Strong semiclassical limit from Hartree and Hartree-Fock to Vlasov-Poisson equation

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STRONG SEMICLASSICAL LIMIT FROM HARTREE AND HARTREE-FOCK TO VLASOV-POISSON EQUATION

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ABSTRACT. In this paper we consider the semiclassical limit from the Hartree to the Vlasov equation with general singular interaction potential including the Coulomb and gravitational interactions, and we prove explicit bounds in the strong topologies of Schatten norms. Moreover, in the case of Fermions, we provide estimates on the size of the exchange term in the Hartree-Fock equation and also obtain a rate of convergence for the semiclassical limit from the Hartree-Fock to the Vlasov equation in Schatten norms. Our results hold for general initial data in some Sobolev space and are global in time.

Keywords: Hartree equation, Hartree-Fock equation, Vlasov equation, Coulomb interaction, gravitational interaction, semiclassical limit.

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1. Introduction

The problem of deriving the Vlasov equation, a kinetic equation describing the time evolution of the probability density of particles in interaction, such as particles in a plasma or in a galaxy, from the dynamics of N quantum interacting particles in a joint mean-field and semiclassical approximation is a classical question in mathematical physics and the first rigorous results were obtained in the '80s (Cf. [49, 63]).

The Vlasov equation is a nonlinear transport equation for the probability density $f: \mathbb{R}_+ \times \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$

(1)
$$\partial_t f + \xi \cdot \nabla_x f + E \cdot \nabla_{\xi} f = 0,$$

with $E := -\nabla K * \rho_f$ the self induced mean-field force field created by the pair interaction potential $K : \mathbb{R}^d \to \mathbb{R}$ through the formula

$$-(\nabla K * \rho_f)(t, x) = -\int_{\mathbb{R}^d} \nabla K(x - y) \,\rho_f(t, y) \,\mathrm{d}y,$$

where ρ_f is the spatial density associated to f, namely

$$\rho_f(t,x) = \int_{\mathbb{D}^d} f(t,x,\xi) \,\mathrm{d}\xi.$$

When K is the Green function, Equation (1) is called the Vlasov-Poisson system, because K can be obtained as a solution to the Poisson equation $-\Delta K = \rho_f$, thus linking the Vlasov equation to the Poisson one. In dimension 3, it corresponds to the case of the Coulomb potential

$$K(x) = \frac{1}{2\pi |x|},$$

but we will consider more general attractive and repulsive potentials.

The well-posedness of the Vlasov equation (1) is due to Dobrushin [19] for smooth interaction potentials $K \in C_c^2(\mathbb{R}^d)$. Concerning singular interactions, the case of Coulomb and gravitational potentials have been tackled first in [38] and [64], respectively for d=1 and d=2. In d=3, the well-posedness for small data has been proven in [6] and later extended to general initial data by Pfaffelmoser [55] and by Lions and Perthame [44]. In recent years improvements on the conditions of propagation of momenta and on the uniqueness condition have been addressed in [50, 51, 18, 45, 47, 36]. In this paper we will closely refer to the Lions and Perthame paper [44], that is the one that better adapt to the comparison with the quantum dynamics because of its Eulerian viewpoint.

The Vlasov equation (1) is supposed to emerge as a joint mean-field and semiclassical limit from the dynamics of N interacting quantum particles. This has been first proven in [49, 63], respectively for analytic and C^2 interaction potentials, using the BBGKY approach in the fermionic setting. The case of Bosons has been studied in [33], in the mean-field limit combined with a semiclassical limit, through the analysis of the dynamics of factored WKB states.

It is well known that the many-body dynamics can be approximated in the mean-field limit by the Hartree equation

(2)
$$i\hbar \,\partial_t \boldsymbol{\rho} = [H, \boldsymbol{\rho}],$$

an evolution equation for the one-particle density matrix ρ on the one-particle space $L^2(\mathbb{R}^d)$, with $\text{Tr}(\rho) = 1$. In Equation (2), $\hbar := \frac{h}{2\pi}$ is h the Planck constant, and H

is the Hamiltonian

$$(3) H = -\frac{\hbar^2}{2} \Delta + K * \rho,$$

where Δ is the Laplace operator, K is the two-body interaction potential and $\rho(x) = \rho(x,x)$ the diagonal of the kernel of the operator ρ . The mathematical literature on this subject is rather extensive. See for example [8, 21, 7, 24, 58, 34, 56, 17, 39, 29, 48, 30, 32, 31, 16] for the case of Bosons and [20, 23, 12, 10, 5, 53, 57, 52, 59] for the case of Fermions. We recall that the interest in the mean-field regime is due to the fact that many systems of interest in quantum mechanics are usually made of N particles, where the number of particles N typically ranges between 10^2 and 10^{23} .

In the case of Fermions, a more precise mean-field approximation for the manybody quantum dynamics is given by the Hartree-Fock equation

$$i\hbar \,\partial_t \boldsymbol{\rho} = [H_{HF}, \boldsymbol{\rho}],$$

with $H_{HF} = -\hbar^2 \Delta + K * \rho - X$, where X is the so called exchange term defined as the operator of kernel

(5)
$$X(x,y) = K(x-y) \rho(x,y),$$

in contrast with the direct term $K * \rho$.

The Hartree and Hartree-Fock equations are quantum models. It is therefore natural to investigate their semiclassical limit as $\hbar \to 0$. First results in this direction provide the convergence from the Hartree dynamics towards the Vlasov equation in abstract sense, without rate of convergence and in weak topologies, but including the case of singular interaction potentials, such as the Coulomb one (Cf. [43, 46, 25, 22]). Explicit bounds on the convergence rate in stronger topologies have been established in [54, 4, 1, 2, 11, 30]. They all deal with smooth interaction potentials. More recently, the case of singular interactions, including the Coulomb potential, has been considered in [41, 40], where the convergence from the Hartree to the Vlasov equation is achieved in weak topology using quantum Wasserstein-Monge-Kantorovich distance, providing explicit bounds on the convergence rate. In strong topology (trace norm and Hilbert-Schmidt norm) explicit bounds on the convergence from the Hartree dynamics to the Vlasov equation with inverse power law of the form $K(x) = |x|^{-a}$ with $a \in (0, 1/2)$ have been proven in [61], and a proof that includes the Coulomb potential has been provided in [60] but under restrictive assumptions on the initial data.

The aim of this paper is to establish a strong convergence result from both the Hartree and the Hartree-Fock equations towards the Vlasov dynamics for a large class of regular initial states. Our results apply to a wide class of initial data at positive temperature, thus giving a thorough answer to the question of strong convergence of the Hartree equation to the Vlasov system for singular interactions in the case of mixed states (i.e. states that are relevant at positive temperature).

