with} \quad \int_{\mathbf{R}^d} |\psi^{in}(x)|^2 dx = 1,$$

and let Ψ_N be the solution of the Cauchy problem (2) — which exists for all times provided that V is such that

$$-\frac{1}{2}\epsilon \sum_{k=1}^N \Delta_{x_k} + \frac{1}{N\epsilon} \sum_{k,l=1}^N V(x_k - x_l)$$

has a self-adjoint extension as an unbounded operator on $L^2((\mathbf{R}^d)^N)$. Under various assumptions on ψ^{in} and V , it is known that

$$\int_{(\mathbf{R}^d)^{N-1}} \Psi_N(t, x, z_2, \dots, z_N) \overline{\Psi_N(t, y, z_2, \dots, z_N)} dz_2 \dots dz_N \rightarrow \psi(t, x) \overline{\psi(t, y)}$$

in some appropriate sense as $N \rightarrow \infty$, where ψ is the solution of the Hartree equation

$$(3) \quad \begin{cases} i\partial_t \psi = -\frac{1}{2}\epsilon \Delta_x \psi + \frac{1}{\epsilon} \psi(t, x) \int_{\mathbf{R}^d} V(x - z) |\psi(t, z)|^2 dz, \\ \psi|_{t=0} = \psi^{in}. \end{cases}$$

See [26, 4, 7, 1, 8, 9, 11, 25, 22, 23, 16] for various results in this direction, obtained under different assumptions on the regularity of the interaction potential V . Most of the physically relevant particle interactions, especially the case where V is the

Coulomb potential, are covered by these results, but not always with a quantitative error estimate.

1.2. The classical limit. The classical limit is the asymptotic regime where $\epsilon \rightarrow 0$ while N is kept fixed in (2) — or simply $\epsilon \rightarrow 0$ in (3). The formalism of the *Wigner transform* is perhaps the most convenient way to formulate this limit. Given $\Phi \equiv \Phi(X) \in \mathbf{C}$, an element of $L^2(\mathbf{R}^n)$, its Wigner transform at scale ϵ is

$$W_\epsilon[\Phi](X, \Xi) := \frac{1}{(2\pi)^n} \int_{\mathbf{R}^n} \Phi\left(X + \frac{1}{2}\epsilon Y\right) \overline{\Phi\left(X - \frac{1}{2}\epsilon Y\right)} e^{-i\Xi \cdot Y} dY.$$

Assume that the initial data in (2) is a family Ψ_ϵ^{in} such that

$$W_\epsilon[\Psi_\epsilon^{in}] \rightarrow F^{in} \quad \text{in } \mathcal{S}'((\mathbf{R}^d \times \mathbf{R}^d)^N) \text{ as } \epsilon \rightarrow 0.$$

Then, for all $t \in \mathbf{R}$, the family of solutions Ψ_ϵ of the Cauchy problem (2) satisfies

$$W_\epsilon[\Psi_\epsilon(t, \cdot)] \rightarrow F(t, \cdot, \cdot) \quad \text{in } \mathcal{S}'((\mathbf{R}^d \times \mathbf{R}^d)^N) \text{ as } \epsilon \rightarrow 0,$$

where $F \equiv F(t, x_1, \dots, x_N, \xi_1, \dots, \xi_N) \geq 0$ is the solution of the following Cauchy problem for the N -body Liouville equation of classical mechanics

$$(4) \quad \begin{cases} \partial_t F + \sum_{k=1}^N \xi_k \cdot \nabla_{x_k} F - \frac{1}{N} \sum_{k,l=1}^N \nabla V(x_k - x_l) \cdot \nabla_{\xi_k} F = 0, \\ F|_{t=0} = F^{in}. \end{cases}$$

The classical limit of the Hartree equation (3) can be formulated similarly. Assume that the initial data in (3) is a family ψ_ϵ^{in} such that

$$W_\epsilon[\psi_\epsilon^{in}] \rightarrow f^{in} \quad \text{in } \mathcal{S}'(\mathbf{R}^d \times \mathbf{R}^d) \text{ as } \epsilon \rightarrow 0.$$

Then, for all $t \in \mathbf{R}$, the family of solutions ψ_ϵ of the Hartree equation (3) satisfies

$$W_\epsilon[\psi_\epsilon(t, \cdot)] \rightarrow f(t, \cdot, \cdot) \quad \text{in } \mathcal{S}'(\mathbf{R}^d \times \mathbf{R}^d) \text{ as } \epsilon \rightarrow 0,$$

where $f \equiv f(t, x, \xi) \geq 0$ is the solution of the following Cauchy problem for the Vlasov equation of classical mechanics with interaction potential V :

$$(5) \quad \begin{cases} \partial_t f + \xi \cdot \nabla_x f - \left(\int_{\mathbf{R}^d} \nabla V(x - z) f(t, z) dz \right) \cdot \nabla_\xi f = 0, \\ f|_{t=0} = f^{in}. \end{cases}$$

See [17, 12] for results on the classical limit of quantum mechanics involving the Wigner transform.

1.3. The mean field limit in classical mechanics. There is also a notion of mean field limit in classical mechanics, which can be formulated as follows. Assume that the initial data in (4) is

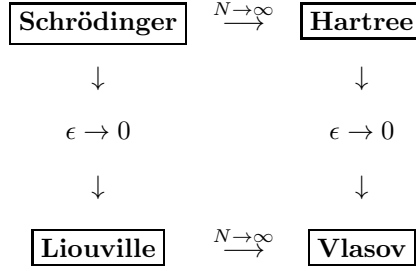
$$F_N^{in}(x_1, \dots, x_N, \xi_1, \dots, \xi_N) = \prod_{k=1}^N f^{in}(x_k, \xi_k),$$

where f^{in} is a probability density on $\mathbf{R}^d \times \mathbf{R}^d$. Under various assumptions on the potential V , the solution F_N of (4) satisfies

$$\int_{(\mathbf{R}^d \times \mathbf{R}^d)^{N-1}} F_N(t, x, x_2, \dots, x_N, \xi, \xi_2, \dots, \xi_N) dx_2 d\xi_2 \dots dx_N d\xi_N \rightarrow f(t, x, \xi)$$

in some appropriate sense as $N \rightarrow \infty$, where f is the solution of the Cauchy problem for the Vlasov equation (5). See [21, 5, 6] for the missing details. All these references address the problem of the mean field limit in terms of the empirical measure of the N -particle system. Typically these results cover the case where $V \in C^{1,1}(\mathbf{R})$, but the case of a Coulomb, or Newtonian interaction remains open at the time of this writing. For a formulation of the same results in terms of the BBGKY hierarchy, see [14, 19].

The situation described above can be summarized in the following diagram: the horizontal arrows correspond to the mean field limit, while the vertical arrows correspond to the classical limit.



However, these various limits are established by very different methods. The classical limits of either the N -body Schrödinger equation or of the Hartree equation are obtained by a compactness argument and the uniqueness of the solution of the Cauchy problems (4) or (5). Error estimates for these limits require rather stringent assumptions on the regularity of the potential V and on the type of initial wave or distribution functions considered. The mean field limit in quantum mechanics (the upper horizontal arrow) comes from trace norm estimates on the infinite hierarchy of equations obtained from the BBGKY hierarchy in the large N limit. The trace norm is the quantum analogue of the total variation norm on the probability measures appearing in the classical setting. In general, the total variation norm is not convenient in the context of the mean field limit, since it does not capture the distance between neighboring point particles. This suggests that the trace norm is not appropriate to obtain controls on the large N (mean field) limit which remain uniform in the vanishing ϵ (classical) limit.

Another notable difficulty with this problem is that the mean field limit in classical mechanics is obtained by proving the weak convergence of the N -particle empirical measure in the single-particle phase space to the solution of the Vlasov equation. Since there does not seem to be any natural analogue of the notion of empirical measure for a quantum N -particle system, the analogy between the quantum and the classical mean field limits is far from obvious.

Our main result, stated as Theorem 2.4 below, is a new quantitative estimate for the mean field limit $N \rightarrow \infty$ of quantum mechanics which is uniform in the classical limit $\epsilon \rightarrow 0$.

2. MAIN RESULT

Let d be a positive integer. Henceforth we set $\mathfrak{H} := L^2(\mathbf{R}^d)$, and $\mathfrak{H}_N := \mathfrak{H}^{\otimes N} \simeq L^2((\mathbf{R}^d)^N)$ for each $N \geq 1$. We designate by $\mathcal{L}(\mathfrak{H})$ the algebra of bounded linear

operators on the Hilbert space \mathfrak{H} . We also denote by $\mathcal{D}(\mathfrak{H}_N)$ the set of operators $A \in \mathcal{L}(\mathfrak{H}_N)$ such that

$$A = A^* \geq 0, \quad \text{and} \quad \text{trace}(A) = 1.$$

We are concerned with the N -body Schrödinger equation written in terms of density matrices, i.e. the von Neumann equation

$$(6) \quad \begin{cases} i\partial_t \rho_{\epsilon,N} = \left[-\frac{1}{2}\epsilon \sum_{k=1}^N \Delta_k + \frac{1}{N\epsilon} \sum_{k,l=1}^N V_{kl}, \rho_{\epsilon,N} \right], \\ \rho_{\epsilon,N}|_{t=0} = (\rho_\epsilon^{in})^{\otimes N}. \end{cases}$$

where $\rho_{\epsilon,N}(t) \in \mathcal{D}(\mathfrak{H})$, while

$$\Delta_j := I_{\mathfrak{H}}^{\otimes(j-1)} \otimes \Delta \otimes I_{\mathfrak{H}}^{\otimes(N-j)},$$

and

$$(7) \quad (V_{jk}\psi)(x_1, \dots, x_N) := V(x_k - x_j)\psi(x_1, \dots, x_N), \quad \text{for each } \psi \in \mathfrak{H}_N.$$

We designate by $I_{\mathfrak{H}}$ the identity on the Hilbert space \mathfrak{H} .

On the other hand, we consider the corresponding mean field equation, i.e. the Hartree equation written in terms of the density matrix $\rho_\epsilon(t) \in \mathcal{D}(\mathfrak{H})$

$$(8) \quad \begin{cases} i\partial_t \rho_\epsilon = \left[-\frac{1}{2}\epsilon \Delta + \frac{1}{\epsilon} V_{\rho_\epsilon}, \rho_\epsilon \right], \\ \rho_\epsilon|_{t=0} = \rho_\epsilon^{in}, \end{cases}$$

where V_{ρ_ϵ} designates both the function

$$V_{\rho_\epsilon}(t, x) := \int_{\mathbf{R}^d} V(x - z) \rho_\epsilon(t, z, z) dz$$

and the time-dependent multiplication operator defined on \mathfrak{H} by

$$(V_{\rho_\epsilon} \psi)(t, x) := V_{\rho_\epsilon}(t, x) \psi(x).$$

Next we formulate the mean field limit in terms of density operators. For each N -particle density operator $\rho_N \in \mathcal{D}(\mathfrak{H}_N)$, we define its first n -particle marginal density operator, denoted by ρ_N^n for each integer n such that $1 \leq n \leq N$, by the following conditions:

$$\begin{cases} \rho_N^n \in \mathcal{D}(\mathfrak{H}_n), \quad \text{and} \\ \text{trace}_{\mathfrak{H}_n}(A \rho_N^n) = \text{trace}_{\mathfrak{H}_N}((A \otimes I_{\mathfrak{H}_{N-n}}) \rho_N) \quad \text{for each } A \in \mathcal{L}(\mathfrak{H}_n). \end{cases}$$

In the mean field limit, i.e. for $N \rightarrow \infty$ while $\epsilon > 0$ is kept fixed, one expects that the sequence $\rho_{\epsilon,N}^1$ of first marginals of the density operators $\rho_{\epsilon,N}$ solutions of (6) converges in some sense to the solution ρ_ϵ of (8). The difference between $\rho_{\epsilon,N}^1$ and ρ_ϵ is measured in terms of a quantity analogous to the Monge-Kantorovich distance used in the context of optimal transport.

First we define the notion of coupling between two density operators.

Definition 2.1. Let d be a positive integer and let $\mathfrak{H} := L^2(\mathbf{R}^d)$. For each $\rho, \bar{\rho} \in \mathcal{D}(\mathfrak{H})$, let $\mathcal{Q}(\rho, \bar{\rho})$ be the set of $R \in \mathcal{D}(\mathfrak{H}_2)$ such that

$$\begin{cases} \text{trace}_{\mathfrak{H}_2}((A \otimes I_{\mathfrak{H}}) R) = \text{trace}_{\mathfrak{H}}(A \rho) \\ \text{trace}_{\mathfrak{H}_2}((I_{\mathfrak{H}} \otimes A) R) = \text{trace}_{\mathfrak{H}}(A \bar{\rho}) \end{cases}$$

for each $A \in \mathcal{L}(\mathfrak{H})$.

Next we define two unbounded operators on $\mathfrak{H}_2 \simeq L^2(\mathbf{R}^d \times \mathbf{R}^d)$, as follows:

$$(9) \quad \begin{cases} (Q\psi)(x_1, x_2) := (x_1 - x_2)\psi(x_1, x_2), \\ (P\psi)(x_1, x_2) := -i\epsilon(\nabla_{x_1} - \nabla_{x_2})\psi(x_1 - x_2), \end{cases}$$

so that

$$(10) \quad (P^*P\psi)(x_1 - x_2) = -\epsilon^2(\operatorname{div}_{x_1} - \operatorname{div}_{x_2})(\nabla_{x_1} - \nabla_{x_2})\psi(x_1, x_2).$$

The quantum analogue of the Monge-Kantorovich distance with exponent 2 is defined as follows. For the definition of Monge-Kantorovich distances, also called Wasserstein distances, see formula (15) in section 3, or chapter 7 in [28], or chapter 6 in [29].

Definition 2.2. For each $\rho, \bar{\rho} \in \mathcal{D}(\mathfrak{H})$, we set

$$MK_2^\epsilon(\rho, \bar{\rho}) := \inf_{R \in \mathcal{Q}(\rho, \bar{\rho})} \operatorname{trace}_{\mathfrak{H}_2}((Q^*Q + P^*P)R)^{1/2}$$

with the following convention:

$$\operatorname{trace}_{\mathfrak{H}_2}((Q^*Q + P^*P)R) := \operatorname{trace}_{\mathfrak{H}_2}(R^{1/2}(Q^*Q + P^*P)R^{1/2})$$

if $R^{1/2}(Q^*Q + P^*P)R^{1/2}$ is a trace-class operator, and

$$\operatorname{trace}_{\mathfrak{H}_2}((Q^*Q + P^*P)R) := +\infty$$

otherwise.

The quantity MK_2^ϵ is not a distance on $\mathcal{D}(\mathfrak{H})$. In fact, for each density operator ρ on \mathfrak{H} , one has $MK_2^\epsilon(\rho, \rho) > 0$ (see formula (11) below). However, MK_2^ϵ can be compared with the Monge-Kantorovich distance with exponent 2 (see formula (15) below) as $\epsilon \rightarrow 0$, at least for a certain class of operators.

Henceforth, we denote by $\mathcal{P}(\mathbf{R}^d)$ the set of Borel probability measures on \mathbf{R}^d . For each $q > 0$, we define

$$\mathcal{P}_q(\mathbf{R}^d) := \left\{ \mu \in \mathcal{P}(\mathbf{R}^d) \text{ s.t. } \int_{\mathbf{R}^d} |x|^q \mu(dx) < \infty \right\}.$$

Theorem 2.3 (Properties of MK_2^ϵ). Let d be a positive integer and let $\mathfrak{H} := L^2(\mathbf{R}^d)$. For each $\rho, \bar{\rho} \in \mathcal{D}(\mathfrak{H})$ and each $\epsilon > 0$, one has

$$(11) \quad MK_2^\epsilon(\rho, \bar{\rho})^2 \geq 2d\epsilon.$$

(1) Let $\epsilon > 0$ and let ρ_1^ϵ and ρ_2^ϵ be Töplitz operators at scale ϵ on $L^2(\mathbf{R}^d)$ with symbols $(2\pi\epsilon)^d \mu_1$ and $(2\pi\epsilon)^d \mu_2$, where $\mu_1, \mu_2 \in \mathcal{P}_2(\mathbf{R}^{2d})$. Then

$$\begin{aligned} MK_2^\epsilon(\rho_1^\epsilon, \rho_2^\epsilon)^2 &\leq \inf_{\pi \in \Pi(\mu_1, \mu_2)} \operatorname{trace}_{\mathfrak{H} \otimes \mathfrak{H}}((Q^*Q + P^*P) \operatorname{OP}_\epsilon^T((2\pi\epsilon)^{2d} \pi)) \\ &= \operatorname{dist}_{\operatorname{MK}, 2}(\mu_1, \mu_2)^2 + 2d\epsilon. \end{aligned}$$

(2) Let ρ_1^ϵ and $\rho_2^\epsilon \in \mathcal{D}(\mathfrak{H})$, with Husimi transforms at scale ϵ denoted respectively $\tilde{W}_\epsilon[\rho_1^\epsilon]$ and $\tilde{W}_\epsilon[\rho_2^\epsilon]$. Then

$$MK_2^\epsilon(\rho_1^\epsilon, \rho_2^\epsilon)^2 \geq \operatorname{dist}_{\operatorname{MK}, 2}(\tilde{W}_\epsilon[\rho_1^\epsilon], \tilde{W}_\epsilon[\rho_2^\epsilon])^2 - 2d\epsilon.$$

Assume further that the Wigner transforms at scale ϵ of ρ_1^ϵ and ρ_2^ϵ , denoted respectively $W_\epsilon[\rho_1^\epsilon]$ and $W_\epsilon[\rho_2^\epsilon]$, converge in $\mathcal{S}'(\mathbf{R}^{2d})$ to Wigner measures denoted respectively w_1 and w_2 as $\epsilon \rightarrow 0$. Then

$$\text{dist}_{\text{MK},2}(w_1, w_2) \leq \lim_{\epsilon \rightarrow 0} MK_2^\epsilon(\rho_1^\epsilon, \rho_2^\epsilon).$$

The definitions and basic properties of Töplitz operators, Wigner and Husimi functions are recalled in the appendix.