With respect to the results present in literature, there are several novelties: apart from the large class of initial data for whose evolution we can establish strong convergence with explicit rate towards the Vlasov equation, our techniques allow to consider inverse power law potentials that are more singular than Coulomb and our methods easily extend to very general non radially symmetric potentials. Moreover, the topology we consider is not only the one induced by the trace or Hilbert-Schmidt norm (as it is for instance in [61]), but the ones induced by semiclassical Schatten

norms \mathcal{L}^p , for all $p \in [1, \infty)$. These are obtained by a refinement on the estimate for the \mathcal{L}^p norms of the commutator $[K(\cdot - z), \rho]$ and a careful analysis of the propagation in time of initial conditions leading to bound the quantity

$$\left\|\operatorname{diag}\left|\left[\frac{x}{i\hbar}, oldsymbol{
ho}\right]\right|\right\|_{L^p(\mathbb{R}^d)}$$

uniformly in \hbar , for p > 3. This requires using kinetic interpolation inequalities as in [41] and an extension of the Calderón-Vaillancourt theorem for Weyl operators.

Finally, we extend our results to the Hartree-Fock equation (4), thus proving the strong convergence of the Hartree-Fock dynamics to the Vlasov one. As a corollary, we get explicit estimates on the difference between the Hartree and Hartree-Fock dynamics in Schatten norms, thus giving a rigorous proof of the fact that the exchange term in the Hartree-Fock dynamics is subleading with respect to the direct one also when the interaction potential is singular (this was proved in [12] in the case of smooth potentials).

Notice that the Hartree equation can be seen as a mean-field limit in both the bosonic and the fermionic setting, the difference being that in the fermionic setting, the anti-symmetry of the N-particles wave functions forces the number of particles N and the semiclassical parameter \hbar to satisfy

(6)
$$h \le N^{-1/d} \|f_{\hbar}\|_{L^{2}(\mathbb{R}^{2d})}^{-2/d}$$

where f_{\hbar} is the Wigner transform of the normalized one particle marginal of the N-body density operator solving the N-body Schrödinger equation. Notice that, because of Inequality (6), the explicit bounds on the convergence rates given by our results also provide information on the accuracy of the semiclassical approximation in terms of the number of particles.

Despite our results give a good answer to the problem of the semiclassical limit from the Hartree and Hartree-Fock equations to the Vlasov one with general singular potentials in the context of positive temperature states, a certain number of questions related to the derivation of the Vlasov equation from quantum dynamics remain open:

- i) The mean-field limit from a system of N quantum particles interacting through a singular potential in the case of mixed states. Up to our knowledge, this problem is open in both the bosonic and the fermionic setting.
- ii) In the bosonic setting, where N and \hbar are independent parameters, the joint mean-field and semiclassical limit is an open problem when the interaction is singular. Namely, no uniform convergence in the semiclassical parameter \hbar has been proven so far.
- iii) We believe our results give optimal bounds on the convergence rate in trace norm \mathcal{L}^1 . The question whether the bounds we obtain for the semiclassical Hilbert-Schmidt norm \mathcal{L}^2 , and thus the L^2 convergence for the associated Wigner functions, are optimal is open. The exact same question can be asked for the bounds in Theorem 3 about the convergence of the Hartree-Fock equation to the Vlasov one. In both cases, we believe the bounds we get are not optimal and there is room for improvements.

The paper is structured as follows: in Subsections 1.1 and 1.2 we state our main results and introduce the notations we will use throughout the paper; in Section 2 we explain our strategy by making a comparison with the classical Vlasov dynamics and find a new (up to our knowledge) stability estimate for the Vlasov

system; Section 3 contains the main results concerning the regularity of the Weyl transform of a solution to the Vlasov equation, that will be crucial to prove the theorems stated in the subsection 1.1; Sections 4 is devoted to prove Theorem 1 and Theorem 2 respectively; in Section 5 we present the proof of Theorem 3, based on estimates on the exchange term. Two Appendices on the propagation of regularity for the Vlasov equation and on basic operators identity complement the paper.

1.1. Main results.

1.1.1. Operators and function spaces. We denote by $L^p = L^p(\mathbb{R}^d)$ the classical Lebesgue spaces, by $L^{p,q} = L^{p,q}(\mathbb{R}^d)$ the classical Lorentz spaces for $(p,q) \in [1,\infty]^2$ (see for example [13]) and we define the space of positive and trace class operators by

$$\mathcal{L}^1_+ := \{ \boldsymbol{\rho} \in \mathcal{L}(L^2), \boldsymbol{\rho} = \boldsymbol{\rho}^* \ge 0, \operatorname{Tr}(\boldsymbol{\rho}) < \infty \},$$

where $\mathcal{L}(L^2)$ denotes the space of linear operators on L^2 , and the quantum Lebesgue norms (or semiclassical Schatten norms) \mathcal{L}^p by

$$\|\boldsymbol{\rho}\|_{\mathcal{L}^p} := h^{-d/p'} \|\boldsymbol{\rho}\|_p = h^{-d/p'} \left(\operatorname{Tr}(|\boldsymbol{\rho}|^p) \right)^{\frac{1}{p}}.$$

where $\|\boldsymbol{\rho}\|_p$ denotes the usual Schatten norm (i.e. without dependency in h).

In this work, we consider the semiclassical limit to solutions of the Vlasov equation with regular data in the sense that the initial condition will be bounded in some weighted Sobolev space. Therefore, we will use the following notation for smooth polynomial weight functions

$$\langle y \rangle = \sqrt{1 + |y|^2},$$

and for $\sigma \in \mathbb{N}$, we define the spaces $W_k^{\sigma,p}(\mathbb{R}^{2d})$ as the spaces equipped with the norm

$$||f||_{W_k^{\sigma,p}(\mathbb{R}^{2d})} = \left\| \langle z \rangle^k f(z) \right\|_{L^p(\mathbb{R}^{2d})} + \left\| \langle z \rangle^k \nabla_z^{\sigma} f(z) \right\|_{L^p(\mathbb{R}^{2d})},$$

where $z=(x,\xi)$ so that $\langle z\rangle^2=1+|x|^2+|\xi|^2$. We also use the standard notations in the cases $\sigma=0$ or p=2

$$\begin{split} L_k^p(\mathbb{R}^{2d}) &:= W_k^{0,p}(\mathbb{R}^{2d}) \\ H_k^\sigma(\mathbb{R}^{2d}) &:= W_k^{\sigma,2}(\mathbb{R}^{2d}). \end{split}$$

1.1.2. Wigner and Weyl transforms. We can associate to each density operator ρ a function of the phase space called the Wigner transform and which is defined (for h = 1) by

$$w_{\rho}(x,\xi) := \int_{\mathbb{R}^d} e^{-2i\pi y \cdot \xi} \rho\left(x + \frac{y}{2}, x - \frac{y}{2}\right) dy = \mathcal{F}(\tilde{\rho}_x)(\xi),$$

where $\tilde{\rho}_x(y) = \rho(x+y/2, x-y/2)$ and we used the following convention for the Fourier transform

$$\mathcal{F}(u)\left(\xi\right) := \int_{\mathbb{R}^d} e^{-2i\pi x \cdot \xi} u(x) \, \mathrm{d}x.$$

This function of the phase space is however not a probability distribution since it is generally not non-negative. We refer to [43] for more properties of the Wigner transform. Given ρ , we will write its semiclassical Wigner transform

$$w_{\hbar}(\boldsymbol{\rho})(x,\xi) = \frac{1}{h^d} w_{\boldsymbol{\rho}} \left(x, \frac{\xi}{h} \right).$$

Conversely, to each function of the phase space, we can associate an operator through the Weyl transformation, which is the inverse of the Wigner transform. It is defined as the operator such that for any $\varphi \in C_c^{\infty}$

$$\rho_{\hbar}^{W}(g) \varphi := \iint_{\mathbb{R}^{2d}} g\left(\frac{x+y}{2}, \xi\right) e^{-i(y-x)\cdot\xi/\hbar} \varphi(y) \,\mathrm{d}y \,\mathrm{d}\xi.$$

1.1.3. Theorems. Our main result is the following.

Theorem 1. Let $d \in \{2,3\}$, $a \in (\max\{\frac{d}{2}-2,-1\},d-2]$ and suppose K is given by one of the following expressions

(7)
$$K(x) = \frac{\pm 1}{|x|^a} \text{ or } K(x) = \pm \ln(|x|).$$

In the second case we set a := 0. Let $f \ge 0$ be a solution of the Vlasov equation (1) and $\rho \ge 0$ be a solution of the Hartree equation (2) with respective initial conditions

(8)
$$f^{\text{in}} \in W_m^{\sigma+1,\infty}(\mathbb{R}^{2d}) \cap H_{\sigma}^{\sigma+1}(\mathbb{R}^{2d})$$

(9)
$$\boldsymbol{\rho}^{\mathrm{in}} \in \mathcal{L}^1$$

where $(m,\sigma) \in (4\mathbb{N}) \times (2\mathbb{N})$ verify m > d and $\sigma > m + \frac{d}{\mathfrak{b}-1}$ with $\mathfrak{b} = \frac{d}{a+1}$. If $a \leq 0$, we also require $\operatorname{Tr}((|x|^2 - \hbar^2 \Delta) \, \boldsymbol{\rho}^{\mathrm{in}})$ to be bounded. Then, there exists $\lambda_f(t) \in C^0(\mathbb{R}_+, \mathbb{R}_+)$ and $C_f(t) \in C^0(\mathbb{R}_+, \mathbb{R}_+)$ depending only on d, a and on the initial condition of the solution of the Vlasov equation such that

(10)
$$\operatorname{Tr}(|\boldsymbol{\rho} - \boldsymbol{\rho}_f|) \le (\operatorname{Tr}(|\boldsymbol{\rho}^{\text{in}} - \boldsymbol{\rho}_f^{\text{in}}|) + C_f(t)\,\hbar)\,e^{\lambda_f(t)}$$

where $\rho_f = \rho_h^W(f)$. An upper bound for the expression of the functions λ_f and C_f is given by

$$\lambda_f(t) \le C_{d,a} \int_0^t \|\nabla_{\xi} f\|_{W^{n_0,\infty}(\mathbb{R}^{2d}) \cap H^{\sigma}_{\sigma}(\mathbb{R}^{2d})} \, \mathrm{d}s$$

$$C_f(t) \le C_{d,a} \int_0^t \|\rho_f(s)\|_{L^1 \cap H^{\nu}} \|\nabla_{\xi}^2 f(s)\|_{H^m_m(\mathbb{R}^{2d})} e^{-\lambda_f(s)} \, \mathrm{d}s,$$

which remain bounded at any time $t \ge 0$, and where $\nu = \left(\frac{m}{2} + a + 2 - d\right)_+$ and $n_0 = \lfloor d/2 \rfloor + 1$.

Remark 1.1. Condition (7) includes in particular the Coulomb or Newton potential in dimensions d=3 and d=2. In these cases, the conditions of regularity (8) of the initial data of the Vlasov equation become $f^{\text{in}} \in W_4^{13,\infty}(\mathbb{R}^{2d}) \cap H_{12}^{13}(\mathbb{R}^{2d})$ when d=3 and a=1, and $f^{\text{in}} \in W_4^{9,\infty}(\mathbb{R}^{2d}) \cap H_8^9(\mathbb{R}^{2d})$ when d=2 and a=0. These conditions are of course not optimal: for example the fact that we ask for m/2 and σ to be even numbers is mostly to simplify some computations.

Remark 1.2. To see more explicitly that Inequality (10) gives a good semiclassical approximation estimate, one can take $\rho^{in} = \rho_f^{in}$ and fix some T > 0, which yields for any $t \in [0,T]$

(11)
$$\operatorname{Tr}(|\boldsymbol{\rho} - \boldsymbol{\rho}_f|) \lesssim C_T \,\hbar,$$

for some constant $C_T > 0$. In this case, since ρ_f^{in} has to be regular in the sense that it is the Weyl transform of a regular classical phase space distribution, then $\rho^{\text{in}} = \rho_f^{\text{in}}$ implies that ρ^{in} also has to be regular. However remark that Inequality (10) is actually stronger since it is telling that the initial condition of the Hartree equation

does not need to be regular but just initially close to some regular density matrix. In particular, taking ρ^{in} and ρ^{in}_f such that $\text{Tr}\left(\left|\rho^{\text{in}}-\rho^{\text{in}}_f\right|\right) \leq C\hbar$ also implies the simplified Inequality (11).

Remark 1.3. Observe that Theorem 1 implies the convergence of the spatial density of particles $\rho \to \rho_f$ in L^1 . Indeed, by duality we have

(12)
$$\|\rho - \rho_f\|_{L^1} = \sup_{\substack{O \in L^{\infty}(\mathbb{R}^d) \\ \|O\|_{L^{\infty}} \le 1}} \left| \int O(x) \left(\rho(x) - \rho_f(x) \right) dx \right| \le \operatorname{Tr} \left(\left| \boldsymbol{\rho} - \boldsymbol{\rho}_f \right| \right) ,$$

since every bounded function $x \mapsto O(x)$ also defines a multiplication operator with operator norm $\|O\|_{L^{\infty}}$.