Statement (2) in Theorem 2.3 implies in particular that the quantity MK_2^ϵ is not vanishing for all density matrices as $\epsilon \rightarrow 0^+$. This property is obviously essential; otherwise, the quantity MK_2^ϵ would not be of much practical interest for controlling the error in the mean field limit. Statement (1) in Theorem 2.3 will be used in choosing the initial quantum states to which our error estimate for the mean field limit will apply.

The main result in this paper is the following theorem.

Theorem 2.4. *Assume that the space dimension d satisfies $d \geq 3$. For each $\epsilon > 0$, let $\rho_\epsilon^{\text{in}}$ be a Töplitz operator at scale ϵ on \mathfrak{H} with symbol $(2\pi\epsilon)^d \mu^{\text{in}} \in \mathcal{P}_2(\mathbf{C}^d)$. Let $\rho_{\epsilon,N}$ be the solution of the quantum N -body Cauchy problem (6) with initial data $(\rho_\epsilon^{\text{in}})^{\otimes N}$, and let ρ_ϵ be the solution of the quantum mean field Cauchy problem (8). Then, for each integer n such that $1 \leq n \leq N$ and each $t \geq 0$, one has*

$$\begin{aligned} & MK_2^\epsilon(\rho_\epsilon(t)^{\otimes n}, \rho_{\epsilon,N}^{\mathbf{n}}(t))^2 \\ & \leq n \left(2d\epsilon + C_d C_{d,\epsilon}[\mu^{\text{in}}, V](t) \|\nabla V\|_{L^\infty} \text{Lip}(\nabla V) N^{-1/d} \right) \exp((3 + 4 \text{Lip}(\nabla V)^2) t), \end{aligned}$$

where C_d is a positive constant depending only on the space dimension d , while

$$C_{d,\epsilon}[\mu^{\text{in}}, V](t) := (1+t)e^t \left(\int_{\mathbf{C}^d} |z|^2 \mu^{\text{in}}(dz) + d\epsilon + 2\|V\|_{L^\infty} \right).$$

This estimate is not optimal, since, for $t = 0$ and $n = 1$, the right hand side of (12) is not equal to

$$2d\epsilon = MK_2^\epsilon(\rho_\epsilon^{\text{in}}, \rho_\epsilon^{\text{in}})^2 = MK_2^\epsilon(\rho_\epsilon(0), \rho_{\epsilon,N}^{\mathbf{1}}(0))^2.$$

Observe indeed that these equalities follow directly from Theorem 2.3 (1).

In addition, one cannot deduce the mean field limit of the quantum N -body problem (6) from the bound on $MK_2^\epsilon(\rho_\epsilon(t), \rho_{\epsilon,N}^{\mathbf{1}}(t))$ obtained in Theorem 2.4 in the case where $\epsilon > 0$ is kept fixed, because of the term $2d\epsilon \exp((3 + 4 \text{Lip}(\nabla V)^2)t)$ on the right hand side.

On the other hand, the mean field limit alone, i.e. for ϵ fixed, has been proved by other methods in this case (see [26, 4]). Moreover, quantitative estimates for that limit for ϵ fixed and $N \rightarrow \infty$ have been obtained in [25, 22, 2]. Therefore, only the case where both $N \rightarrow \infty$ and $\epsilon \rightarrow 0$ remains to be treated, and the present work answers precisely this question.

Indeed, the estimate in Theorem 2.4, together with the first lower bound in Theorem 2.3 (2), implies that the mean field limit, i.e. the convergence

$$\rho_{\epsilon,N}^{\mathbf{n}}(t) \rightarrow \rho_\epsilon(t)^{\otimes n}$$

for each $n \geq 1$ as $N \rightarrow \infty$ is uniform as $\epsilon \rightarrow 0$ and over long times intervals, in the following sense. Let c, c' satisfy $0 < c < c' < 1$, and set

$$T(c, \eta, N) := \frac{1}{4}c(1 + \text{Lip}(\nabla V)^2)^{-1} \min\left(\ln \frac{1}{\eta}, \frac{1}{d} \ln N\right),$$

$$n(c', \eta, N) := \left\lceil \min\left(\epsilon^{-(1-c')}, N^{\frac{1}{d}(1-c')}\right) \right\rceil,$$

(where $[x]$ designates the largest integer less than or equal to x). Then one has

$$\sup_{1 \leq n \leq n(c', \eta, N)} \sup_{0 \leq t \leq T(c, \eta, N)} \sup_{0 < \epsilon < \eta} \text{dist}_{\text{MK}, 2}(\tilde{W}_\epsilon[\rho_\epsilon(t)^{\otimes n}], \tilde{W}_\epsilon[\rho_{\epsilon, N}^n(t)]) \rightarrow 0$$

in the limit as $\frac{1}{N} + \eta \rightarrow 0$.

The case $d = 2$ involves a logarithmic correction in N in (12), and requires controlling some moment of the density of order higher than 2 (see the remarks following Theorem 1 in [10], and Lemma 5.1 below). We have left this question aside to avoid additional technicalities.

Earlier works have discussed the mean field limit of the quantum N -body problem in the small ϵ regime, more precisely, in the case where $\epsilon = \epsilon(N) \rightarrow 0$ as $N \rightarrow \infty$. The case $\epsilon(N) = N^{-1/3}$ has been investigated in [20, 27]. In [13], for each sequence $\epsilon \equiv \epsilon(N) \rightarrow 0$ as $N \rightarrow \infty$ and each monokinetic solution of the Vlasov equation (5) — i.e. a solution of the form $f(t, x, \xi) = \rho(t, x)\delta(\xi - u(t, x))$ — Theorem 1.1 gives an asymptotic approximation rate for the convergence of the Wigner transform at scale $\epsilon(N)$ of $\rho_{\epsilon, N}^1$ to f in the sense of distributions for $t \in [0, T]$. A priori, the time T and the convergence rate depend on the Vlasov solution f and on the sequence $\epsilon(N)$. On the diagram of section 1.3, this result corresponds to the left vertical and bottom horizontal arrow along distinguished sequences $(\epsilon(N), N)$ over time intervals which may depend on the dependence of ϵ in terms of N .

On the contrary, Theorem 2.4 provides a quantitative estimate of the distance between the solution of the Hartree equation and the first marginal of the solution of the quantum N -body problem, for a rather general class of initial data. This estimate implies that the mean field limit, i.e. the top horizontal arrow, is uniform as $\epsilon \rightarrow 0$, over arbitrary long time intervals. This estimate is the quantum analogue of the Dobrushin estimate [6] for the classical mean field limit — see section 3.

The new ideas used in the proof of Theorem 2.4 are

- (a) the use of the quantity MK_2^ϵ , which behaves well with the Töplitz quantization, and can be conveniently compared with the Monge-Kantorovich distance with exponent 2 on symbols, to which it is obviously analogous;
- (b) an “Eulerian” version of Dobrushin’s estimate, which avoids the traditional presentation in terms of particle trajectories as in Dobrushin’s original work [6], and can therefore be easily adapted to the quantum dynamics;
- (c) the adaptation of Dobrushin’s estimate to the N -particle Liouville equation, thereby avoiding the need of any quantum analogue of the classical notion of N -particle empirical measure;
- (d) and a new estimate by Fournier-Guillin [10], which improves previously known quantitative variants of the law of large numbers, such as [15] cited in [24].

The Eulerian version of Dobrushin’s inequality (item (b) on the list above) significantly simplifies the original argument, and allows extending Dobrushin’s inequality to Monge-Kantorovich distances with arbitrary finite exponents (see [18] for the original argument for the Monge-Kantorovich distance with exponent 2).

Estimating directly the Monge-Kantorovich distance between the first marginal of the N -particle distribution function and the solution of the mean field equation (item (c) on the list above) avoids using the fact that the N -particle empirical measure is an exact solution of the mean field equation, an important feature in Dobrushin's original approach [6]. This feature is very peculiar to the mean field limit in classical Hamiltonian mechanics, and we do not know of any quantum analogue of the notion of N -particle empirical measure which would exactly satisfy the mean field quantum dynamics. In other words, the mean field limit in quantum mechanics cannot be reduced to the continuous dependence of solutions of the quantum mean field equation in terms of their initial data, in some appropriate weak topology.

The outline of the paper is as follows: in the next section, we present items (b)-(c)-(d) above on the mean field limit for the classical Liouville equation, leading to the Vlasov equation. The resulting estimate in Theorem 3.1 below improves earlier quantitative bounds of the same type obtained in [14, 19]. The proof of the uniform in ϵ estimate in Theorem 2.4 for the quantum mean field limit occupies section 5. The properties of the quantity MK_2^ϵ used in this estimate, stated in Theorem 2.3, are proved in section 4. The material on Töplitz quantization, Wigner and Husimi functions used in the proof of Theorem 2.3 is recalled in the Appendix.

3. THE MEAN FIELD LIMIT IN CLASSICAL MECHANICS

As a warm-up, we first discuss the mean field limit for the N -body problem in classical mechanics, leading to the Vlasov equation. The approach proposed in [21, 5, 6] is based on the fact that the phase-space empirical measure of a N -particle system governed by the Newton equations of classical mechanics is a weak solution of the Vlasov equation (5). The estimate of the distance between the N -particle and the mean field dynamics obtained by Dobrushin [6] can be formulated in terms of propagation of chaos for the sequence of marginals of the N -particle distribution, as explained in [14, 19].

The approach proposed below bears directly on the N -particle distribution, i.e. the solution of the Liouville equation (4), and avoids any reference to the N -particle empirical measure. Besides, the core of our argument also avoids using particle trajectories and is based on a computation formulated exclusively in terms of Eulerian coordinates. For that reason, this approach can be adapted to the quantum problem, at variance with the Dobrushin procedure [6], also used in [14, 19].

For $\mu, \nu \in \mathcal{P}(\mathbf{R}^d)$, we denote by $\Pi(\mu, \nu)$ the set of couplings of μ et ν , i.e. the set of Borel probability measures π on $\mathbf{R}^d \times \mathbf{R}^d$ with first and second marginals

$$(13) \quad \pi_1 = \mu \quad \text{and} \quad \pi_2 = \nu.$$

In other words,

$$(14) \quad \iint_{\mathbf{R}^d \times \mathbf{R}^d} (\phi(x) + \psi(y)) \pi(dxdy) = \int_{\mathbf{R}^d} \phi(x) \mu(dx) + \int_{\mathbf{R}^d} \psi(y) \nu(dy)$$

for each $\phi, \psi \in C_b(\mathbf{R}^d)$. The identity (14) can be used as a definition of the first and second marginals of π in (13). Finally, we recall the definition of the Monge-Kantorovich distance of exponent $p \geq 1$ on $\mathcal{P}_p(\mathbf{R}^d)$:

$$(15) \quad \text{dist}_{\text{MK},p}(\mu, \nu) := \inf_{\pi \in \Pi(\mu, \nu)} \left(\iint_{\mathbf{R}^d \times \mathbf{R}^d} |x - y|^p \pi(dxdy) \right)^{1/p}.$$

Theorem 3.1. *Assume that $V \in C_b^2(\mathbf{R}^d)$ satisfies (1). Let p satisfy $1 \leq p \neq d/2$, and let $f^{in} \in \mathcal{P}_q(\mathbf{R}^d \times \mathbf{R}^d)$ with $q > 2p$. Let F_N be the solution of the Cauchy problem (4) for the N -body Liouville equation with initial data*

$$F_N^{in} := (f^{in})^{\otimes N},$$

and let f be the solution of the Cauchy problem for the Vlasov equation (5) with initial data f^{in} . For each integer n such that $1 \leq n \leq N$, let

$$F_N^n(t) = \int F_N(t, dy_{n+1} \dots dy_N d\eta_{n+1} \dots d\eta_N) \in \mathcal{P}_q(\mathbf{R}^{dn} \times \mathbf{R}^{dn})$$

be the n -th marginal of F_N (i.e. the marginal corresponding to the phase space distribution of the n first particles). Then

$$\begin{aligned} & \text{dist}_{\text{MK},p}(f(t)^{\otimes n}, F_N^n(t))^p \\ & \leq 2^{p-1} K_p C_{d,p,q} \text{Lip}(\nabla V)^p e^{2K_p(1+2^{p-1} \text{Lip}(\nabla V)^p)t} t m_q(t)^{p/q} n N^{-\min(1/2, p/d)}, \end{aligned}$$

where $K_p := \min(1, p-1)$ and $C_{d,p,q}$ is some positive constant depending only on d, p, q , while

$$m_q(t) = \sup_{0 \leq s \leq t} \iint_{\mathbf{R}^d \times \mathbf{R}^d} |x|^q f(s, dx d\xi).$$

The proof of Theorem 3.1 occupies the remaining part of the present section.

3.1. On the growth of moments of the solution of the Vlasov equation.

Let f be a solution of (5). We designate by $\rho[f]$ the macroscopic density associated to f , i.e.

$$\rho[f](t) := \int_{\mathbf{R}^d} f(t, d\xi).$$

The notation $V \star_x \rho[f]$ designates the function

$$V \star_x \rho[f](t, x) := \int_{\mathbf{R}^d} V(x-z) \rho[f](t, dz) = \iint_{\mathbf{R}^d \times \mathbf{R}^d} V(x-z) f(t, dz d\xi).$$

We recall that, if f is a solution of (5) such that $f|_{t=0}$ is a probability density on $\mathbf{R}^d \times \mathbf{R}^d$ (with respect to the Lebesgue measure), then $f(t)$ is also a probability density on $\mathbf{R}^d \times \mathbf{R}^d$. In addition, the proof of Theorem 3.1 requires some information on the moments of solutions (5) recalled in the next lemma. For each $q \geq 2$, we set

$$M_q(t) := \iint (|x|^q + |\xi|^q) f(t, dx d\xi).$$

Lemma 3.2. *For each $t \geq 0$ and each $q \geq 2$, the solution f of (5) satisfies*

$$M_q(t) \leq M_q(0) e^{(q-1)(1+2 \text{Lip}(\nabla V))t}.$$

In particular

$$f(0) \in \mathcal{P}_q(\mathbf{R}^d \times \mathbf{R}^d) \Rightarrow f(t) \in \mathcal{P}_q(\mathbf{R}^d \times \mathbf{R}^d)$$

for each $t \geq 0$.