Remark 1.4. Our assumptions on the solution of the Hartree equation imply the global well-posedness of solutions as proved in [15] where the trace norm corresponds to the $L^2(\lambda)$ norm (see also [26, 27, 43]). Even if these assumptions are weak, remark however that the operator ρ^{in} has to be at a finite trace norm distance of the operator ρ^{in} which by construction is bounded in higher Sobolev spaces (as can be deduced from Proposition 3.2). The additional moment bound when $a \leq 0$ ensures that the energy is finite, which allows to propagate the space moments (see e.g. [41, Remark 3.1]). This is sufficient to give a meaning to the pair interaction potential which is growing at infinity in this case.

From the bound in Theorem 1 we also obtain estimates in other semiclassical Lebesgue spaces.

Theorem 2. Take the same assumptions and notations as in Theorem 1, define $\mathfrak{b} = \frac{d}{a+1}$ and assume moreover that

$$f^{\mathrm{in}} \in W^{\sigma+1,\infty}_{\sigma}(\mathbb{R}^{2d}) \cap H^{\sigma+1}_{\sigma}(\mathbb{R}^{2d})$$

and that $\sigma > n_0 + \frac{d}{\mathfrak{b}}$. Then for any $p \in [1, \mathfrak{b})$ it holds

(13)
$$\|\boldsymbol{\rho} - \boldsymbol{\rho}_f\|_{\mathcal{L}_p} \le \|\boldsymbol{\rho}^{\text{in}} - \boldsymbol{\rho}_f^{\text{in}}\|_{\mathcal{L}_p} + \left(\text{Tr}\left(\left|\boldsymbol{\rho}^{\text{in}} - \boldsymbol{\rho}_f^{\text{in}}\right|\right) + c(t)\hbar\right)e^{\lambda(t)},$$

where c and λ are continuous functions on \mathbb{R}_+ depending on d, a, p and f^{in} . For any $q \in [\mathfrak{b}, \infty)$, assuming also that $\boldsymbol{\rho}^{\mathrm{in}} \in \mathcal{L}^{\infty}$, this leads to the following estimate

(14)
$$\|\boldsymbol{\rho} - \boldsymbol{\rho}_f\|_{\mathcal{L}^q} \le c_2(t) \left(\|\boldsymbol{\rho}^{\text{in}} - \boldsymbol{\rho}_f^{\text{in}}\|_{\mathcal{L}^p}^{\frac{p}{q}} + \text{Tr}\left(|\boldsymbol{\rho}^{\text{in}} - \boldsymbol{\rho}_f^{\text{in}}| \right)^{\frac{p}{q}} + \hbar^{\frac{p}{q}} \right) e^{\frac{p}{q}\lambda(t)},$$

where $\rho_f = \rho_{\hbar}^W(f)$ and $c_2 \in C^0(\mathbb{R}_+, \mathbb{R}_+)$ can also be computed explicitly and depends on the initial conditions.

Remark 1.5. In particular, if we assume $ho^{\rm in}=
ho^{\rm in}_{\rm f}$, or more generally

$$\operatorname{Tr}(\left| \boldsymbol{\rho}^{\operatorname{in}} - \boldsymbol{\rho}_f^{\operatorname{in}} \right|) \leq C\hbar \quad and \quad \left\| \boldsymbol{\rho}^{\operatorname{in}} - \boldsymbol{\rho}_f^{\operatorname{in}} \right\|_{\mathcal{L}^2} \leq C\hbar,$$

then we have a rate $\hbar^{\mathfrak{b}/2-\varepsilon}$ with $\varepsilon>0$ as small as we want, that for the Coulomb potential in dimension d=3 reads

$$\|f_{\boldsymbol{\rho}} - f\|_{L^2(\mathbb{R}^{2d})} = \|\boldsymbol{\rho} - \boldsymbol{\rho}_f\|_{\mathcal{L}^2} \le C_T \, \hbar^{3/4 - \varepsilon}$$

where $f_{\rho} = w_{\hbar}(\rho)$ is the Wigner transform of ρ and for any $t \in [0,T]$ for some fixed T > 0. Remark that Theorem 1 does not imply convergence of the operators, but is only a quantitative estimate, where both ρ and $\rho_{\hbar}^{W}(f)$ depend on \hbar , whereas

the above equation is both a quantitative estimate and a convergence result since it implies the **convergence of** f_{ρ} **to** f **in** $L^{\infty}_{loc}(\mathbb{R}_+, L^2(\mathbb{R}^{2d}))$.

With the same assumptions, in the case when d=2, then the Coulomb kernel is of the form $K(x)=C\ln(|x|)$, and $\mathfrak{b}=2$, implying that Inequality (13) holds for any $p\in[1,2)$ and that we almost get the conjectured optimal rate of convergence for p=2

$$||f_{\rho} - f||_{L^{2}(\mathbb{R}^{2d})} \le C_{T} \, \hbar^{1-\varepsilon}.$$

Remark 1.6. All our results generalize to more general non-radial pair interactions. For $s \in (0,d)$, define the weak Sobolev space $\dot{H}_w^{\sigma,1}$ as the completion of C_c^{∞} with respect to the norm

$$||u||_{\dot{H}^{s,1}} := ||\Delta^{\frac{s}{2}}u||_{\mathrm{TV}},$$

where $\|\cdot\|_{TV}$ denotes the total variation norm over the space \mathcal{M} of bounded measures. By the formula of the inverse of the powers of Laplacian, we deduce that it is the space of functions that can be written

(15)
$$u(x) = \int_{\mathbb{R}^d} \frac{1}{|x - w|^{d-s}} \, \mu(\mathrm{d}w),$$

for some measure $\mu \in \mathcal{M}$. Remark that this space contains the interaction kernel

$$K(x) = \frac{1}{|x|^a} \text{ with } a = d - s,$$

when a > 0, which follows by taking $\mu = \delta_0$. In particular, the Coulomb potential in dimension d = 3 verifies

$$\frac{1}{|x|} \in \dot{H}_w^{2,1}.$$

However, this space contains also more general potentials. It contains for example the Sobolev space $\dot{H}^{s,1} = \dot{F}^s_{2,1}$ which is defined by the norm $\left\|\Delta^{\frac{s}{2}}u\right\|_{L^1}$. When $n \in \mathbb{N}$, then $\dot{H}^{n,1} = \dot{W}^{n,1}$ is a classical homogeneous Sobolev space.