Proof. We deduce from the Vlasov equation that

$$\begin{aligned} \frac{dM_q}{dt} &= \iint (q\xi \cdot x |x|^{q-2} - q \nabla V_{\rho[f]}(x) \cdot \xi |\xi|^{q-2}) f(t, dx d\xi) \\ &\leq (q-1) M_q(t) - q \iint \nabla V_{\rho[f]}(x) \cdot \xi |\xi|^{q-2} f(t, dx d\xi) \end{aligned}$$

since

$$q|x||\xi|^{q-1} \leq |x|^q + (q-1)|\xi|^q$$

by Young's inequality. Then

$$\begin{aligned} & q \left| \iint \nabla V_{\rho[f]}(x) \cdot \xi |\xi|^{q-2} f(t, dx d\xi) \right| \\ &= q \left| \iiint \nabla V(x-y) \cdot \xi |\xi|^{q-2} f(t, dy d\eta) f(t, dx d\xi) \right| \\ &\leq q \operatorname{Lip}(\nabla V) \iiint |x-y| |\xi|^{q-1} f(t, dy d\eta) f(t, dx d\xi) \\ &\leq q \operatorname{Lip}(\nabla V) \iint |x| |\xi|^{q-1} f(t, dx d\xi) \\ &\quad + q \operatorname{Lip}(\nabla V) \iint \int |y| |\xi|^{q-1} f(t, dy d\eta) f(t, dx d\xi) \\ &\leq (q-1) \operatorname{Lip}(\nabla V) m_q(t) \\ &\quad + (q-1) \operatorname{Lip}(\nabla V) \iint \int (|y|^q + |\xi|^q) f(t, dy d\eta) f(t, dx d\xi) \\ &= 2(q-1) \operatorname{Lip}(\nabla V) M_q(t). \end{aligned}$$

In the first inequality, we have used the fact that

$$|\nabla V(x-y)| \leq \operatorname{Lip}(\nabla V) |x-y|$$

since $\nabla V(0) = 0$ by (1). Eventually, we arrive at the inequality

$$\frac{dM_q}{dt} \leq (q-1)(1 + 2 \operatorname{Lip}(\nabla V)) M_q$$

from which the announced conclusion immediately follows. \square

3.2. The dynamics of couplings. Let $\pi_N^{in} \in \Pi((f^{in})^{\otimes N}, (f^{in})^{\otimes N})$ satisfy

$$(16) \quad T_\sigma \# \pi_N^{in} = \pi_N^{in}, \quad \text{for each } \sigma \in \mathfrak{S}_N,$$

where

$$\begin{aligned} & T_\sigma(x_1, \xi_1, \dots, x_N, \xi_N, y_1, \eta_1, \dots, y_N, \eta_N) \\ &= (x_{\sigma(1)}, \xi_{\sigma(1)}, \dots, x_{\sigma(N)}, \xi_{\sigma(N)}, y_{\sigma(1)}, \eta_{\sigma(1)}, \dots, y_{\sigma(N)}, \eta_{\sigma(N)}). \end{aligned}$$

It will be convenient to use the following notation

$$(17) \quad \begin{aligned} X_N &:= (x_1, \dots, x_N), \quad \Xi_N := (\xi_1, \dots, \xi_N), \\ Y_N &:= (y_1, \dots, y_N), \quad H_N := (\eta_1, \dots, \eta_N), \end{aligned}$$

Let f be the solution of the Cauchy problem (5) with initial data f^{in} , and let

$$\mathbf{H}_N^{\rho[f]}(X_N, \Xi_N) := \sum_{j=1}^N \left(\frac{1}{2} |\xi_j|^2 + V_{\rho[f]}(x_j) \right)$$

be the mean field Hamiltonian. On the other hand, let

$$\mathcal{H}_N(Y_N, H_N) := \sum_{k=1}^N \frac{1}{2} |\eta_k|^2 + \frac{1}{N} \sum_{k,l=1}^N V(y_k - y_l)$$

be the microscopic (N -particle) Hamiltonian. Finally, we denote by $\{\cdot, \cdot\}_N$ the Poisson bracket on $(\mathbf{R}^d \times \mathbf{R}^d)^N$ defined by

$$\{\phi, \psi\}_N := \sum_{j=1}^N (\nabla_{\xi_j} \phi \cdot \nabla_{x_j} \psi - \nabla_{\xi_j} \psi \cdot \nabla_{x_j} \phi).$$

The following observation is the key to the Eulerian formulation of the Dobrushin type estimates, which we shall adapt to the quantum case.

Lemma 3.3. *Let $t \mapsto \pi_N(t) \in \mathcal{P}_2((\mathbf{R}^d \times \mathbf{R}^d)^N \times (\mathbf{R}^d \times \mathbf{R}^d)^N)$ be the solution of the Cauchy problem*

$$\begin{cases} \partial_t \pi_N + \{\mathbf{H}_N^{\rho[f(t)]}(X_N, \Xi_N) + \mathcal{H}_N(Y_N, H_N), \pi_N\}_{2N} = 0, \\ \pi_N|_{t=0} = \pi_N^{in}. \end{cases}$$

Then

$$\pi_N(t) \in \Pi(f(t)^{\otimes N}; F_N(t)), \quad \text{for each } t \in \mathbf{R},$$

and

$$T_\sigma \pi_N(t) = \pi_N(t) \quad \text{for each } t \in \mathbf{R} \text{ and each } \sigma \in \mathfrak{S}_N.$$

Proof. Let $\phi \equiv \phi(X_N, \Xi_N)$ and $\psi \equiv \psi(Y_N, H_N) \in C_c^\infty((\mathbf{R}^d \times \mathbf{R}^d)^N)$ be two test functions. Then

$$\begin{aligned} & \frac{d}{dt} \iint \phi(X_N, \Xi_N) \pi_{N,1}(t, dX_N d\Xi_N) \\ &= \frac{d}{dt} \iiint \phi(X_N, \Xi_N) \pi_N(t, dX_N d\Xi_N dY_N dH_N) \\ &= \iiint \{\mathbf{H}_N^{\rho[f(t)]}, \phi\}_N(X_N, \Xi_N) \pi_N(t, dX_N d\Xi_N dY_N dH_N) \\ &= \iiint \{\mathbf{H}_N^{\rho[f(t)]}, \phi\}_N(X_N, \Xi_N) \pi_{N,1}(t, dX_N d\Xi_N) \end{aligned}$$

since

$$\{\mathcal{H}_N(Y_N, H_N), \phi(X_N, \Xi_N)\}_{2N} = 0.$$

The penultimate chain of equalities shows that the first marginal $\pi_{N,1}$ of π_N corresponding to the phase space variables (X_N, Ξ_N) is a solution of the equation

$$\partial_t \pi_{N,1} + \{\mathbf{H}_N^{\rho[f(t)]}, \pi_{N,1}\}_N = 0.$$

On the other hand, an elementary computation shows that the solution f of (5) satisfies

$$\partial_t f^{\otimes N} + \{\mathbf{H}_N^{\rho[f(t)]}, f^{\otimes N}\}_N = 0.$$

Since $\pi_{N,1}$ and $f^{\otimes N}$ are solutions of the same Liouville equation and

$$\pi_{N,1}(0) = (f^{in})^{\otimes N} = f(0)^{\otimes N}$$

we conclude from the uniqueness of the solution of the Cauchy problem for a transport equation with Lipschitz continuous coefficients that $\pi_{N,1}(t) = f(t)^{\otimes N}$ for all $t \geq 0$.

Similarly

$$\begin{aligned}
& \frac{d}{dt} \iint \psi(Y_N, H_N) \pi_{N,2}(t, dY_N dH_N) \\
&= \frac{d}{dt} \iiint \psi(Y_N, H_N) \pi_N(t, dX_N d\Xi_N dY_N dH_N) \\
&= \iiint \{\mathcal{H}_N, \psi\}_N(Y_N, H_N) \pi_N(t, dX_N d\Xi_N dY_N dH_N) \\
&= \iiint \{\mathcal{H}_N, \psi\}_N(Y_N, H_N) \pi_{N,2}(t, dY_N dH_N),
\end{aligned}$$

since

$$\{\mathbf{H}_N^{\rho[f(t)]}(X_N, \Xi_N), \psi(Y_N, H_N)\}_{2N} = 0.$$

This shows that the second marginal $\pi_{N,2}$, corresponding to the phase space variables (Y_N, H_N) , is a solution to the same Liouville equation (4) as F_N . Since

$$\pi_{N,2}(0) = (f^{in})^{\otimes N} = F_N(0)$$

we conclude that $\pi_{N,2}(t) = F_N(t)$ for each $t \geq 0$, by uniqueness of the solution of (4).

Finally the time-dependent Hamiltonian

$$\mathbf{h}_f : (X_N, \Xi_N, Y_N, H_N) \mapsto \mathbf{H}_N^{\rho[f(t)]}(X_N, \Xi_N) + \mathcal{H}_N(Y_N, H_N)$$

satisfies

$$\mathbf{h}_f \circ T_\sigma = \mathbf{h}_f \quad \text{pour tout } \sigma \in \mathfrak{S}_N.$$

Hence

$$\partial_t(\pi_N - T_\sigma \# \pi_N)(t) + \{\mathbf{h}_f, (\pi_N - T_\sigma \# \pi_N)(t)\}_{2N} = 0.$$

Since $(\pi_N - T_\sigma \# \pi_N)(0)$ by (16), we conclude that

$$\pi_N(t) = T_\sigma \# \pi_N(t)$$

for all $t \geq 0$, by uniqueness of the solution of the Cauchy problem for the Liouville equation with Hamiltonian \mathbf{h}_f . \square

3.3. The Eulerian variant of the Dobrushin estimate. Set

$$D_N^p(t) := \int \frac{1}{N} \sum_{j=1}^N (|x_j - y_j|^p + |\xi_j - \eta_j|^p) \pi_N(t, dX_N d\Xi_N dY_N dH_N).$$

We recall that $p \geq 1$ and that $p \neq d/2$. Then

$$\begin{aligned}
\frac{dD_N^p}{dt} &= \int \left\{ \mathbf{H}_N^{\rho[f(t)]}(X_N, \Xi_N), \frac{1}{N} \sum_{j=1}^N (|x_j - y_j|^p + |\xi_j - \eta_j|^p) \right\}_{2N} d\pi_N(t) \\
&\quad + \int \left\{ \mathcal{H}_N(Y_N, H_N), \frac{1}{N} \sum_{j=1}^N (|x_j - y_j|^p + |\xi_j - \eta_j|^p) \right\}_{2N} d\pi_N(t).
\end{aligned}$$

First

$$\begin{aligned}
& \left\{ \mathbf{H}_N^{\rho[f(t)]}(X_N, \Xi_N), \frac{1}{N} \sum_{j=1}^N (|x_j - y_j|^p + |\xi_j - \eta_j|^p) \right\}_{2N} \\
&= \frac{1}{N} \sum_{j=1}^N \left\{ \frac{1}{2} |\xi_j|^2, |x_j - y_j|^p \right\}_{2N} + \frac{1}{N} \sum_{j=1}^N \{V_{\rho[f]}(x_j), |\xi_j - \eta_j|^p\}_{2N} \\
&= \frac{p}{N} \sum_{j=1}^N \xi_j \cdot (x_j - y_j) |x_j - y_j|^{p-2} - \frac{p}{N} \sum_{j=1}^N \nabla V_{\rho[f]}(x_j) \cdot (\xi_j - \eta_j) |\xi_j - \eta_j|^{p-2},
\end{aligned}$$

while

$$\begin{aligned}
& \left\{ \mathcal{H}_N(Y_N, H_N), \frac{1}{N} \sum_{j=1}^N (|x_j - y_j|^p + |\xi_j - \eta_j|^p) \right\}_{2N} \\
&= \frac{1}{N} \sum_{j=1}^N \left\{ \frac{1}{2} |\eta_j|^2, |x_j - y_j|^p \right\}_{2N} + \frac{1}{N^2} \sum_{j,k=1}^N \{V(y_j - y_k), |\xi_j - \eta_j|^p\}_{2N} \\
&= \frac{p}{N} \sum_{j=1}^N \eta_j \cdot (y_j - x_j) |y_j - x_j|^{p-2} - \frac{p}{N^2} \sum_{j,k=1}^N \nabla V(y_j - y_k) \cdot (\eta_j - \xi_j) |\eta_j - \xi_j|^{p-2}.
\end{aligned}$$

Therefore

$$\begin{aligned}
\frac{dD_N^p}{dt} &= -\frac{p}{N} \sum_{j=1}^N \int (\xi_j - \eta_j) \cdot (x_j - y_j) |x_j - y_j|^{p-2} d\pi_N \\
&\quad - \frac{p}{N} \sum_{j=1}^N \int (\xi_j - \eta_j) \cdot \left(\nabla V_{\rho[f]}(x_j) - \frac{1}{N} \sum_{k=1}^N \nabla V(y_j - y_k) \right) |\xi_j - \eta_j|^{p-2} d\pi_N.
\end{aligned}$$

At this point we use Young's inequality in the form

$$pab^{p-1} \leq a^p + (p-1)b^p \leq \max(1, p-1)(a^p + b^p)$$

for each $a, b > 0$ and each $p \geq 1$. Denoting

$$K_p := \max(1, p-1),$$

one has

$$\begin{aligned}
\frac{dD_N^p}{dt} &\leq \frac{K_p}{N} \sum_{j=1}^N \int (|\xi_j - \eta_j|^p + |x_j - y_j|^p) d\pi_N + \frac{K_p}{N} \sum_{j=1}^N \int |\xi_j - \eta_j|^p d\pi_N \\
&\quad + \frac{K_p}{N} \sum_{j=1}^N \int \left| \nabla V_{\rho[f]}(x_j) - \frac{1}{N} \sum_{k=1}^N \nabla V(y_j - y_k) \right|^p d\pi_N \\
&\leq 2K_p D_N^p + \frac{K_p}{N} \sum_{j=1}^N \int \left| \nabla V_{\rho[f]}(x_j) - \frac{1}{N} \sum_{k=1}^N \nabla V(y_j - y_k) \right|^p d\pi_N.
\end{aligned}$$

Let us decompose this last term as follows

$$\begin{aligned} \nabla V_{\rho[f]}(x_j) - \frac{1}{N} \sum_{k=1}^N \nabla V(y_j - y_k) &= \nabla V_{\rho[f]}(x_j) - \frac{1}{N} \sum_{k=1}^N \nabla V(x_j - x_k) \\ &\quad + \frac{1}{N} \sum_{k=1}^N (\nabla V(x_j - x_k) - \nabla V(y_j - y_k)) , \end{aligned}$$

so that, by convexity of the function $z \mapsto z^p$ on $(0, \infty)$ for $p \geq 1$,

$$\begin{aligned} &\left| \nabla V_{\rho[f]}(x_j) - \frac{1}{N} \sum_{k=1}^N \nabla V(y_j - y_k) \right|^p \\ &\leq 2^{p-1} \left| \nabla V_{\rho[f]}(x_j) - \frac{1}{N} \sum_{k=1}^N \nabla V(x_j - x_k) \right|^p \\ &\quad + 2^{p-1} \left| \frac{1}{N} \sum_{k=1}^N (\nabla V(x_j - x_k) - \nabla V(y_j - y_k)) \right|^p . \end{aligned}$$

Then, by the same convexity argument as above

$$\begin{aligned} &\left| \frac{1}{N} \sum_{k=1}^N (\nabla V(x_j - x_k) - \nabla V(y_j - y_k)) \right|^p \\ &\leq \frac{1}{N} \sum_{k=1}^N |\nabla V(x_j - x_k) - \nabla V(y_j - y_k)|^p \\ &\leq \frac{\text{Lip}(\nabla V)^p}{N} \sum_{k=1}^N |(x_j - x_k) - (y_j - y_k)|^p \\ &\leq \frac{2^{p-1} \text{Lip}(\nabla V)^p}{N} \sum_{k=1}^N (|x_j - y_j|^p + |x_k - y_k|^p) . \end{aligned}$$

Hence

$$\begin{aligned} \frac{dD_N^p}{dt} &\leq 2K_p D_N^p + \frac{2^{p-1} K_p \text{Lip}(\nabla V)^p}{N^2} \sum_{j,k=1}^N \int (|x_j - y_j|^p + |x_k - y_k|^p) d\pi_N \\ &\quad + \frac{2^{p-1} K_p}{N} \sum_{j=1}^N \int \left| \nabla V_{\rho[f]}(x_j) - \frac{1}{N} \sum_{k=1}^N \nabla V(x_j - x_k) \right|^p d\pi_N . \end{aligned}$$

Since

$$\frac{1}{N^2} \sum_{j,k=1}^N \int (|x_j - y_j|^p + |x_k - y_k|^p) d\pi_N = \frac{2}{N} \sum_{l=1}^N \int |x_l - y_l|^p d\pi_N \leq 2D_N^p ,$$

the inequality above can be recast as

$$\begin{aligned} \frac{dD_N^p}{dt} &\leq 2K_p (1 + 2^{p-1} \text{Lip}(\nabla V)^p) D_N^p \\ &\quad + \frac{2^{p-1} K_p}{N} \sum_{j=1}^N \int \left| \nabla V_{\rho[f]}(x_j) - \frac{1}{N} \sum_{k=1}^N \nabla V(x_j - x_k) \right|^p d\pi_N . \end{aligned}$$

Let us examine the last term on the right hand side of this inequality. Since $\pi_N(t) \in \Pi(f(t)^{\otimes N}, F_N(t))$ by Lemma 3.3

$$\begin{aligned} & \int \left| \nabla V_{\rho[f]}(x_j) - \frac{1}{N} \sum_{k=1}^N \nabla V(x_j - x_k) \right|^p d\pi_N \\ &= \int \left| \nabla V_{\rho[f]}(x_j) - \frac{1}{N} \sum_{k=1}^N \nabla V(x_j - x_k) \right|^p f^{\otimes N}(t, dX_N). \end{aligned}$$

Observe that this term involves only the factorized distribution $f^{\otimes N}$. This is the “consistency” error in the sense of numerical analysis. In other words, it measures by how much $f^{\otimes N}$ fails to be an exact solution of the N -body Liouville equation (4). This term is controlled by a quantitative variant of the law of large numbers, as explained below.