Let us sketch briefly how one should adapt the proofs to obtain the results in these spaces. The key point in which we heavily use the explicit form of the potential is in the proof of Proposition 4.2, where we write the inverse power law potential as a combination of Gaussian functions. Because of Equation (15), we can use the exact same decomposition for $|x - w|^{s-d}$ with μ a bounded measure, and write

$$\left\| \left[K(\cdot - z), \boldsymbol{\rho} \right] \right\|_1 \leq \sup_{w \in \mathbb{R}^d} \left(\left\| \left[|\cdot - z - w|^{s-d}, \boldsymbol{\rho} \right] \right\|_1 \right) \left\| \boldsymbol{\mu} \right\|_{\mathrm{TV}},$$

and then use the Proposition 4.2 exchanging z with z + w.

Hence, all our results also hold with the assumption $K \in \dot{H}_w^{d-a}$ instead of $K(x) = |x|^{-a}$ when a > 0, except Theorem 3 below, since we need an assumption on K^2 to prove inequalities (39a) and (39b). For this theorem, the assumption $K(x) = |x|^{-a}$ can therefore be replaced by $K \in \dot{H}_w^{d-a}$ and $K^2 \in \dot{H}_w^{d-2a}$ when $a \geq 0$.

Our third result concerns the Hartree-Fock equation. We write both cases p=1 and p>1 in one theorem in this case.

Theorem 3. Let ρ be a solution of the Hartree-Fock equation (4) and f be a solution of the Vlasov equation (1) satisfying the same initial conditions as in Theorem 1, and as in Theorem 2 if p > 1. If a > 0, we assume additionally that the

solution has finite kinetic energy, i.e.

$$-\operatorname{Tr}(\hbar^2\Delta\boldsymbol{\rho}^{\mathrm{in}})$$

is bounded uniformly with respect to \hbar . Then, for any $p \in [1, \mathfrak{b})$, there exists functions $c \in C^0(\mathbb{R}_+, \mathbb{R}_+)$ and $\lambda \in C^0(\mathbb{R}_+, \mathbb{R}_+)$ depending on the d, a, p and f^{in} such that

$$\left\|\boldsymbol{\rho}_{HF}-\boldsymbol{\rho}_{f}\right\|_{\mathcal{L}^{p}}\leq\left\|\boldsymbol{\rho}^{\mathrm{in}}-\boldsymbol{\rho}_{f}^{\mathrm{in}}\right\|_{\mathcal{L}^{p}}+\left(\mathrm{Tr}\left(\left|\boldsymbol{\rho}^{\mathrm{in}}-\boldsymbol{\rho}_{f}^{\mathrm{in}}\right|\right)+c(t)\,\hbar^{\min\left\{1,\tilde{s}-1\right\}}\right)e^{\lambda(t)}\,,$$

where $\rho_f = \rho_{\hbar}^W(f)$, $\tilde{s} = d - a_+ - d\left(\frac{1}{2} - \frac{1}{p}\right)_+$. For $q \in [\mathfrak{b}, \infty)$, assuming again also that $\rho^{\mathrm{in}} \in \mathcal{L}^{\infty}$, we can still get the following estimate

$$\|\boldsymbol{\rho}_{HF} - \boldsymbol{\rho}_f\|_{\mathcal{L}^q} \leq c_2(t) \left(\|\boldsymbol{\rho}^{\text{in}} - \boldsymbol{\rho}_f^{\text{in}}\|_{\mathcal{L}^p}^{\frac{p}{q}} + \text{Tr}(|\boldsymbol{\rho}^{\text{in}} - \boldsymbol{\rho}_f^{\text{in}}|)^{\frac{p}{q}} + \hbar^{\frac{p}{q} \min\{1,\tilde{s}-1\}} \right) e^{\frac{p}{q}\lambda(t)}.$$

where $c_2(t)$ can also be computed explicitly and depends on the initial conditions.

Remark 1.7. For a > d-2, we have no propagation of regularity and therefore our results hold true only in a conditional form. Namely, if the solution to the Vlasov equation is sufficiently regular, then the bounds of Theorem 1 and Theorem 2 are still satisfied. More precisely, if d=3, such conditional results hold for any $a \in (1,2)$. As for Theorem 3, a conditional result is still true. However, due to the control on the exchange term X, we can address a smaller class of potentials. In particular in dimension d=3 we have $a \in (1,3/2)$. Our results in dimension 2 and 3 can be summarized as follows.

Settings			Hartree	Hartree-Fock
d=2	and	$a \in (-1, 0]$	global	global
d=2	and	$a \in (0,1]$	conditional	conditional
d=3	and	$a \in \left(-\frac{1}{2}, 1\right]$	global	global
d=3	and	$a \in \left(1, \frac{3}{2}\right]$	conditional	conditional
d=3	and	$a \in \left(\frac{3}{2}, 2\right)$	conditional	??

Remark 1.8. Notice that Theorem 2 and Theorem 3 give a semiclassical estimate between the solutions of the Hartree equation (2) and the solutions of the Hartree-Fock equation (4). Indeed, let ρ_H and ρ_{HF} be respectively a solution to the Hartree and Hartree-Fock equation, and let ρ_f be a solution to the Weyl transformed Vlasov equation. Then, for $p \in [1, \infty)$, we have

$$\left\|oldsymbol{
ho}_{H}-oldsymbol{
ho}_{HF}
ight\|_{\mathcal{L}^{p}}\leq\left\|oldsymbol{
ho}_{H}-oldsymbol{
ho}_{f}
ight\|_{\mathcal{L}^{p}}+\left\|oldsymbol{
ho}_{HF}-oldsymbol{
ho}_{f}
ight\|_{\mathcal{L}^{p}},$$

where the first term in the r.h.s. is bounded by Theorem 2 and the second term in the r.h.s. can be estimated by Theorem 3.