First

$$\begin{aligned} & \left| \nabla V_{\rho[f]}(x_j) - \frac{1}{N} \sum_{k=1}^N \nabla V(x_j - x_k) \right|^p \\ &= \left| \int \nabla V(x_j - \bar{x}) \rho[f](t, d\bar{x}) - \int \nabla V(x_j - \bar{x}) \mu_{X_N}(d\bar{x}) \right|^p \end{aligned}$$

where the notation

$$\mu_{X_N} := \frac{1}{N} \sum_{k=1}^N \delta_{x_k}$$

designates the empirical measure of the N particles with positions X_N . Thus

$$\begin{aligned} \left| \nabla V_{\rho[f]}(x_j) - \frac{1}{N} \sum_{k=1}^N \nabla V(x_j - x_k) \right|^p &\leq \text{Lip}(\nabla V)^p \text{dist}_{\text{MK},1}(\rho[f](t), \mu_{X_N})^p \\ &\leq \text{Lip}(\nabla V)^p \text{dist}_{\text{MK},p}(\rho[f](t), \mu_{X_N})^p, \end{aligned}$$

by the ordering of Monge-Kantorovich distances (see formula (7.3) in [28], which is a straightforward consequence of the Hölder, or Jensen inequality). Thus

$$\begin{aligned} \frac{dD_N}{dt} &\leq 2K_p(1 + 2^{p-1} \text{Lip}(\nabla V)^p) D_N^p \\ &+ 2^{p-1} K_p \text{Lip}(\nabla V)^p \int \text{dist}_{\text{MK},p}(\rho[f](t), \mu_{X_N})^p \rho[f]^{\otimes N}(t, dX_N). \end{aligned}$$

At this point, we apply Theorem 1 in [10]: assuming that $f(t) \in \mathcal{P}_q(\mathbf{R}^d \times \mathbf{R}^d)$ with $q > 2p$ and $1 \leq p \neq d/2$, one has

$$\int \text{dist}_{\text{MK},p}(\rho[f](t), \mu_{X_N})^p \rho[f]^{\otimes N}(t, dX_N) \leq C_{d,p,q} m_q^{1/q}(t) N^{-\min(1/2, p/d)}.$$

Assuming that $f^{in} \in \mathcal{P}_q(\mathbf{R}^d \times \mathbf{R}^d)$ with $q > 2p$, one has $m_q(t) < \infty$ for each $t \geq 0$, by Lemma 3.2. Thus

$$\begin{aligned} \frac{dD_N^p}{dt} &\leq 2K_p(1 + 2^{p-1} \text{Lip}(\nabla V)^p) D_N^p \\ &+ 2^{p-1} K_p C_{d,p,q} \text{Lip}(\nabla V)^p m_q^{p/q}(t) N^{-\min(1/2, p/d)}, \end{aligned}$$

and we deduce from Gronwall's inequality that

(18)

$$\begin{aligned} D_N^p(t) &\leq D_N^p(0) e^{2K_p(1+2^{p-1} \text{Lip}(\nabla V)^p)t} \\ &\quad + 2^{p-1} K_p C_{d,p,q} \text{Lip}(\nabla V)^p e^{2K_p(1+2^{p-1} \text{Lip}(\nabla V)^p)t} t m_q^{p/q}(t) N^{-\min(1/2, p/d)}. \end{aligned}$$

Remark 3.4. Observe that one can always obtain a right hand side of order $O(N^{-1/2})$ in (18), corresponding to the optimal rate predicted by the central limit theorem, provided that one controls moments of f of order $q > d$.

3.4. End of the proof of Theorem 3.1. By Lemma 3.3,

$$T_\sigma \# \pi_N(t) = \pi_N(t)$$

for each $t \geq 0$ and each permutation $\sigma \in \mathfrak{S}_N$. Thus, for each $k = 1, \dots, N$, one has

$$\begin{aligned} &\int (|x_k - y_k|^p + |\xi_k - \eta_k|^p) \pi_N(t, dX_N d\Xi_N dY_N dH_N) \\ &= \int (|x_1 - y_1|^p + |\xi_1 - \eta_1|^p) \pi_N(t, dX_N d\Xi_N dY_N dH_N), \end{aligned}$$

so that

$$\begin{aligned} D_N^p(t) &= \int (|x_j - y_j|^p + |\xi_j - \eta_j|^p) \pi_N(t, dX_N d\Xi_N dY_N dH_N) \\ &= \frac{1}{n} \int \sum_{j=1}^n (|x_j - y_j|^p + |\xi_j - \eta_j|^p) \pi_N(t, dX_N d\Xi_N dY_N dH_N) \end{aligned}$$

Denoting

$$(19) \quad X_N^k := (x_k, \dots, x_N), \quad \Xi_N^k := (\xi_k, \dots, \xi_N)$$

for each $k = 1, \dots, N$, we set

$$p_N^n(t, dX_n d\Xi_n dY_n dH_n) := \int \pi_N(t, dX_N^n d\Xi_N^n dY_N^n dH_N^n).$$

By Fubini's theorem, for each $\phi \in C_b((\mathbf{R}^{2d})^n)$, one has

$$\begin{aligned} \int \phi(X_n, \Xi_n) p_N^n(t, dX_n d\Xi_n dY_n dH_n) &= \int \phi(X_n, \Xi_n) \pi_N(t, dX_N d\Xi_N dY_N dH_N) \\ &= \int \phi(X_n, \Xi_n) f(t)^{\otimes N} (dX_N d\Xi_N) \\ &= \int \phi(X_n, \Xi_n) f(t)^{\otimes n} (dX_n d\Xi_n), \end{aligned}$$

while

$$\begin{aligned} \int \phi(Y_n, H_n) p_N^n(t, dX_n d\Xi_n dY_n dH_n) &= \int \phi(Y_n, H_n) \pi_N(t, dX_N d\Xi_N dY_N dH_N) \\ &= \int \phi(Y_n, H_n) F_N(t, dY_N dH_N) \\ &= \int \phi(Y_n, H_n) F_N^n(t, dY_n dH_n), \end{aligned}$$

so that

$$p_N^n(t) \in \Pi(f(t)^{\otimes n}, F_N^n(t)) \quad \text{for each } t \geq 0.$$

Therefore

$$\begin{aligned} D_N^p(t) &= \frac{1}{n} \int \sum_{j=1}^n (|x_j - y_j|^p + |\xi_j - \eta_j|^p) p_N^n(t, dX_n d\Xi_n dY_n dH_n) \\ &\geq \frac{1}{n} \text{dist}_{\text{MK},p}(f(t)^{\otimes n}, F_N^n(t))^p. \end{aligned}$$

Thus the inequality (18) implies that

$$\begin{aligned} (20) \quad &\text{dist}_{\text{MK},p}(f(t)^{\otimes n}, F_N^n(t))^p \leq n D_N^p(0) e^{2K_p(1+2^{p-1} \text{Lip}(\nabla V)^p)t} \\ &+ 2^{p-1} K_p C_{d,p,q} \text{Lip}(\nabla V)^p e^{2K_p(1+2^{p-1} \text{Lip}(\nabla V)^p)t} t m_q^{p/q}(t) n N^{-\min(1/2, p/d)}. \end{aligned}$$

for each $t \geq 0$, each $N \geq n \geq 1$ and each $\pi_N^{\text{in}} \in \Pi((f^{\text{in}})^{\otimes N}, F_N^{\text{in}})$ satisfying

$$T_\sigma \pi_N^{\text{in}} = \pi_N^{\text{in}} \quad \text{for all } \sigma \in \mathfrak{S}_N.$$

Let us choose the initial coupling of the form

$$\pi_N^{\text{in}} := (f^{\text{in}})^{\otimes N} (dX_N d\Xi_N) \delta_{(X_N, \Xi_N)}(Y_N, H_N),$$

i.e.

$$\pi_N := \mathbf{D} \# (f^{\text{in}})^{\otimes N}, \quad \text{where } \mathbf{D} : (X_N, \Xi_N) \mapsto (X_N, \Xi_N, X_N, \Xi_N).$$

Then

$$D_N^p(0) = \frac{1}{N} \sum_{j=1}^N \int (|x_k - y_k|^p + |\xi_k - \eta_k|^p) \pi_N^{\text{in}}(dX_N d\Xi_N dY_N dH_N) = 0,$$

since π_N^{in} is supported in the diagonal

$$\{(X_N, \Xi_N, Y_N, H_N) \text{ s.t. } X_N = Y_N \text{ et } \Xi_N = H_N\}.$$

Inserting this last piece of information in (20) leads to the inequality in the statement of Theorem 3.1.

4. PROOF OF THEOREM 2.3: PROPERTIES OF MK_2^ϵ

4.1. The general lower bound (11). The lower bound (11) can be viewed as a variant of the uncertainty principle. More precisely

$$Q^*Q + P^*P = (Q + iP)^*(Q + iP) + i(P^*Q - Q^*P) \geq i(P^*Q - Q^*P).$$

On the other hand,

$$(P^*Q - Q^*P) = -i\epsilon(\text{div}_{x_1}(x_1) + \text{div}_{x_2}(x_2)) = -2i d\epsilon I_{\mathfrak{H}_2},$$

so that

$$Q^*Q + P^*P \geq 2d\epsilon I_{\mathfrak{H}_2}.$$

Therefore, for each $R \in \mathcal{D}(\mathfrak{H}_2)$, one has

$$\begin{aligned} \text{trace}_{\mathfrak{H}_2}((Q^*Q + P^*P)R) &= \text{trace}_{\mathfrak{H}_2}(R^{1/2}(Q^*Q + P^*P)R^{1/2}) \\ &\geq 2d\epsilon \text{trace}_{\mathfrak{H}_2}(R) = 2d\epsilon. \end{aligned}$$

4.2. Upper bound for Töplitz operators. The goal of this section is to prove statement (1) in Theorem 2.3.

In the course of the proof, we shall need the following intermediate result.

Lemma 4.1 (Construction of quantum couplings). *Let $\epsilon > 0$ and let ρ_1^ϵ and ρ_2^ϵ be Töplitz operators at scale ϵ on $L^2(\mathbf{R}^d)$ with symbols $(2\pi\epsilon)^d\mu_1$ and $(2\pi\epsilon)^d\mu_2$, where $\mu_1, \mu_2 \in \mathcal{P}(\mathbf{R}^{2d})$. For each coupling $\pi \in \Pi(\mu_1, \mu_2)$, the Töplitz operator $\text{OP}_\epsilon^T((2\pi\epsilon)^{2d}\pi)$ belongs to $\mathcal{Q}(\rho_1^\epsilon, \rho_2^\epsilon)$.*

Proof of Lemma 4.1. Let $\mu_1, \mu_2 \in \mathcal{P}_2(\mathbf{R}^{2d})$. Set $\rho_j^\epsilon = \text{OP}_\epsilon^T((2\pi\epsilon)^d\mu_j)$ for $j = 1, 2$. Everywhere in this section, the identification $\mathbf{R}^{2d} \ni (q, p) \mapsto q + ip \in \mathbf{C}^d$ is implicitly assumed. For each $\pi \in \Pi(\mu_1, \mu_2)$, one has

$$\text{OP}_\epsilon^T((2\pi\epsilon)^{2d}\pi) = \int_{\mathbf{R}^{4d}} |(z_1, z_2), \epsilon\rangle \langle (z_1, z_2), \epsilon| \pi(dz_1 dz_2),$$

where the wave function $|(z_1, z_2), \epsilon\rangle$ is defined in formula (34) in the Appendix. In this section and in the Appendix, we use the bra-ket notation. Recalling that $\mathfrak{H} = L^2(\mathbf{R}^d)$, for each $A \in \mathcal{L}(\mathfrak{H})$, one has

$$\begin{aligned} & \text{trace}_{\mathfrak{H} \otimes \mathfrak{H}}((A \otimes I_{\mathfrak{H}}) \text{OP}_\epsilon^T((2\pi\epsilon)^{2d}\pi)) \\ &= \int_{\mathbf{R}^{4d}} \text{trace}_{\mathfrak{H} \otimes \mathfrak{H}}((A \otimes I_{\mathfrak{H}}) |(z_1, z_2), \epsilon\rangle \langle (z_1, z_2), \epsilon|) \pi(dz_1 dz_2) \\ &= \int_{\mathbf{R}^{4d}} \text{trace}_{\mathfrak{H}}(A |z_1, \epsilon\rangle \langle z_1, \epsilon|) \pi(dz_1 dz_2) = \int_{\mathbf{R}^{2d}} \text{trace}_{\mathfrak{H}}(A |z_1, \epsilon\rangle \langle z_1, \epsilon|) \mu_1(dz_1) \\ &= \text{trace}_{\mathfrak{H}}(A \rho_1^\epsilon), \end{aligned}$$

because

$$|(z_1, z_2), \epsilon\rangle \langle (z_1, z_2), \epsilon| = |z_1, \epsilon\rangle \langle z_1, \epsilon| \otimes |z_2, \epsilon\rangle \langle z_2, \epsilon|.$$

Hence

$$\begin{aligned} & \text{trace}_{\mathfrak{H} \otimes \mathfrak{H}}((A \otimes I_{\mathfrak{H}}) |(z_1, z_2), \epsilon\rangle \langle (z_1, z_2), \epsilon|) \\ &= \text{trace}_{\mathfrak{H}}(A |z_1, \epsilon\rangle \langle z_1, \epsilon|) \text{trace}_{\mathfrak{H}}(|z_2, \epsilon\rangle \langle z_2, \epsilon|) \\ &= \text{trace}_{\mathfrak{H}}(A |z_1, \epsilon\rangle \langle z_1, \epsilon|) \langle z_2, \epsilon | z_2, \epsilon \rangle \\ &= \text{trace}_{\mathfrak{H}}(A |z_1, \epsilon\rangle \langle z_1, \epsilon|). \end{aligned}$$

Similarly

$$\text{trace}_{\mathfrak{H} \otimes \mathfrak{H}}((I_{\mathfrak{H}} \otimes A) \text{OP}_\epsilon^T((2\pi\epsilon)^{2d}\pi)) = \text{trace}_{\mathfrak{H}}(A \rho_2^\epsilon),$$

so that

$$(21) \quad \pi \in \Pi(\mu_1, \mu_2) \Rightarrow \text{OP}_\epsilon^T((2\pi\epsilon)^{2d}\pi) \in \mathcal{Q}(\rho_1^\epsilon, \rho_2^\epsilon).$$

□

Proof of Theorem 2.3 (1). For each $\pi \in \Pi(\mu_1, \mu_2)$, by Lemma 4.1 and the definition of MK_2^ϵ , one has

$$MK_2^\epsilon(\rho_1, \rho_2)^2 \leq \text{trace}_{\mathfrak{H} \otimes \mathfrak{H}}((Q^*Q + P^*P) \text{OP}_\epsilon^T((2\pi\epsilon)^{2d}\pi)),$$

where we recall that

$$(22) \quad \begin{aligned} Q\psi(x_1, x_2) &= (x_1 - x_2)\psi(x_1, x_2), \\ P\psi(x_1, x_2) &= -i\epsilon(\nabla_{x_1} - \nabla_{x_2})\psi(x_1, x_2), \end{aligned}$$

so that

$$Q^*Q\psi(x_1, x_2) = |x_1 - x_2|^2\psi(x_1, x_2),$$

and

$$P^*P\psi(x_1, x_2) = -\epsilon^2(\operatorname{div}_{x_1} - \operatorname{div}_{x_2})(\nabla_{x_1} - \nabla_{x_2})\psi(x_1, x_2).$$

In other words

$$Q^*Q + P^*P = \operatorname{OP}_\epsilon^T(|q_1 - q_2|^2 + |p_1 - p_2|^2) - 2d\epsilon I_{\mathfrak{H}_2}$$

— see formula (37) in Appendix A, with $f(y_1, y_2) = |y_1 - y_2|^2$, and $\Delta f = 4d$. By formula (44) in Appendix A, one has

$$\begin{aligned} & \operatorname{trace}_{\mathfrak{H} \otimes \mathfrak{H}}((Q^*Q + P^*P) \operatorname{OP}_\epsilon^T(\pi)) \\ &= \int_{(\mathbf{R}^d)^4} (|x_1 - x_2|^2 + |\xi_1 - \xi_2|^2) \pi(dx_1 d\xi_1 dx_2 d\xi_2) + 2d\epsilon. \end{aligned}$$

Therefore, for each $\pi \in \Pi(\mu_1, \mu_2)$, one has

$$MK_2^\epsilon(\rho_1, \rho_2)^2 \leq \int_{(\mathbf{R}^d)^4} (|x_1 - x_2|^2 + |\xi_1 - \xi_2|^2) \pi(dx_1 d\xi_1 dx_2 d\xi_2) + 2d\epsilon.$$

Observing that the left hand side of this inequality is independent of the coupling $\pi \in \Pi(\mu_1, \mu_2)$, we conclude that

$$\begin{aligned} MK_2^\epsilon(\rho_1, \rho_2)^2 &\leq \inf_{\pi \in \Pi(\mu_1, \mu_2)} \int_{(\mathbf{R}^d)^4} (|x_1 - x_2|^2 + |\xi_1 - \xi_2|^2) \pi(dx_1 d\xi_1 dx_2 d\xi_2) + 2d\epsilon \\ &= \operatorname{dist}_{\operatorname{MK}, 2}(\mu_1, \mu_2)^2 + 2d\epsilon \end{aligned}$$

which is the sought inequality. \square

4.3. Asymptotic lower bound for MK_2^ϵ . The core of the argument leading to the lower bound in Theorem 2.3 (2) combines Kantorovich duality with the convergence of Husimi functions to Wigner measures.

Proof of Theorem 2.3 (2). Let $a, b \in C_b(\mathbf{R}^d)$ satisfy

$$(23) \quad a(x_1, \xi_1) + b(x_2, \xi_2) \leq |x_1 - x_2|^2 + |\xi_1 - \xi_2|^2 \quad \text{for all } x_1, x_2, \xi_1, \xi_2 \in \mathbf{R}^d.$$

Hence¹

$$\begin{aligned} (\operatorname{OP}_\epsilon^T(a) \otimes I_{\mathfrak{H}} + I_{\mathfrak{H}} \otimes \operatorname{OP}_\epsilon^T(b)) &= \operatorname{OP}_\epsilon^T(a \otimes 1 + 1 \otimes b) \\ &\leq \operatorname{OP}_\epsilon^T(c) = Q^*Q + P^*P + 2d\epsilon I_{\mathfrak{H}_2}. \end{aligned}$$

Thus, for each $R^\epsilon \in \mathcal{Q}(\rho_1^\epsilon, \rho_2^\epsilon)$, one has

$$\begin{aligned} & \operatorname{trace}_{\mathfrak{H} \otimes \mathfrak{H}}((Q^*Q + P^*P)R^\epsilon) \\ &\geq \operatorname{trace}_{\mathfrak{H} \otimes \mathfrak{H}}((\operatorname{OP}_\epsilon^T(a) \otimes I_{\mathfrak{H}} + I_{\mathfrak{H}} \otimes \operatorname{OP}_\epsilon^T(b))R^\epsilon) - 2d\epsilon \\ &= \operatorname{trace}_{\mathfrak{H}}(\operatorname{OP}_\epsilon^T(a)\rho_1^\epsilon) + \operatorname{trace}_{\mathfrak{H}}(\operatorname{OP}_\epsilon^T(b)\rho_2^\epsilon) - 2d\epsilon. \end{aligned}$$

Taking the inf of the left hand side as R^ϵ runs through $\mathcal{Q}(\rho_1^\epsilon, \rho_2^\epsilon)$, one arrives at the inequality

$$(24) \quad MK_2^\epsilon(\rho_1^\epsilon, \rho_2^\epsilon)^2 \geq \operatorname{trace}_{\mathfrak{H}}(\operatorname{OP}_\epsilon^T(a)\rho_1^\epsilon) + \operatorname{trace}_{\mathfrak{H}}(\operatorname{OP}_\epsilon^T(b)\rho_2^\epsilon) - 2d\epsilon.$$

¹Denoting $a \otimes 1$, $1 \otimes b$ and c the functions $(x_1, \xi_1, x_2, \xi_2) \mapsto a(x_1, \xi_1)$, $(x_1, \xi_1, x_2, \xi_2) \mapsto b(x_2, \xi_2)$ and $(x_1, \xi_1, x_2, \xi_2) \mapsto |x_1 - x_2|^2 + |\xi_1 - \xi_2|^2$ respectively.

Next the traces on the right hand side are expressed in terms of the Husimi functions of ρ_1^ϵ and ρ_2^ϵ by formula (43):

$$\begin{aligned} \text{trace}_{\mathfrak{H}}(\text{OP}_\epsilon^T(a)\rho_1^\epsilon) &= \iint a(x_1, \xi_1) \tilde{W}_\epsilon[\rho_1^\epsilon](x_1, \xi_1) dx_1 d\xi_1, \\ \text{trace}_{\mathfrak{H}}(\text{OP}_\epsilon^T(b)\rho_2^\epsilon) &= \iint b(x_2, \xi_2) \tilde{W}_\epsilon[\rho_2^\epsilon](x_2, \xi_2) dx_2 d\xi_2. \end{aligned}$$

Hence

$$\begin{aligned} MK_2^\epsilon(\rho_1^\epsilon, \rho_2^\epsilon)^2 &\geq \iint a(x_1, \xi_1) \tilde{W}_\epsilon[\rho_1^\epsilon](x_1, \xi_1) dx_1 d\xi_1 \\ &\quad + \iint b(x_2, \xi_2) \tilde{W}_\epsilon[\rho_2^\epsilon](x_2, \xi_2) dx_2 d\xi_2 - 2d\epsilon. \end{aligned}$$

Taking the sup of both sides of this equality over all $a, b \in C_b(\mathbf{R}^d \times \mathbf{R}^d)$ satisfying (23) shows that

$$\begin{aligned} &MK_2^\epsilon(\rho_1^\epsilon, \rho_2^\epsilon)^2 \\ &\geq \sup_{\substack{a \otimes 1 + 1 \otimes b \leq c \\ a, b \in C_b(\mathbf{R}^d \times \mathbf{R}^d)}} \left(\iint a \tilde{W}_\epsilon[\rho_1^\epsilon] dx_1 d\xi_1 + \iint b \tilde{W}_\epsilon[\rho_2^\epsilon] dx_2 d\xi_2 \right) - 2d\epsilon \\ &= \text{dist}_{\text{MK}, 2}(\tilde{W}_\epsilon[\rho_1^\epsilon], \tilde{W}_\epsilon[\rho_2^\epsilon])^2 - 2d\epsilon, \end{aligned}$$

where the last equality follows from Kantorovich duality (Theorem 1 in chapter 1 of [28]). This gives the first inequality in Theorem 2.3 (2).

Since the sequence of Wigner transforms of the density matrices ρ_j^ϵ satisfies

$$W_\epsilon[\rho_j^\epsilon] \rightarrow w_j \quad \text{in } \mathcal{S}'(\mathbf{R}^d \times \mathbf{R}^d) \text{ as } \epsilon \rightarrow 0$$

for $j = 1, 2$, one has

$$\tilde{W}_\epsilon[\rho_j^\epsilon] \rightarrow w_j \text{ weakly in the sense of measures on } \mathbf{R}^d \times \mathbf{R}^d$$

for $j = 1, 2$, by Theorem III.1 (1) in [17]. By the first inequality in Theorem 2.3 (2) already established above and Remark 6.12 in [29],

$$\liminf_{\epsilon \rightarrow 0} MK_2^\epsilon(\rho_1^\epsilon, \rho_2^\epsilon)^2 \geq \liminf_{\epsilon \rightarrow 0} \text{dist}_{\text{MK}, 2}(W_\epsilon[\rho_1^\epsilon], W_\epsilon[\rho_2^\epsilon])^2 \geq \text{dist}_{\text{MK}, 2}(w_1, w_2)^2.$$

This concludes the proof of Theorem 2.3. \square

5. PROOF OF THEOREM 2.4

The quantum N -body Hamiltonian is

$$\mathcal{H}_{\epsilon, N} := \sum_{j=1}^N -\frac{1}{2}\epsilon^2 \Delta_j + \frac{1}{N} \sum_{1 \leq j, k \leq N} V_{jk},$$

an unbounded self-adjoint operator on $\mathfrak{H}_N := \mathfrak{H}^{\otimes N} = L^2((\mathbf{R}^d)^N)$. We denote by Δ_j the Laplacian acting on the variable x_j , and by V_{jk} the multiplication by $V(x_j - x_k)$. The N -body von Neumann equation for the density matrix is

$$(25) \quad i\epsilon \partial_t \rho_{\epsilon, N} := [\mathcal{H}_{\epsilon, N}, \rho_{\epsilon, N}],$$

with initial data

$$\rho_{\epsilon, N}|_{t=0} = (\rho^{in})^{\otimes N}$$

for $\rho^{in} \in \mathcal{D}(\mathfrak{H})$.

On the other hand, for each $\rho \in \mathcal{D}(\mathfrak{H})$, we consider the mean-field Hamiltonian

$$\mathbf{H}_\epsilon^\rho := -\frac{1}{2}\epsilon^2\Delta + V_\rho$$

where V_ρ designates the operator defined on \mathfrak{H} as the multiplication by the function

$$x \mapsto \int V(x-x')\rho(x',x')dx' =: V_\rho(x).$$

The Hartree equation for the density matrix ρ_ϵ is

$$(26) \quad i\epsilon\partial_t\rho_\epsilon = [\mathbf{H}_\epsilon^{\rho_\epsilon}, \rho_\epsilon], \quad \rho_\epsilon|_{t=0} = \rho^{in}.$$

By a straightforward computation, the solution ρ_ϵ of the Hartree equation (26) satisfies

$$(27) \quad i\epsilon\partial_t\rho_\epsilon^{\otimes N} = [\mathbf{H}_{\epsilon,N}^{\rho_\epsilon}, \rho_\epsilon^{\otimes N}], \quad \rho_\epsilon^{\otimes N}|_{t=0} = (\rho^{in})^{\otimes N},$$

where

$$\mathbf{H}_{\epsilon,N}^\rho := \mathbf{H}_\epsilon^\rho \otimes I_{\mathfrak{H}_{N-1}} + I \otimes \mathbf{H}_\epsilon^\rho \otimes I_{\mathfrak{H}_{N-2}} + \dots + I_{\mathfrak{H}_{N-1}} \otimes \mathbf{H}_\epsilon^\rho.$$

5.1. Controlling the second order moment of the density.

Lemma 5.1. *Let ρ_ϵ be the solution of the Cauchy problem for the Hartree equation with initial data $\rho^{in} \in \mathcal{D}(\mathfrak{H})$ such that*

$$\text{trace}(|x|^2 - \Delta)\rho^{in} < \infty.$$

Then, for each $\epsilon > 0$, one has

$$\text{trace}(|x|^2\rho_\epsilon(t)) \leq (\text{trace}(|x|^2\rho^{in}) + te^t(\text{trace}(-\epsilon^2\Delta\rho^{in}) + 2\|V\|_{L^\infty})).$$

Proof.

$$\begin{aligned} \frac{d}{dt} \int |x|^2 |\rho_\epsilon(t, x, x)|^2 dx &= \frac{d}{dt} \text{trace}(|x|^2\rho_\epsilon(t)) \\ &= -\frac{i}{\epsilon} \text{trace}([\tfrac{1}{2}\epsilon^2\Delta - V_{\rho_\epsilon}, |x|^2]\rho_\epsilon(t)) \\ &= -i \text{trace}([\tfrac{1}{2}\epsilon\Delta, |x|^2]\rho_\epsilon(t)). \end{aligned}$$

Next

$$\begin{aligned} |\text{trace}([\tfrac{1}{2}\epsilon\Delta, |x|^2]\rho_\epsilon(t))| &= |\text{trace}(\epsilon(x \cdot \nabla + \text{div}(x \cdot))\rho_\epsilon(t))| \\ &\leq \text{trace}((|x|^2 - \epsilon^2\Delta)\rho_\epsilon(t)). \end{aligned}$$

On the other hand,

$$\begin{aligned} \text{trace}((-\tfrac{1}{2}\epsilon^2\Delta + V_{\rho_\epsilon})\partial_t\rho_\epsilon) &= -i \text{trace}((-\tfrac{1}{2}\epsilon^2\Delta + V_{\rho_\epsilon})[-\tfrac{1}{2}\epsilon^2\Delta + V_{\rho_\epsilon}, \rho_\epsilon]) \\ &= i \text{trace}([-\tfrac{1}{2}\epsilon^2\Delta + V_{\rho_\epsilon}, -\tfrac{1}{2}\epsilon^2\Delta + V_{\rho_\epsilon}]\rho_\epsilon) = 0, \end{aligned}$$

and since V is even,

$$\begin{aligned} \text{trace}(V_{\rho_\epsilon}\partial_t\rho_\epsilon) &= \iint V(x-z)\rho_\epsilon(t, z, z)\partial_t\rho_\epsilon(t, x, x)dx dz \\ &= \tfrac{1}{2}\partial_t \iint V(x-z)\rho_\epsilon(t, z, z)\rho_\epsilon(t, x, x)dx dz. \end{aligned}$$

Therefore

$$\frac{d}{dt} \left(\text{trace}(-\epsilon^2\Delta\rho_\epsilon(t)) + \iint V(x-z)\rho_\epsilon(t, z, z)\rho_\epsilon(t, x, x)dx dz \right) = 0.$$

This implies that

$$\text{trace}(-\epsilon^2 \Delta \rho_\epsilon(t)) \leq \text{trace}(-\epsilon^2 \Delta \rho^{in}) + 2\|V\|_{L^\infty}.$$

Thus

$$\begin{aligned} \text{trace}(|x|^2 \rho_\epsilon(t)) &\leq \text{trace}(|x|^2 \rho^{in}) + \int_0^t |\text{trace}([\tfrac{1}{2}\epsilon \Delta, |x|^2] \rho_\epsilon(s))| ds \\ &\leq \text{trace}(|x|^2 \rho^{in}) + \int_0^t \text{trace}(-\epsilon^2 \Delta \rho_\epsilon(s)) ds \\ &\quad + \int_0^t \text{trace}(|x|^2 \rho_\epsilon(s)) ds \\ &\leq \text{trace}(|x|^2 \rho^{in}) + t(\text{trace}(-\epsilon^2 \Delta \rho^{in}) + 2\|V\|_{L^\infty}) \\ &\quad + \int_0^t \text{trace}(|x|^2 \rho_\epsilon(s)) ds, \end{aligned}$$

and we conclude with Gronwall's inequality. \square

5.2. The quantum dynamics of couplings. Let $R_{\epsilon,N}^{in} \in \mathcal{Q}((\rho^{in})^{\otimes N}, (\rho^{in})^{\otimes N})$, and let $t \mapsto R_{\epsilon,N}(t) \in \mathcal{D}(\mathfrak{H}_{2N})$ be the solution of the Cauchy problem

$$(28) \quad i\epsilon \partial_t R_{\epsilon,N} = [\mathbf{H}_{\epsilon,N}^{\rho_\epsilon} \otimes I_{\mathfrak{H}_N} + I_{\mathfrak{H}_N} \otimes \mathcal{H}_{\epsilon,N}, R_{\epsilon,N}], \quad R_{\epsilon,N}|_{t=0} = R_{\epsilon,N}^{in}.$$

For each $\sigma \in \mathfrak{S}_N$, we denote by \mathcal{T}_σ the unitary operator on \mathfrak{H}_{2N} defined by

$$\mathcal{T}_\sigma \Psi(x_1, \dots, x_N, y_1, \dots, y_N) = \Psi(x_{\sigma^{-1}(1)}, \dots, x_{\sigma^{-1}(N)}, y_{\sigma^{-1}(1)}, \dots, y_{\sigma^{-1}(N)})$$

for each $\Psi \in \mathfrak{H}_{2N}$. We shall henceforth assume that

$$(29) \quad \mathcal{T}_\sigma R_{\epsilon,N}^{in} \mathcal{T}_\sigma^* = R_{\epsilon,N}^{in}, \quad \text{for each } \sigma \in \mathfrak{S}_N.$$

Lemma 5.2. *For each $t \geq 0$, one has $R_{\epsilon,N}(t) \in \mathcal{Q}((\rho_\epsilon(t))^{\otimes N}, \rho_{\epsilon,N}(t))$. Moreover*

$$(30) \quad \mathcal{T}_\sigma R_{\epsilon,N}(t) \mathcal{T}_\sigma^* = R_{\epsilon,N}(t) \quad \text{for each } \sigma \in \mathfrak{S}_N \text{ and } t \geq 0.$$

Proof. By definition

$$R_{\epsilon,N}(t) = U_{\epsilon,N}(t/\epsilon) R_{\epsilon,N}^{in} U_{\epsilon,N}(t/\epsilon)^*$$

where

$$\frac{d}{dt} U_{\epsilon,N}(t) = -i(\mathbf{H}_{\epsilon,N}^{\rho_\epsilon} \otimes I_{\mathfrak{H}_N} + I_{\mathfrak{H}_N} \otimes \mathcal{H}_{\epsilon,N}) U_{\epsilon,N}(t), \quad U_{\epsilon,N}(0) = I_{\mathfrak{H}_{2N}}.$$

Since $\mathbf{H}_{\epsilon,N}^{\rho_\epsilon} \otimes I_{\mathfrak{H}_N} + I_{\mathfrak{H}_N} \otimes \mathcal{H}_{\epsilon,N}$ is self-adjoint, $U_{\epsilon,N}(t)$ is unitary for each $t \geq 0$. Therefore

$$R_{\epsilon,N}(t) = R_{\epsilon,N}(t)^* \geq 0 \quad \text{and} \quad \text{trace}_{\mathfrak{H}_{2N}}(R_{\epsilon,N}(t)) = \text{trace}_{\mathfrak{H}_{2N}}(R_{\epsilon,N}^{in}) = 1$$

for each $t \geq 0$.