1.2. Quantum gradients of the phase space.

The strategy of this paper consists in getting the semiclassical analogue of the estimates of the classical mechanics, and in particular the case of kinetic models. The quantum analogue of the classical momentum variable ξ is the operator

$$\mathbf{p} = -i\hbar\nabla$$
,

which is an unbounded operator on L^2 . From this we get in particular that $|\boldsymbol{p}|^2 := \boldsymbol{p}^*\boldsymbol{p} = -\hbar^2\Delta$ and we can express the Hamiltonian (3) as $H = \frac{|\boldsymbol{p}|^2}{2} + V(x)$. Since

our method here uses regular initial conditions, we define the following operators which are the quantum equivalent of the gradient with respect to the variables x and ξ of the phase space:

$$oldsymbol{
abla}_{x}oldsymbol{
ho}:=\left[
abla,oldsymbol{
ho}
ight]=\left[rac{oldsymbol{p}}{i\hbar},oldsymbol{
ho}
ight]
onumber \ oldsymbol{
abla}_{\xi}oldsymbol{
ho}:=\left[rac{x}{i\hbar},oldsymbol{
ho}
ight].$$

These formulas can be seen from the point of view of the correspondence principle as the quantum equivalent of the Poisson bracket definition of the classical gradients. Another point of view is to remark that they are Weyl transforms, since we have

$$egin{aligned} oldsymbol{
abla}_x oldsymbol{
ho} &= oldsymbol{
ho}_{\hbar}^W (
abla_x w_{\hbar}(oldsymbol{
ho})) \,, \ oldsymbol{
abla}_{\xi} oldsymbol{
ho} &= oldsymbol{
ho}_{\hbar}^W (
abla_{\xi} w_{\hbar}(oldsymbol{
ho})) \,. \end{aligned}$$

One should not confuse $\nabla \in \mathcal{L}(L^2)$ with $\nabla_x \in \mathcal{L}(\mathcal{L}(L^2))$.

2. The classical case: L^1 weak-strong stability

In the classical case, the method we use to prove the semiclassical limit can be seen as an equivalent of the following L^1 weak-strong stability estimate for the Vlasov equation, which tells that we just need to have a control of the gradient of only one of the solutions to get a bound on the integral of their difference. For functions of the phase space of the form $f = f(x, \xi)$, we use the shortcut notation $L^p_x L^{q,r}_\xi = L^p(\mathbb{R}^d, L^{q,r}(\mathbb{R}^d))$. The next proposition can be seen as the classical equivalent of Theorem 1.

Proposition 2.1. Let $\mathfrak{b} \in (1,\infty]$ and $\nabla K \in L^{\mathfrak{b},\infty}$ and assume f_1 and f_2 are two solutions of the Vlasov equation (1) in $L^{\infty}([0,T],L^1(\mathbb{R}^{2d}))$ for some T>0. Then, under the condition

(16)
$$\nabla_{\xi} f_2 \in L^1([0,T], L_x^{\mathfrak{b}',1} L_{\xi}^1),$$

one has the following stability estimate

$$\|f_1 - f_2\|_{L^1(\mathbb{R}^{2d})} \leq \left\|f_1^{\text{in}} - f_2^{\text{in}}\right\|_{L^1(\mathbb{R}^{2d})} e^{C\int_0^T \|\nabla_\xi f_2\|_{L_x^{\mathfrak{b}',1}L_{\xi}^{1}} \mathrm{d}t},$$

where $C = \|\nabla K\|_{L^{\mathfrak{b},\infty}}$.

Remark 2.1. In the case of the Coulomb interaction, $\mathfrak{b} = \frac{3}{2}$, the condition on f_2 becomes

$$\int_{\mathbb{R}^d} |\nabla_{\xi} f_2| \, \mathrm{d}\xi \in L^1([0,T], L_x^{3,1}),$$

 $which\ by\ real\ interpolation\ follows\ in\ particular\ if$

$$\|\nabla_{\xi} f_2\|_{L^1_{\varepsilon}} \in L^1([0,T], L^{3+\varepsilon}_x \cap L^{3-\varepsilon}_x),$$

for some $\varepsilon \in (0,2]$. In particular, the case $\varepsilon = 2$ yields $(3-\varepsilon, 3+\varepsilon) = (1,5)$, which corresponds to the equivalent of the hypotheses required on the solutions in [60]. A quantum version of this hypothesis can also be found in [57].

Remark 2.2. This result allows ∇K to be more singular than the case of the Coulomb potential. However, it is a conditional result, since one still has to show that condition (16) holds. If the potential is the Coulomb potential or a less singular potential, then one can prove that this condition holds if the data is initially in some

weighted Sobolev space by Proposition A.1 in appendix. If the potential is more singular than the Coulomb potential, then such a result is unclear.

Proof of Proposition 2.1. Let $f:=f_1-f_2$ and define for $k\in\{1,2\},\ \rho_k=\int_{\mathbb{R}^d}f_k\,\mathrm{d}\xi$ and $E_k=\nabla V_k=\nabla K*\rho_k$. Then it holds

$$\partial_t f + \xi \cdot \nabla_x f + E_1 \cdot \nabla_{\xi} f = (E_2 - E_1) \cdot \nabla_{\xi} f_2,$$

so that by defining $\rho := \rho_1 - \rho_2$, we obtain

$$\partial_t \iint_{\mathbb{R}^{2d}} |f| \, \mathrm{d}x \, \mathrm{d}\xi = \iint_{\mathbb{R}^{2d}} (\nabla K * \rho \cdot \nabla_{\xi} f_2) \operatorname{sign}(f) \, \mathrm{d}x \, \mathrm{d}\xi$$
$$= - \int_{\mathbb{R}^d} \rho \, \nabla K \, \dot{*} \left(\int_{\mathbb{R}^d} \operatorname{sign}(f) \, \nabla_{\xi} f_2 \, \mathrm{d}\xi \right)$$
$$\leq ||f||_{L^1} \, \left\| \nabla K * \int_{\mathbb{R}^d} |\nabla_{\xi} f_2| \, \mathrm{d}\xi \right\|_{L^{\infty}}.$$

We conclude by remarking that by Hölder's inequality for Lorentz spaces (see for example [37, Formula (2.7)]), for any $g \in L^{\mathfrak{b}',1}$, the following inequality holds

(17)
$$\|\nabla K * g\|_{L^{\infty}} \leq \sup_{z \in \mathbb{R}^d} \int_{\mathbb{R}^d} |\nabla K(z - \cdot)g| \leq \|\nabla K\|_{L^{\mathfrak{b}, \infty}} \|g\|_{L^{\mathfrak{b}', 1}},$$

so that the result follows by taking $g=\|\nabla_\xi f_2\|_{L^1_\xi}$ and then using Grönwall's Lemma.

The next proposition is the classical equivalent of the first part of Theorem 2.

Proposition 2.2. Let $\mathfrak{b} > 1$ and $\nabla K \in L^{\mathfrak{b},\infty}$ and assume f_1 and f_2 are two solutions of the Vlasov equation (1) in $L^{\infty}([0,T],L^1(\mathbb{R}^{2d}))$ for some T>0. Then, if $\nabla_{\xi} f_2 \in L^1([0,T],L^{q,1}_xL^p_{\xi})$, the following inequality holds

$$||f_1 - f_2||_{L^p(\mathbb{R}^{2d})} \le ||f_1^{\text{in}} - f_2^{\text{in}}||_{L^p(\mathbb{R}^{2d})} e^{C \int_0^T ||\nabla_{\xi} f_2||_{L_x^{q,1}(L_\xi^p)} dt},$$

where $C = \|\nabla K\|_{L^{\mathfrak{b},\infty}}$ and

$$\frac{1}{q} = \frac{1}{p} - \frac{1}{\mathfrak{b}}.$$

Remark 2.3. We observe that Formula (18) implies $p \leq \mathfrak{b}$. In the case of the Coulomb interaction in dimension d=3 we have $\mathfrak{b}=\frac{3}{2}$, thus the estimate works at most with $p=\frac{3}{2}$.