The marginals of the density $R_{\epsilon,N}$ in the product $\mathfrak{H}_{2N} = \mathfrak{H}_N \otimes \mathfrak{H}_N$ are defined by analogy with (13)-(14) in Definition 2.1:

$$(31) \quad \begin{cases} R_{\epsilon,N,1} \in \mathcal{D}(\mathfrak{H}_N) & \text{and } \text{trace}_{\mathfrak{H}_N}(AR_{\epsilon,N,1}) = \text{trace}_{\mathfrak{H}_{2N}}((A \otimes I_{\mathfrak{H}_N})R_{\epsilon,N}), \\ R_{\epsilon,N,2} \in \mathcal{D}(\mathfrak{H}_N) & \text{and } \text{trace}_{\mathfrak{H}_N}(AR_{\epsilon,N,2}) = \text{trace}_{\mathfrak{H}_{2N}}((I_{\mathfrak{H}_N} \otimes A)R_{\epsilon,N}), \end{cases}$$

for each $A \in \mathcal{L}(\mathfrak{H}_N)$.

Let $A \in \mathcal{L}(\mathfrak{H}_N)$ be such that

$$\left[\sum_{j=1}^N \Delta_{x_j}, A \right] \in \mathcal{L}(\mathfrak{H}_N);$$

then

$$\begin{aligned} i\epsilon \partial_t \text{trace}_{\mathfrak{H}_N}(AR_{\epsilon,N,1}) &= i\epsilon \partial_t \text{trace}_{\mathfrak{H}_{2N}}((A \otimes I_{\mathfrak{H}_N})R_{\epsilon,N}) \\ &= -\text{trace}_{\mathfrak{H}_{2N}}([\mathbf{H}_{\epsilon,N}^{\rho_\epsilon} \otimes I_{\mathfrak{H}_N} + I_{\mathfrak{H}_N} \otimes \mathcal{H}_{\epsilon,N}, (A \otimes I_{\mathfrak{H}_N})]R_{\epsilon,N}) \\ &= -\text{trace}_{\mathfrak{H}_{2N}}([\mathbf{H}_{\epsilon,N}^{\rho_\epsilon}, A] \otimes I_{\mathfrak{H}_N})R_{\epsilon,N}) \\ &= -\text{trace}_{\mathfrak{H}_N}([\mathbf{H}_{\epsilon,N}^{\rho_\epsilon}, A]R_{\epsilon,N,1}) \\ &= \text{trace}_{\mathfrak{H}_N}(A[\mathbf{H}_{\epsilon,N}^{\rho_\epsilon}, R_{\epsilon,N,1}]) \end{aligned}$$

and

$$R_{\epsilon,N,1}|_{t=0} = R_{\epsilon,N,1}^{in} = (\rho^{in})^{\otimes N}.$$

By uniqueness of the solution of the Cauchy problem (27), one concludes that

$$R_{\epsilon,N,1}(t) = \rho_\epsilon(t)^{\otimes N}, \quad \text{for each } t \geq 0.$$

Similarly

$$\begin{aligned} i\epsilon \partial_t \text{trace}_{\mathfrak{H}_N}(AR_{\epsilon,N,2}) &= i\epsilon \partial_t \text{trace}_{\mathfrak{H}_{2N}}((I_{\mathfrak{H}_N} \otimes A)R_{\epsilon,N}) \\ &= -\text{trace}_{\mathfrak{H}_{2N}}([\mathbf{H}_{\epsilon,N}^{\rho_\epsilon} \otimes I_{\mathfrak{H}_N} + I_{\mathfrak{H}_N} \otimes \mathcal{H}_{\epsilon,N}, (I_{\mathfrak{H}_N} \otimes A)]R_{\epsilon,N}) \\ &= -\text{trace}_{\mathfrak{H}_{2N}}((I_{\mathfrak{H}_N}) \otimes [\mathcal{H}_{\epsilon,N}, A])R_{\epsilon,N}) \\ &= -\text{trace}_{\mathfrak{H}_N}([\mathcal{H}_{\epsilon,N}, A]R_{\epsilon,N,2}) \\ &= \text{trace}_{\mathfrak{H}_N}(A[\mathcal{H}_{\epsilon,N}, R_{\epsilon,N,2}]) \end{aligned}$$

and

$$R_{\epsilon,N,2}|_{t=0} = R_{\epsilon,N,2}^{in} = (\rho^{in})^{\otimes N}.$$

By uniqueness of the solution of the Cauchy problem for the von Neumann equation (25), one concludes that

$$R_{\epsilon,N,2}(t) = \rho_{\epsilon,N}(t), \quad \text{for each } t \geq 0.$$

Finally, let $\sigma \in \mathfrak{S}_N$;

$$\begin{aligned} i\epsilon \partial_t (\mathcal{T}_\sigma R_{\epsilon,N}(t) \mathcal{T}_\sigma^*) &= \mathcal{T}_\sigma [\mathbf{H}_{\epsilon,N}^{\rho_\epsilon} \otimes I_{\mathfrak{H}_N} + I_{\mathfrak{H}_N} \otimes \mathcal{H}_{\epsilon,N}, R_{\epsilon,N}] \mathcal{T}_\sigma^* \\ &= [\mathcal{T}_\sigma (\mathbf{H}_{\epsilon,N}^{\rho_\epsilon} \otimes I_{\mathfrak{H}_N} + I_{\mathfrak{H}_N} \otimes \mathcal{H}_{\epsilon,N}) \mathcal{T}_\sigma^*, \mathcal{T}_\sigma R_{\epsilon,N} \mathcal{T}_\sigma^*] \\ &= [\tau_\sigma \mathbf{H}_{\epsilon,N}^{\rho_\epsilon} \tau_\sigma^* \otimes I_{\mathfrak{H}_N} + I_{\mathfrak{H}_N} \otimes \tau_\sigma \mathcal{H}_{\epsilon,N} \tau_\sigma^*, \mathcal{T}_\sigma R_{\epsilon,N} \mathcal{T}_\sigma^*] \\ &= [\mathbf{H}_{\epsilon,N}^{\rho_\epsilon} \otimes I_{\mathfrak{H}_N} + I_{\mathfrak{H}_N} \otimes \mathcal{H}_{\epsilon,N}, \mathcal{T}_\sigma R_{\epsilon,N} \mathcal{T}_\sigma^*] \end{aligned}$$

where τ_σ is the unitary operator on \mathfrak{H}_N defined by the formula

$$\tau_\sigma \Phi(z_1, \dots, z_N) = \Phi(z_{\sigma^{-1}(1)}, \dots, z_{\sigma^{-1}(N)}),$$

since one has obviously

$$\tau_\sigma \mathbf{H}_{\epsilon,N}^{\rho_\epsilon} \tau_\sigma^* = \mathbf{H}_{\epsilon,N}^{\rho_\epsilon} \quad \text{and} \quad \tau_\sigma \mathcal{H}_{\epsilon,N} \tau_\sigma^* = \mathcal{H}_{\epsilon,N}.$$

On the other hand

$$\mathcal{T}_\sigma R_{\epsilon,N}(0) \mathcal{T}_\sigma^* = \mathcal{T}_\sigma R_{\epsilon,N}^{in}(0) \mathcal{T}_\sigma^* = R_{\epsilon,N}^{in} = R_{\epsilon,N}(0),$$

so that, by uniqueness of the solution of the Cauchy problem (28),

$$\mathcal{T}_\sigma R_{\epsilon,N}(t) \mathcal{T}_\sigma^* = R_{\epsilon,N}(t) \quad \text{for each } t \geq 0 \text{ and each } \sigma \in \mathfrak{S}_N.$$

□

5.3. **The Dobrushin type estimate.** Set

$$D_{\epsilon,N}(t) := \text{trace} \left(\frac{1}{N} \sum_{j=1}^N (Q_j^* Q_j + P_j^* P_j) R_{\epsilon,N}(t) \right).$$

We compute

$$\begin{aligned} \frac{dD_{\epsilon,N}}{dt} &= -\frac{1}{\epsilon} \text{trace} \left(i \frac{1}{N} \sum_{j=1}^N (Q_j^* Q_j + P_j^* P_j) [\mathbf{H}_{\epsilon,N}^{\rho_\epsilon} \otimes I_{\mathfrak{H}_N} + I_{\mathfrak{H}_N} \otimes \mathcal{H}_{\epsilon,N}, R_{\epsilon,N}] \right) \\ &= \frac{1}{\epsilon} \text{trace} \left(i \left[\mathbf{H}_{\epsilon,N}^{\rho_\epsilon} \otimes I_{\mathfrak{H}_N} + I_{\mathfrak{H}_N} \otimes \mathcal{H}_{\epsilon,N}, \frac{1}{N} \sum_{j=1}^N (Q_j^* Q_j + P_j^* P_j) \right] R_{\epsilon,N} \right) \\ &= \frac{1}{\epsilon} \text{trace} \left(i \left[\mathbf{H}_{\epsilon,N}^{\rho_\epsilon} \otimes I_{\mathfrak{H}_N} - \mathcal{H}_{\epsilon,N} \otimes I_{\mathfrak{H}_N}, \frac{1}{N} \sum_{j=1}^N (Q_j^* Q_j + P_j^* P_j) \right] R_{\epsilon,N} \right) \\ &\quad + \frac{1}{\epsilon} \text{trace} \left(i \left[\mathcal{H}_{\epsilon,N} \otimes I_{\mathfrak{H}_N} + I_{\mathfrak{H}_N} \otimes \mathcal{H}_{\epsilon,N}, \frac{1}{N} \sum_{j=1}^N (Q_j^* Q_j + P_j^* P_j) \right] R_{\epsilon,N} \right). \end{aligned}$$

Consider the second term on the right hand side of this equality. One has

$$\begin{aligned} &[\mathcal{H}_{\epsilon,N} \otimes I_{\mathfrak{H}_N} + I_{\mathfrak{H}_N} \otimes \mathcal{H}_{\epsilon,N}, (Q_j^* Q_j + P_j^* P_j)] \\ &= [-\frac{1}{2}\epsilon^2(\Delta_j \otimes I_{\mathfrak{H}} + I_{\mathfrak{H}} \otimes \Delta_j), Q_j^* Q_j]_j \\ &\quad + \frac{1}{N} \sum_{k=1}^N [V_{jk} \otimes I_{\mathfrak{H}} + I_{\mathfrak{H}} \otimes V_{jk}, P_j^* P_j]_j \end{aligned}$$

where the index j on the brackets in the right hand side indicate that the corresponding operators act on the variables x_j et y_j . In other words

$$A_j = I_{\mathfrak{H}}^{\otimes(j-1)} \otimes A \otimes I_{\mathfrak{H}}^{\otimes(N-j)}$$

for each operator A on \mathfrak{H} .

Obviously

$$\begin{aligned} &[-\frac{1}{2}\epsilon^2(\Delta_j \otimes I_{\mathfrak{H}} + I_{\mathfrak{H}} \otimes \Delta_j), Q_j^* Q_j] \\ &= -\frac{1}{2}\epsilon^2(\text{div}_{x_j}[\nabla_{x_j}, Q_j^* Q_j] + [\nabla_{x_j}, Q_j^* Q_j] \cdot \nabla_{x_j}) \\ &\quad -\frac{1}{2}\epsilon^2(\text{div}_{y_j}[\nabla_{y_j}, Q_j^* Q_j] + [\nabla_{y_j}, Q_j^* Q_j] \cdot \nabla_{y_j}) \\ &= -i\epsilon(P_j^* Q_j + Q_j^* P_j). \end{aligned}$$

On the other hand

$$\begin{aligned} [V_{jk} \otimes I_{\mathfrak{H}} + I_{\mathfrak{H}} \otimes V_{jk}, P_j^* P_j] &= [V_{jk} \otimes I_{\mathfrak{H}} + I_{\mathfrak{H}} \otimes V_{jk}, P_j^*] P_j \\ &\quad + P_j^* [V_{jk} \otimes I_{\mathfrak{H}} + I_{\mathfrak{H}} \otimes V_{jk}, P_j] \\ &= i\epsilon(\nabla V(x_j - x_k) - \nabla V(y_j - y_k)) P_j \\ &\quad + i\epsilon P_j^* (\nabla V(x_j - x_k) - \nabla V(y_j - y_k)). \end{aligned}$$

Therefore

$$\begin{aligned}
& \frac{1}{\epsilon} \operatorname{trace} \left(i \left[\mathcal{H}_{\epsilon,N} \otimes I_{\mathfrak{H}_N} + I_{\mathfrak{H}_N} \otimes \mathcal{H}_{\epsilon,N}, \frac{1}{N} \sum_{j=1}^N (Q_j^* Q_j + P_j^* P_j) \right] R_{\epsilon,N} \right) \\
&= \operatorname{trace} \left(\frac{1}{N} \sum_{j=1}^N (P_j^* Q_j + Q_j^* P_j) R_{\epsilon,N} \right) \\
&- \operatorname{trace} \left(\frac{1}{N^2} \sum_{1 \leq j, k \leq N} P_j^* (\nabla V(x_j - x_k) - \nabla V(y_j - y_k)) R_{\epsilon,N} \right) \\
&- \operatorname{trace} \left(\frac{1}{N^2} \sum_{1 \leq j, k \leq N} (\nabla V(x_j - x_k) - \nabla V(y_j - y_k)) P_j R_{\epsilon,N} \right).
\end{aligned}$$

By the Cauchy-Schwarz inequality

$$| \operatorname{trace} ((P_j^* Q_j + Q_j^* P_j) R_{\epsilon,N}) | \leq \operatorname{trace} ((P_j^* P_j + Q_j^* Q_j) R_{\epsilon,N}) ,$$

while

$$\begin{aligned}
& \operatorname{trace} ((P_j^* (\nabla V(x_j - x_k) - \nabla V(y_j - y_k)) + (\nabla V(x_j - x_k) - \nabla V(y_j - y_k)) P_j) R_{\epsilon,N}) \\
& \leq \operatorname{trace} (P_j^* P_j R_{\epsilon,N}) + \operatorname{trace} (|\nabla V(x_j - x_k) - \nabla V(y_j - y_k)|^2 R_{\epsilon,N}) .
\end{aligned}$$

Eventually

$$\begin{aligned}
& \frac{1}{\epsilon} \operatorname{trace} \left(i \left[\mathcal{H}_{\epsilon,N} \otimes I_{\mathfrak{H}_N} + I_{\mathfrak{H}_N} \otimes \mathcal{H}_{\epsilon,N}, \frac{1}{N} \sum_{j=1}^N (Q_j^* Q_j + P_j^* P_j) \right] R_{\epsilon,N} \right) \\
& \leq \operatorname{trace} \left(\frac{1}{N} \sum_{j=1}^N (P_j^* P_j + Q_j^* Q_j) R_{\epsilon,N} \right) + \operatorname{trace} \left(\frac{1}{N^2} \sum_{1 \leq j, k \leq N} P_j^* P_j R_{\epsilon,N} \right) \\
& \quad + \operatorname{trace} \left(\frac{1}{N^2} \sum_{1 \leq j, k \leq N} |\nabla V(x_j - x_k) - \nabla V(y_j - y_k)|^2 R_{\epsilon,N} \right) \\
& \leq 2D_{\epsilon,N} + \operatorname{Lip}(\nabla V)^2 \operatorname{trace} \left(\frac{1}{N^2} \sum_{1 \leq j, k \leq N} |(x_j - x_k) - (y_j - y_k)|^2 R_{\epsilon,N} \right) \\
& \leq 2D_{\epsilon,N} + \operatorname{Lip}(\nabla V)^2 \operatorname{trace} \left(\frac{2}{N^2} \sum_{1 \leq j, k \leq N} (|x_j - y_j|^2 + |x_k - y_k|^2) R_{\epsilon,N} \right) \\
& = 2D_{\epsilon,N} + \operatorname{Lip}(\nabla V)^2 \operatorname{trace} \left(\frac{4}{N} \sum_{l=1}^N |x_l - y_l|^2 R_{\epsilon,N} \right) \\
& \leq (2 + 4 \operatorname{Lip}(\nabla V)^2) D_{\epsilon,N} ,
\end{aligned}$$

so that

$$\begin{aligned} \frac{dD_{\epsilon,N}}{dt} &\leq (2 + 4 \text{Lip}(\nabla V)^2) D_{\epsilon,N} \\ &+ \frac{1}{\epsilon} \text{trace} \left(i \left[\mathbf{H}_{\epsilon,N}^{\rho_\epsilon} \otimes I_{\mathfrak{H}_N} - \mathcal{H}_{\epsilon,N} \otimes I_{\mathfrak{H}_N}, \frac{1}{N} \sum_{j=1}^N (Q_j^* Q_j + P_j^* P_j) \right] R_{\epsilon,N} \right). \end{aligned}$$