Proof. We define the two parameters semigroup $S_{t,s}$ such that $S_{s,s} = 1$ and

$$\partial_t S_{t,s} q = \Lambda_t S_{t,s} q$$
,

where

$$\Lambda_t S_{t,s} g := -\xi \cdot \nabla_x S_{t,s} g - E_1(t) \cdot \nabla_\xi S_{t,s} g,$$

with $E_1(t) = E_1(t,x) = -\nabla K * \rho_1$ with $\rho_1(t,x) = \int f_1(t,x,\xi) d\xi$. Now remark that the flow property of $S_{t,s}$ implies that $\partial_s S_{t,s} = -S_{t,s} \Lambda_s$. Thus, using the notation

$$\tilde{\Lambda} := -\xi \cdot \nabla_{\tau} - E_2 \cdot \nabla_{\varepsilon}$$

and taking $f_1(s) = f_1(s, x, \xi)$ and $f_2(s) = f_2(s, x, \xi)$ two solutions of the Vlasov equation, we get

$$\begin{split} \partial_{s} S_{t,s}(f_{1} - f_{2})(s) &= -S_{t,s} \Lambda_{s}(f_{1} - f_{2})(s) + S_{t,s} \Lambda_{s} f_{1}(s) - S_{t,s} \tilde{\Lambda}_{s} f_{2}(s) \\ &= S_{t,s} \left(\Lambda_{s} - \tilde{\Lambda}_{s} \right) f_{2}(s) \\ &= S_{t,s} \left((E_{2}(s) - E_{1}(s)) \cdot \nabla_{\varepsilon} f_{2}(s) \right), \end{split}$$

and by integrating with respect to s and denoting $f := f_1 - f_2$ and $E := E_1 - E_2$, we obtain the following Duhamel formula

$$f(t) = S_{t,0} f^{\text{in}} + \int_0^t S_{t,s} (E(s) \cdot \nabla_{\xi} f_2(s)) \, ds.$$

Since the semigroup $S_{t,s}$ preserves all Lebesgue norms of the phase space, taking the L^p norm yields

$$||f(t)||_{L^{p}_{x,\xi}} \le ||f^{\text{in}}||_{L^{p}_{x,\xi}} + \int_{0}^{t} ||E(s) \cdot \nabla_{\xi} f_{2}(s)||_{L^{p}_{x,\xi}} \, \mathrm{d}s.$$

To bound the expression inside the time integral we write

$$\begin{split} \|E(s) \cdot \nabla_{\xi} f_{2}(s)\|_{L^{p}_{x,\xi}} &= \|(\rho * \nabla K) \cdot \nabla_{\xi} f_{2}(s)\|_{L^{p}_{x,\xi}} \\ &\leq \int_{\mathbb{R}^{d}} |\rho(z)| \, \|\nabla K(\cdot - z) \cdot \nabla_{\xi} f_{2}(s)\|_{L^{p}_{x,\xi}} \, \mathrm{d}z \\ &\leq \int_{\mathbb{R}^{d}} |\rho(z)| \, \Big\| |\nabla K(\cdot - z)| \, \|\nabla_{\xi} f_{2}(s)\|_{L^{p}_{v}} \, \Big\|_{L^{p}_{x}} \, \mathrm{d}z \\ &\leq \|\rho\|_{L^{1}} \, \|\nabla K\|_{L^{\mathfrak{b},\infty}} \, \|\nabla_{\xi} f_{2}(s)\|_{L^{q,1}_{x}L^{p}_{x}} \, , \end{split}$$

where we used again Hölder's inequality for Lorentz spaces.

3. Regularity of the Weyl Transform

In this section, we want to prove that if the solution f of the Vlasov equation is sufficiently well-behaved, then we can obtain uniform in \hbar bounds for the quantum equivalent of the norm $\|\nabla_{\xi} f\|_{L^{p}_{x}L^{1}_{\xi}}$ expressed in term of the Weyl transform of f.

Proposition 3.1. Let $(n, n_1) \in \mathbb{N}^2$ be even numbers such that n > d/2 and define $\sigma := 2n + n_1$ and $n_0 = \lfloor d/2 \rfloor + 1$. Then, for any $f \in W^{n_0 + 1, \infty}(\mathbb{R}^{2d}) \cap H^{\sigma + 1}_{\sigma}(\mathbb{R}^{2d})$, there exists a constant $\mathcal{C}_{d, n_1} > 0$ depending only on d and n_1 such that

$$\left\|\operatorname{diag}\left(\left|\nabla_{\xi}\boldsymbol{\rho}_{\hbar}^{W}(f)\right|\right)\right\|_{L^{p}} \leq \mathcal{C}_{d,n_{1}} \left\|\nabla_{\xi}f\right\|_{W^{n_{0},\infty}(\mathbb{R}^{2d})\cap H_{\sigma}^{\sigma}(\mathbb{R}^{2d})}$$

for any $p \in [1, 1 + \frac{n_1}{d}]$.

The strategy is to use a special case of the quantum kinetic interpolation inequality proved in [41, Theorem 6]. For the operator $|\nabla_{\varepsilon} \rho|$, This reads

(19)
$$\|\operatorname{diag}(|\nabla_{\xi}\boldsymbol{\rho}|)\|_{L^{p}} \leq \mathcal{C} \operatorname{Tr}(|\nabla_{\xi}\boldsymbol{\rho}||\boldsymbol{p}|^{n_{1}})^{\theta} \|\nabla_{\xi}\boldsymbol{\rho}\|_{\mathcal{L}^{\infty}}^{1-\theta},$$

where p is given by $p = 1 + \frac{n_1}{d}$ and $\theta = \frac{1}{p}$. The corresponding kinetic inequality is

$$\|\nabla_{\xi} f\|_{L_{x}^{p}(L_{\xi}^{1})} \leq C \left(\iint_{\mathbb{R}^{2d}} |\nabla_{\xi} f| |\xi|^{n_{1}} dx d\xi \right)^{\theta} \|\nabla_{\xi} f\|_{L_{x,\xi}^{\infty}}^{1-\theta}.$$