Next observe that

$$\begin{aligned} &\left[\mathbf{H}_{\epsilon,N}^{\rho_\epsilon} \otimes I_{\mathfrak{H}_N} - \mathcal{H}_{\epsilon,N} \otimes I_{\mathfrak{H}_N}, \frac{1}{N} \sum_{j=1}^N (Q_j^* Q_j + P_j^* P_j) \right] \\ &= \frac{1}{N} \sum_{j=1}^N [V_{\rho_\epsilon}(x_j), P_j^* P_j] - \frac{1}{N^2} \sum_{1 \leq k < l \leq N} [V(x_k - x_l), (P_k^* P_k + P_l^* P_l)] \\ &= \frac{1}{N} \sum_{j=1}^N ([V_{\rho_\epsilon}, P_j^*] P_j + P_j^* [V_{\rho_\epsilon}(x_j), P_j]) \\ &\quad - \frac{1}{N^2} \sum_{1 \leq k < l \leq N} ([V(x_k - x_l), P_k^*] P_k + P_k^* [V(x_k - x_l), P_k]) \\ &\quad - \frac{1}{N^2} \sum_{1 \leq k < l \leq N} ([V(x_k - x_l), P_l^*] P_l + P_l^* [V(x_k - x_l), P_l]) \\ &= \frac{1}{N} \sum_{j=1}^N ([V_{\rho_\epsilon}(x_j), P_j^*] P_j + P_j^* [V_{\rho_\epsilon}(x_j), P_j]) \\ &\quad - \frac{1}{N^2} \sum_{1 \leq k, l \leq N} ([V(x_k - x_l), P_k^*] P_k + P_k^* [V(x_k - x_l), P_k]). \end{aligned}$$

Moreover

$$[V_{\rho_\epsilon}(x_j), P_j^*] P_j + P_j^* [V_{\rho_\epsilon}(x_j), P_j] = i\epsilon(\nabla V_{\rho_\epsilon}(x_j) P_j + P_j^* \nabla V_{\rho_\epsilon}(x_j)),$$

while

$$\begin{aligned} &[V(x_k - x_l), P_k^*] P_k + P_k^* [V(x_k - x_l), P_k] \\ &= i\epsilon(\nabla V(x_k - x_l) P_k + P_k^* \nabla V(x_k - x_l)). \end{aligned}$$

Therefore

$$\begin{aligned}
& \frac{i}{\epsilon} \left[\mathbf{H}_{\epsilon,N}^{\rho_\epsilon} \otimes I_{\mathfrak{H}_N} - \mathcal{H}_{\epsilon,N} \otimes I_{\mathfrak{H}_N}, \frac{1}{N} \sum_{j=1}^N (Q_j^* Q_j + P_j^* P_j) \right] \\
&= -\frac{1}{N} \sum_{j=1}^N (\nabla V_{\rho_\epsilon}(x_j) P_j + P_j^* \nabla V_{\rho_\epsilon}(x_j)) \\
&+ \frac{1}{N^2} \sum_{1 \leq k, l \leq N} (\nabla V(x_k - x_l) P_k + P_k^* \nabla V(x_k - x_l)) \\
&= -\frac{1}{N} \sum_{j=1}^N \left(\nabla V_{\rho_\epsilon}(x_j) - \frac{1}{N} \sum_{k=1}^N \nabla V(x_j - x_k) \right) P_j \\
&- \frac{1}{N} \sum_{j=1}^N P_j^* \left(\nabla V_{\rho_\epsilon}(x_j) - \frac{1}{N} \sum_{k=1}^N \nabla V(x_j - x_k) \right).
\end{aligned}$$

Thus

$$\begin{aligned}
& \frac{1}{\epsilon} \text{trace} \left(i \left[\mathbf{H}_{\epsilon,N}^{\rho_\epsilon} \otimes I_{\mathfrak{H}_N} - \mathcal{H}_{\epsilon,N} \otimes I_{\mathfrak{H}_N}, \frac{1}{N} \sum_{j=1}^N (Q_j^* Q_j + P_j^* P_j) \right] R_{\epsilon,N} \right) \\
&= -\frac{1}{N} \sum_{j=1}^N \text{trace} \left(\left(\nabla V_{\rho_\epsilon}(x_j) - \frac{1}{N} \sum_{k=1}^N \nabla V(x_j - x_k) \right) P_j R_{\epsilon,N} \right) \\
&- \frac{1}{N} \sum_{j=1}^N \text{trace} \left(P_j^* \left(\nabla V_{\rho_\epsilon}(x_j) - \frac{1}{N} \sum_{k=1}^N \nabla V(x_j - x_k) \right) R_{\epsilon,N} \right) \\
&\leq \frac{1}{N} \sum_{j=1}^N \text{trace} \left(\left| \nabla V_{\rho_\epsilon}(x_j) - \frac{1}{N} \sum_{k=1}^N \nabla V(x_j - x_k) \right|^2 R_{\epsilon,N} \right) \\
&+ \frac{1}{N} \sum_{j=1}^N \text{trace} (P_j^* P_j R_{\epsilon,N}),
\end{aligned}$$

so that

$$\begin{aligned}
& \frac{1}{\epsilon} \text{trace} \left(i \left[\mathbf{H}_{\epsilon,N}^{\rho_\epsilon} \otimes I_{\mathfrak{H}_N} - \mathcal{H}_{\epsilon,N} \otimes I_{\mathfrak{H}_N}, \frac{1}{N} \sum_{j=1}^N (Q_j^* Q_j + P_j^* P_j) \right] R_{\epsilon,N} \right) \\
&\leq D_{\epsilon,N} + \frac{1}{N} \sum_{j=1}^N \text{trace} \left(\left| \nabla V_{\rho_\epsilon}(x_j) - \frac{1}{N} \sum_{k=1}^N \nabla V(x_j - x_k) \right|^2 R_{\epsilon,N} \right).
\end{aligned}$$

Therefore, the differential inequality satisfied by $D_{\epsilon,N}$ is recast as

$$\begin{aligned} \frac{dD_{\epsilon,N}}{dt} &\leq (3 + 4 \text{Lip}(\nabla V)^2) D_{\epsilon,N} \\ &\quad + \frac{1}{N} \sum_{j=1}^N \text{trace} \left(\left| \nabla V_{\rho_\epsilon}(x_j) - \frac{1}{N} \sum_{k=1}^N \nabla V(x_j - x_k) \right|^2 R_{\epsilon,N} \right) \\ &= (3 + 4 \text{Lip}(\nabla V)^2) D_{\epsilon,N} \\ &\quad + \frac{1}{N} \sum_{j=1}^N \text{trace} \left(\left| \nabla V_{\rho_\epsilon}(x_j) - \frac{1}{N} \sum_{k=1}^N \nabla V(x_j - x_k) \right|^2 \rho_\epsilon^{\otimes N} \right). \end{aligned}$$

The last inequality comes from the fact that the multiplication by

$$\left| \nabla V_{\rho_\epsilon}(x_j) - \frac{1}{N} \sum_{k=1}^N \nabla V(x_j - x_k) \right|^2$$

acts on the variables x_1, \dots, x_N only, and that the first marginal $R_{\epsilon,N,1}$ of $R_{\epsilon,N}$ is $\rho_\epsilon^{\otimes N}$ by Lemma 5.2.

Let us finally estimate the term

$$\frac{1}{N} \sum_{j=1}^N \text{trace} \left(\left| \nabla V_{\rho_\epsilon}(x_j) - \frac{1}{N} \sum_{k=1}^N \nabla V(x_j - x_k) \right|^2 \rho_\epsilon^{\otimes N} \right).$$

By a straightforward computation

$$\begin{aligned} &\text{trace} \left(\left| \nabla V_{\rho_\epsilon}(x_j) - \frac{1}{N} \sum_{k=1}^N \nabla V(x_j - x_k) \right|^2 \rho_\epsilon^{\otimes N} \right) \\ &= \int \left| \int \nabla V(x_j - x') \rho_\epsilon(t, x', x') dx' - \frac{1}{N} \sum_{k=1}^N \nabla V(x_j - x_k) \right|^2 \prod_{\ell=1}^N \rho_\epsilon(t, x_\ell, x_\ell) dX_N \\ &= \int \left| \int \nabla V(x_j - x') \rho_\epsilon(t, x', x') dx' - \int \nabla V(x_j - z) \mu_{X_N}(dz) \right|^2 \prod_{\ell=1}^N \rho_\epsilon(t, x_\ell, x_\ell) dX_N, \end{aligned}$$

where

$$\mu_{X_N} := \frac{1}{N} \sum_{k=1}^N \delta_{x_k}.$$

Since $V \in C_b^2(\mathbf{R}^d)$, one has

$$\begin{aligned} &\left| \int \nabla V(x_j - x') \rho(t, x', x') dx' - \int \nabla V(x_j - z) \mu_{X_N}(dz) \right|^2 \\ &\leq 2 \|\nabla V\|_{L^\infty} \text{Lip}(\nabla V) W_1(f_\epsilon(t), \mu_{X_N}), \end{aligned}$$

with

$$f_\epsilon(t, x) := \rho_\epsilon(t, x, x),$$

where ρ_ϵ is the solution of the Hartree equation (26). Since $\rho_\epsilon(t) \in \mathcal{D}(\mathfrak{H})$, then $f_\epsilon(t)$ is a probability density on \mathbf{R}^d for each $\epsilon > 0$ and each $t \geq 0$.

By Theorem 1 in [10] and Lemma 5.1 (with $p = 1$, $q = 2$ and $d \geq 3$), one has

$$\int W_1(f_\epsilon(t), \mu_{X_N}) \prod_{\ell=1}^N f_\epsilon(t, dx_\ell) \leq C_d M_2(t) N^{-1/d}, \quad \text{for } t \geq 0 \text{ and } 0 < \epsilon < 1,$$

with

$$M_2(t) := \sup_{0 < \epsilon < 1} (\text{trace}(|x|^2 \rho_\epsilon^{in}) + t e^t (\text{trace}(-\epsilon^2 \Delta \rho_\epsilon^{in}) + 2 \|V\|_{L^\infty})).$$

Therefore

$$\frac{dD_{\epsilon,N}}{dt}(t) \leq (3 + 4 \text{Lip}(\nabla V)^2) D_{\epsilon,N}(t) + C_d \|\nabla V\|_{L^\infty} \text{Lip}(\nabla V) M_2(t) N^{-1/d}.$$

By Gronwall's inequality, we conclude that

$$D_{\epsilon,N}(t) \leq \left(D_{\epsilon,N}(0) + C_d \|\nabla V\|_{L^\infty} \text{Lip}(\nabla V) M_2(t) N^{-1/d} \right) \exp((3 + 4 \text{Lip}(\nabla V)^2) t).$$

5.4. End of the proof. Let us denote by $R_{\epsilon,N}^{\mathbf{n}}$ the marginal density of $R_{\epsilon,N}$ corresponding to the n first particles. In other words, for each $A \in \mathcal{L}(\mathfrak{H}_{2n})$, we set

$$\text{trace}_{\mathfrak{H}_{2n}}(A R_{\epsilon,N}^{\mathbf{n}}) = \text{trace}_{\mathfrak{H}_{2N}}(S(A \otimes I_{\mathfrak{H}_{2(N-n)}}) S^* R_{\epsilon,N})$$

where

$$S\Psi(x_1, y_1, x_2, y_2, \dots, x_N, y_N) = \Psi(x_1, \dots, x_N, y_1, \dots, y_N).$$

We claim that

$$(32) \quad R_{\epsilon,N}^{\mathbf{n}} \in \mathcal{Q}(\rho_\epsilon^{\otimes n}, \rho_{\epsilon,N}^{\mathbf{n}}).$$

Indeed, for each $B \in \mathcal{L}(\mathfrak{H}_n)$, by Lemma 5.2, one has

$$\begin{aligned} \text{trace}_{\mathfrak{H}_{2n}}((B \otimes I_{\mathfrak{H}_n}) R_{\epsilon,N}^{\mathbf{n}}) &= \text{trace}_{\mathfrak{H}_{2N}}(S(B \otimes I_{\mathfrak{H}_n} \otimes I_{\mathfrak{H}_{2(N-n)}}) S^* R_{\epsilon,N}) \\ &= \text{trace}_{\mathfrak{H}_{2N}}((B \otimes I_{\mathfrak{H}_{N-n}}) \otimes I_{\mathfrak{H}_N}) R_{\epsilon,N}) \\ &= \text{trace}_{\mathfrak{H}_{2N}}((B \otimes I_{\mathfrak{H}_{N-n}}) R_{\epsilon,N,1}) \\ &= \text{trace}_{\mathfrak{H}_N}((B \otimes I_{\mathfrak{H}_{N-n}}) \rho_\epsilon^{\otimes N}) \\ &= \text{trace}_{\mathfrak{H}_n}(B \rho_\epsilon^{\otimes n}), \end{aligned}$$

while

$$\begin{aligned} \text{trace}_{\mathfrak{H}_{2n}}((I_{\mathfrak{H}_n} \otimes B) R_{\epsilon,N}^{\mathbf{n}}) &= \text{trace}_{\mathfrak{H}_{2N}}(S(I_{\mathfrak{H}_n} \otimes B \otimes I_{\mathfrak{H}_{2(N-n)}}) S^* R_{\epsilon,N}) \\ &= \text{trace}_{\mathfrak{H}_{2N}}(I_{\mathfrak{H}_N} \otimes (B \otimes I_{\mathfrak{H}_{N-n}}) R_{\epsilon,N}) \\ &= \text{trace}_{\mathfrak{H}_{2N}}((B \otimes I_{\mathfrak{H}_{N-n}}) R_{\epsilon,N,2}) \\ &= \text{trace}_{\mathfrak{H}_N}((B \otimes I_{\mathfrak{H}_{N-n}}) \rho_{\epsilon,N}) \\ &= \text{trace}_{\mathfrak{H}_n}(B \rho_{\epsilon,N}^{\mathbf{n}}). \end{aligned}$$

Observe further that, for each $j = 1, \dots, N$, one has

$$\begin{aligned} \text{trace}_{\mathfrak{H}_{2N}}((Q_j^* Q_j + P_j^* P_j) R_{\epsilon,N}) &= \text{trace}_{\mathfrak{H}_{2N}}(U_{\sigma_j}^* (Q_1^* Q_1 + P_1^* P_1) U_{\sigma_j} R_{\epsilon,N}) \\ &= \text{trace}_{\mathfrak{H}_{2N}}((Q_1^* Q_1 + P_1^* P_1) U_{\sigma_j} R_{\epsilon,N} U_{\sigma_j}^*) = \text{trace}_{\mathfrak{H}_{2N}}((Q_1^* Q_1 + P_1^* P_1) R_{\epsilon,N}), \end{aligned}$$

because of the identity (30) in Lemma 5.2. Hence, for each $N \geq n \geq 1$, each $\epsilon > 0$ and each $t \geq 0$, one has

$$\begin{aligned} D_{\epsilon,N}(t) &= \text{trace}_{\mathfrak{H}_{2N}}((Q_j^* Q_j + P_j^* P_j) R_{\epsilon,N}(t)) \quad \text{for each } j = 1, \dots, N, \\ &= \frac{1}{n} \text{trace}_{\mathfrak{H}_{2N}} \left(\sum_{j=1}^n (Q_j^* Q_j + P_j^* P_j) R_{\epsilon,N}(t) \right) \\ &= \frac{1}{n} \text{trace}_{\mathfrak{H}_{2n}} \left(\sum_{j=1}^n (Q_j^* Q_j + P_j^* P_j) R_{\epsilon,N}^n(t) \right). \end{aligned}$$

Because of (32), this implies that

$$D_{\epsilon,N}(t) \geq \frac{1}{n} M K_2^\epsilon(\rho_\epsilon(t)^{\otimes n}, \rho_{\epsilon,N}^n(t)),$$

for each $N \geq n \geq 1$, each $\epsilon > 0$ and each $t \geq 0$. In particular,

$$\begin{aligned} (33) \quad & M K_2^\epsilon(\rho_\epsilon(t)^{\otimes n}, \rho_{\epsilon,N}^n(t)) \\ & \leq n \text{trace}_{\mathfrak{H}_2}((Q_1^* Q_1 + P_1^* P_1) R_{\epsilon,N}^1(0)) \exp((3 + 4 \text{Lip}(\nabla V)^2) t) \\ & \quad + C_d \|\nabla V\|_{L^\infty} \text{Lip}(\nabla V) M_2(t) N^{-1/2} n \exp((3 + 4 \text{Lip}(\nabla V)^2) t). \end{aligned}$$

This inequality holds for each $R_{\epsilon,N}^{in}$ satisfying the symmetry (29).

At this point, we choose the initial coupling density $R_{\epsilon,N}^{in}$ as follows. Assume that $\rho_\epsilon^{in} = \text{OP}_\epsilon^T((2\pi\epsilon)^d \mu_\epsilon^{in})$ where $\mu_\epsilon^{in} \in \mathcal{P}_2(\mathbf{C}^d)$. Let $\pi_\epsilon^{in} \in \Pi(\mu_\epsilon^{in}, \mu_\epsilon^{in})$, and let

$$\pi_{\epsilon,N}^{in} = \mathbf{s} \# (\pi_\epsilon^{in})^{\otimes N}$$

where \mathbf{s} is the transformation defined by

$$\mathbf{s} : (\mathbf{C}^d)^{2N} \ni (u_1, v_1, \dots, u_N, v_N) \mapsto (u_1, \dots, u_N, v_1, \dots, v_N) \in (\mathbf{C}^d)^{2N}.$$

Hence

$$\pi_{\epsilon,N}^{in} \in \Pi((\rho_\epsilon^{in})^{\otimes N}, (\rho_\epsilon^{in})^{\otimes N}).$$

Set

$$R_{\epsilon,N}^{in} = \text{OP}_\epsilon^T((2\pi\epsilon)^{2dN} \pi_{\epsilon,N}^{in}),$$

so that

$$R_{\epsilon,N}^{in} \in \mathcal{Q}((\rho_\epsilon^{in})^{\otimes N}, (\rho_\epsilon^{in})^{\otimes N})$$

by Lemma 4.1.

Since

$$|(U_N, V_N), \epsilon\rangle \langle (U_N, V_N), \epsilon| = S |\mathbf{s}^{-1}(U_N, V_N), \epsilon\rangle \langle \mathbf{s}^{-1}(U_N, V_N), \epsilon| S^*$$

and

$$\begin{aligned} & |\mathbf{s}^{-1}(U_N, V_N), \epsilon\rangle \langle \mathbf{s}^{-1}(U_N, V_N), \epsilon| \\ &= |(u_1, v_1), \epsilon\rangle \langle (u_1, v_1), \epsilon| \otimes \dots \otimes |(u_N, v_N), \epsilon\rangle \langle (u_N, v_N), \epsilon|, \end{aligned}$$

one has

$$R_{\epsilon,N}^{in} = S \left(\int_{(\mathbf{C}^d)^2} |(u, v), \epsilon\rangle \langle (u, v), \epsilon| \pi_\epsilon^{in}(dudv) \right)^{\otimes N} S^*$$

and

$$(R_{\epsilon,N}^{in})^{\mathbf{1st}} = \int_{(\mathbf{C}^d)^2} |(u, v), \epsilon\rangle \langle (u, v), \epsilon| \pi_\epsilon^{in}(dudv) = \text{OP}_\epsilon^T((2\pi\epsilon)^{2d} \pi_\epsilon^{in}).$$

In particular $R_{\epsilon,N}^{in} \in \mathcal{Q}((\rho_\epsilon^{in})^{\otimes N}, (\rho_\epsilon^{in})^{\otimes N})$ satisfies symmetry assumption (29).

Taking the inf of both sides of the inequality (33) as π_ϵ^{in} runs through $\Pi(\mu_\epsilon^{in}, \mu_\epsilon^{in})$, one has

$$\begin{aligned} & MK_2^\epsilon(\rho_\epsilon(t)^{\otimes n}, \rho_{\epsilon,N}^n(t)) \\ & \leq n \inf_{\pi_\epsilon^{in} \in \Pi(\mu_\epsilon^{in}, \mu_\epsilon^{in})} \text{trace}_{\mathfrak{H}_2}((Q_1^* Q_1 + P_1^* P_1) \text{OP}_\epsilon^T((2\pi\epsilon)^{2d} \pi_\epsilon^{in})) \exp((3+4 \text{Lip}(\nabla V)^2) t) \\ & \quad + C_d \|\nabla V\|_{L^\infty} \text{Lip}(\nabla V) M_2(t) n N^{-1/2} \exp((3+4 \text{Lip}(\nabla V)^2) t) \\ & \quad = n (\text{dist}_{\text{MK},2}(\mu_\epsilon^{in}, \mu_\epsilon^{in})^2 + 2d\epsilon) \exp((3+4 \text{Lip}(\nabla V)^2) t) \\ & \quad + C_d \|\nabla V\|_{L^\infty} \text{Lip}(\nabla V) M_2(t) n N^{-1/2} \exp((3+4 \text{Lip}(\nabla V)^2) t) \end{aligned}$$

by Theorem 2.3 (2). Finally, the sought inequality follows from observing that $\text{dist}_{\text{MK},2}(\mu_\epsilon^{in}, \mu_\epsilon^{in}) = 0$.

APPENDIX A. TÖPLITZ OPERATORS, WIGNER AND HUSIMI TRANSFORMS

For each $z \in \mathbf{C}^d$ with $\Re(z) = q$ and $\Im(z) = p$, we denote by $|z, \epsilon\rangle$ the wave function (sometimes referred to as a “coherent state”) defined by the formula

$$(34) \quad |z, \epsilon\rangle(x) := (\pi\epsilon)^{-d/4} e^{-(x-q)^2/2\epsilon} e^{ip \cdot x/\epsilon}.$$

With the normalization above, denoting $\mathfrak{H} := L^2(\mathbf{R}^d)$, one has both

$$\langle z, \epsilon | z, \epsilon \rangle := \| |z, \epsilon\rangle \|_{\mathfrak{H}}^2 = \int_{\mathbf{R}^d} | |z, \epsilon\rangle(x) |^2 dx = 1,$$

and

$$(35) \quad \frac{1}{(2\pi\epsilon)^d} \int_{\mathbf{C}^d} |z, \epsilon\rangle \langle z, \epsilon| dz = I_{\mathfrak{H}},$$

where the integral on the left hand side is to be understood in the weak operator sense.

To each positive or finite Borel measure μ on \mathbf{C}^d , we define the Töplitz operator at scale ϵ with symbol μ by the formula

$$\text{OP}_\epsilon^T(\mu) := \frac{1}{(2\pi\epsilon)^d} \int_{\mathbf{C}^d} |z, \epsilon\rangle \langle z, \epsilon| \mu(dz).$$

This is a possibly unbounded operator on \mathfrak{H} , defined by duality by the formula

$$\begin{aligned} \langle u | \text{OP}_\epsilon^T(\mu) v \rangle_{\mathfrak{H}} &:= \frac{1}{(2\pi\epsilon)^d} \int \overline{u(x)} \text{OP}_\epsilon^T(\mu) v(x) dx \\ &= \frac{1}{(2\pi\epsilon)^d} \int_{\mathbf{C}^d} \langle v | z, \epsilon \rangle \langle z, \epsilon | u \rangle \mu(dz) \end{aligned}$$

for all $u, v \in \mathfrak{H}$ such that $z \mapsto \langle z, \epsilon | u \rangle$ and $z \mapsto \langle v | z, \epsilon \rangle$ belong to $L^2(\mathbf{C}^d, \mu)$.

If μ is a positive measure, then

$$(36) \quad \text{OP}_\epsilon^T(\mu) = \text{OP}_\epsilon^T(\mu)^* \geq 0, \quad \text{trace}(\text{OP}_\epsilon^T(\mu)) = \frac{1}{(2\pi\epsilon)^d} \int_{\mathbf{C}^d} \mu(dz).$$

If $f \in L^\infty(\mathbf{C}^d)$, then

$$\text{OP}_\epsilon^T(f) = \frac{1}{(2\pi\epsilon)^d} \int_{\mathbf{C}^d} |z, \epsilon\rangle \langle z, \epsilon| f(z) dz \in \mathcal{L}(\mathfrak{H}), \quad \text{with } \|\text{OP}_\epsilon^T(f)\| \leq \|f\|_{L^\infty}.$$

The following formulas are elementary but fundamental: if f is a quadratic form on \mathbf{R}^d , then

$$(37) \quad \begin{cases} \text{OP}_\epsilon^T(f(q)) = (f(x) + \frac{1}{4}\epsilon(\Delta f)I_{\mathfrak{H}}), \\ \text{OP}_\epsilon^T(f(p)) = (f(-i\epsilon\partial_x) + \frac{1}{4}\epsilon(\Delta f)I_{\mathfrak{H}}), \end{cases}$$

where $f(x)$ designates the unbounded operator defined on $L^2(\mathbf{R}^d)$ by the formula $(f(x)\phi)(x) = f(x)\phi(x)$.

Let A be an unbounded operator on $L^2(\mathbf{R}^d)$, and assume that its Schwartz kernel k_A belongs to $\mathcal{S}'(\mathbf{R}^d \times \mathbf{R}^d)$. In other words, A is the linear map from $\mathcal{S}(\mathbf{R}^d)$ to $\mathcal{S}'(\mathbf{R}^d)$ defined by the formula

$$\langle Au, v \rangle_{\mathcal{S}'(\mathbf{R}^d), \mathcal{S}(\mathbf{R}^d)} = \langle k_A, u \otimes v \rangle_{\mathcal{S}'(\mathbf{R}^d \times \mathbf{R}^d), \mathcal{S}(\mathbf{R}^d \times \mathbf{R}^d)}.$$

The Wigner transform of A at scale ϵ is defined as

$$(38) \quad W_\epsilon[A] := (2\pi)^{-d} \mathcal{F}_2(k_A \circ J_\epsilon), \quad \text{where } J_\epsilon(x, y) = (x + \frac{1}{2}\epsilon y, x - \frac{1}{2}\epsilon y)$$

and where \mathcal{F}_2 is the partial Fourier transform in the second variable. When $k_A \circ J_\epsilon$ is an integrable function, one has

$$W_\epsilon[A](x, \xi) = (2\pi\epsilon)^{-d} \int_{\mathbf{R}^d} e^{-i\xi \cdot y/\epsilon} k_A(x + \frac{1}{2}y, x - \frac{1}{2}y) dy.$$

In particular, for each $q, p \in \mathbf{R}^d$, one has

$$(39) \quad \begin{aligned} & W_\epsilon[|q + ip, \epsilon\rangle\langle q + ip, \epsilon|](x, \xi) \\ &= (2\pi\epsilon)^{-d} \int_{\mathbf{R}^d} (\pi\epsilon)^{-d/2} e^{-i\xi \cdot y/\epsilon} e^{ip \cdot y/\epsilon} e^{-(|x+y/2-q|^2 + |x-y/2-q|^2)/2\epsilon} dy \\ &= (\pi\epsilon)^{-d/2} e^{-|x-q|^2/\epsilon} (2\pi\epsilon)^{-d} \int_{\mathbf{R}^d} e^{i(p-\xi) \cdot y/\epsilon} e^{-|y|^2/4\epsilon} dy \\ &= (\pi\epsilon)^{-d} e^{-(|x-q|^2 + |\xi-p|^2)/\epsilon}, \end{aligned}$$

since

$$\int_{\mathbf{R}^d} (\epsilon/4\pi)^{d/2} e^{-iy \cdot (\xi-p)} e^{-\epsilon y^2/4} e^{-(x-q)^2/\epsilon} dy = e^{-(\xi-p)^2/\epsilon}$$

(which is the classical formula for the Fourier transform of a Gaussian density). Thus, for each positive or finite Borel measure on $\mathbf{R}^d \times \mathbf{R}^d$, one has

$$(40) \quad W_\epsilon[\text{OP}_\epsilon^T(\mu)] = \frac{1}{(2\pi\epsilon)^d} G_{\epsilon/2}^{2d} \star \mu,$$

where G_a^n is the centered Gaussian density on \mathbf{R}^n with covariance matrix aI . With $\mu(dqdp) = dqdp$, or $\mu(dqdp) = f(q)dqdp$, or $\mu(dqdp) = f(p)dqdp$, where f is an arbitrary quadratic form on \mathbf{R}^d , one finds that

$$(41) \quad \begin{cases} W_\epsilon[I_{\mathfrak{H}}](x, \xi) = (2\pi\epsilon)^{-d}, \\ W_\epsilon[f(x)](x, \xi) = (2\pi\epsilon)^{-d} f(x), \\ W_\epsilon[f(-i\epsilon\partial_x)](x, \xi) = (2\pi\epsilon)^{-d} f(\xi). \end{cases}$$

Indeed, when $\mu(dqdp) = g(q, p)dqdp$ with g a polynomial with degree at most m , one has

$$(42) \quad G_{\epsilon/2}^{2d} \star_{x, \xi} g = e^{\epsilon \Delta_{x, \xi}/4} g = \sum_{0 \leq n \leq m/2} \frac{\epsilon^n}{4^n n!} \Delta_{x, \xi}^n g.$$

Thus, for g of degree ≤ 2 , one finds that $G_{\epsilon/2}^{2d} \star_{x,\xi} g = (1 + \frac{1}{4}\epsilon \Delta_{x,\xi})g$. Together with (35) and (37), this formula justifies (41).

The Husimi transform of an operator A at scale ϵ is defined in terms of the Wigner transform of A by the formula

$$\tilde{W}_\epsilon[A] := G_{\epsilon/2}^{2d} \star_{x,\xi} W_\epsilon[A].$$

Let $R \in \mathcal{D}(\mathfrak{H})$; for each $\psi \in L^2(\mathbf{R}^d)$, one has

$$\text{trace}(|\psi\rangle\langle\psi|R) = (2\pi\epsilon)^d \iint \overline{W_\epsilon[\psi](x,\xi)} W_\epsilon[R](x,\xi) dx d\xi$$

by the definition (38) of the Wigner transform, and Plancherel's identity. Specializing this formula to $\psi = |z, \epsilon\rangle$, one finds that

$$\begin{aligned} \text{trace}(|z, \epsilon\rangle\langle z, \epsilon|R) &= \langle z, \epsilon | R | z, \epsilon \rangle \\ &= (2\pi\epsilon)^d \tilde{W}_\epsilon[R](q, p), \quad \text{where } q = \Re(z) \text{ and } p = \Im(z). \end{aligned}$$

More generally, if μ is a positive or finite Borel measure on \mathbf{C}^d , one deduces from the previous identity and the Fubini theorem that

$$(43) \quad \text{trace}(\text{OP}_\epsilon^T(\mu)R) = \int_{\mathbf{C}^d} \tilde{W}_\epsilon[R](z) \mu(dz).$$

(The previous formula is the particular case where $\mu = (2\pi\epsilon)^d \delta_z$.)

In particular, if $R = \text{OP}_\epsilon^T((2\pi\epsilon)^d \pi)$ with $\pi \in \mathcal{P}_2(\mathbf{R}^d \times \mathbf{R}^d)$, for each quadratic form f on \mathbf{R}^d , one has

$$(44) \quad \begin{aligned} &\text{trace}((f(x) + f(-i\epsilon\partial_x)) \text{OP}_\epsilon^T((2\pi\epsilon)^d \pi)) \\ &= \iint_{\mathbf{R}^d \times \mathbf{R}^d} (f(q) + f(p)) \pi(dq dp) + \frac{1}{2}\epsilon \Delta f. \end{aligned}$$

Indeed, applying (43) shows that

$$\begin{aligned} &\text{trace}((f(x) + f(-i\epsilon\partial_x)) \text{OP}_\epsilon^T((2\pi\epsilon)^d \pi)) \\ &= \text{trace}(\text{OP}_\epsilon^T(f(q) + f(p) - \frac{1}{2}\epsilon(\Delta f)) \text{OP}_\epsilon^T((2\pi\epsilon)^d \pi)) \\ &= \iint_{\mathbf{R}^d \times \mathbf{R}^d} (G_{\epsilon/2}^{2d} \star W_\epsilon[\text{OP}_\epsilon^T((2\pi\epsilon)^d \pi)])(q, p) (f(q) + f(p) - \frac{1}{2}\epsilon(\Delta f)) dq dp \\ &= \iint_{\mathbf{R}^d \times \mathbf{R}^d} W_\epsilon[\text{OP}_\epsilon^T((2\pi\epsilon)^d \pi)](q, p) (G_{\epsilon/2}^{2d} \star (f(q) + f(p) - \frac{1}{2}\epsilon(\Delta f))) dq dp \\ &= \iint_{\mathbf{R}^d \times \mathbf{R}^d} (G_{\epsilon/2}^{2d} \star G_{\epsilon/2}^{2d} \star (f(q) + f(p) - \frac{1}{2}\epsilon(\Delta f))) \pi(dq dp), \end{aligned}$$

where the last equality follows from (40). We conclude by observing that

$$\begin{aligned} G_{\epsilon/2}^{2d} \star G_{\epsilon/2}^{2d} \star (f(q) + f(p) - \frac{1}{2}\epsilon(\Delta f)) &= e^{\epsilon \Delta_{q,p}/2} (f(q) + f(p) - \frac{1}{2}\epsilon(\Delta f)) \\ &= (f(q) + f(p) + \frac{1}{2}\epsilon(\Delta f)) \end{aligned}$$

according to (42).

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