To do that, we will need to compare the multiplication by $|p|^n$ and $|x|^n$ of the Weyl transform of a phase space function g with the Weyl transform of the multiplication

of g with $|\mathbf{p}|^n$ and $|x|^n$. This makes appear error terms involving derivatives of g. For example, in the case n=2, it holds

$$\boldsymbol{\rho}_{\hbar}^{W}(g) |\boldsymbol{p}|^{2} = \boldsymbol{\rho}_{\hbar}^{W} \left(|\xi|^{2} g + \frac{i\hbar}{2} \xi \cdot \nabla_{x} g - \frac{\hbar^{2}}{4} \Delta_{x} g \right)$$
$$\boldsymbol{\rho}_{\hbar}^{W}(g) |x|^{2} = \boldsymbol{\rho}_{\hbar}^{W} \left(|x|^{2} g + i\hbar \xi \cdot \nabla_{\xi} g + \frac{\hbar^{2}}{4} \Delta_{\xi} g \right).$$

More generally, one can obtain similar identities when $n \in \mathbb{N}$. In order to write them, we introduce the standard multi-index notations

$$\alpha := (\alpha_{\mathbf{i}})_{\mathbf{i} \in [\![1,d]\!]} \in \mathbb{N}^d,$$

$$|\alpha| := \sum_{i=1}^d \alpha_i \qquad \qquad \alpha! := \alpha_1! \, \alpha_2! \, \dots \, \alpha_d!$$

$$x^{\alpha} := x_1^{\alpha_1} x_2^{\alpha_2} \dots x_d^{\alpha_d} \qquad \qquad \partial_x^{\alpha} := \partial_{x_1}^{\alpha_1} \partial_{x_2}^{\alpha_2} \dots \partial_{x_d}^{\alpha_d}$$

$$\alpha \le \beta \Leftrightarrow \forall \mathbf{i} \in [\![1,d]\!], \, \alpha_{\mathbf{i}} \le \beta_{\mathbf{i}}.$$

We then obtain the following set of identities.

Lemma 3.1. For any $n \in 2\mathbb{N}$ and any tempered distribution g of the phase space, it holds

(20a)
$$\boldsymbol{\rho}_{\hbar}^{W}(g) |\boldsymbol{p}|^{n} = \sum_{|\alpha+\beta|=n} a_{\alpha,\beta} \left(\frac{i\hbar}{2}\right)^{|\beta|} \boldsymbol{\rho}_{\hbar}^{W}(\xi^{\alpha} \, \partial_{x}^{\beta} g)$$

(20b)
$$\boldsymbol{\rho}_{\hbar}^{W}(g) |x|^{n} = \sum_{|\alpha+\beta|=n} b_{\alpha,\beta} \left(-i\hbar\right)^{|\beta|} \boldsymbol{\rho}_{\hbar}^{W} \left(x^{\alpha} \partial_{\xi}^{\beta} g\right)$$

$$(20c) \ \boldsymbol{\rho}_{\hbar}^{W}(g) \left| \boldsymbol{p} \right|^{n_{1}} \left| \boldsymbol{x} \right|^{n} = \sum_{\substack{|\alpha+\beta|=n_{1}\\|\alpha'+\beta'|=n}} a_{\alpha,\beta} b_{\alpha',\beta'} \left(-i\hbar \right)^{\left|\beta'\right|} \left(\frac{i\hbar}{2} \right)^{\left|\beta\right|} \boldsymbol{\rho}_{\hbar}^{W} \left(\boldsymbol{x}^{\alpha'} \partial_{\xi}^{\beta'} \left(\xi^{\alpha} \partial_{x}^{\beta} g \right) \right).$$

where the coefficients $a_{\alpha,\beta}$, $b_{\alpha,\beta}$ and $c = c_{\alpha,\beta,\alpha',\beta',\gamma}$ are nonnegative coefficients that do not depend on \hbar .

Proof of Lemma 3.1. By definition of the Weyl transform, we deduce that for any $\varphi \in C_c^{\infty}$ it holds

$$\rho_{\hbar}^{W}(g) |\mathbf{p}|^{n} \varphi = (i\hbar)^{n} \iint_{\mathbb{R}^{2d}} g\left(\frac{x+y}{2}, \xi\right) e^{-i(y-x)\cdot\xi/\hbar} \Delta^{\frac{n}{2}} \varphi(y) \, \mathrm{d}y \, \mathrm{d}\xi
= (i\hbar)^{n} \iint_{\mathbb{R}^{2d}} \Delta^{\frac{n}{2}}_{y} \left(g\left(\frac{x+y}{2}, \xi\right) e^{-i(y-x)\cdot\xi/\hbar}\right) \varphi(y) \, \mathrm{d}y \, \mathrm{d}\xi.$$

With the multi-index notation, we can expand the powers of the Laplacian of a product of functions in the following way

$$\Delta^{\frac{n}{2}}(fg) = \sum_{|\alpha+\beta|=n} a_{\alpha,\beta} \, \partial^{\alpha} f \, \partial^{\beta} g,$$

where the $a_{\alpha,\beta}^n$ are nonnegative constants depending on n and on the multi-index α , and such that

$$\sum_{|\alpha+\beta|=n} a_{\alpha,\beta} = (4d)^n.$$

Thus, we deduce that the kernel κ of the operator $\rho_{\hbar}^{W}(g) |\mathbf{p}|^{n}$ is given by

$$\kappa(x,y) = \sum_{|\alpha+\beta|=n} a_{\alpha,\beta} \left(i\hbar\right)^{n-|\alpha|} \int_{\mathbb{R}^d} 2^{-|\beta|} \partial_x^{\beta} g\left(\frac{x+y}{2},\xi\right) \xi^{\alpha} e^{-i(y-x)\cdot\xi/\hbar} \,\mathrm{d}\xi,$$

which yields,

$$\boldsymbol{\rho}_{\hbar}^{W}(g) \left| \boldsymbol{p} \right|^{n} = \sum_{|\alpha + \beta| = n} a_{\alpha,\beta} \left(\frac{i\hbar}{2} \right)^{|\beta|} \boldsymbol{\rho}_{\hbar}^{W} \left(\xi^{\alpha} \partial_{x}^{\beta} g \right).$$

This proves Identity (20a). To prove the second identity, we write $u:=\frac{x+y}{2}$ and v:=y-x so that the kernel κ_2 of the operator $\boldsymbol{\rho}_{\hbar}^W(g)\left|x\right|^2$ is given by

$$\kappa_{2}(x,y) = \iint_{\mathbb{R}^{2d}} g\left(\frac{x+y}{2},\xi\right) e^{-i(y-x)\cdot\xi/\hbar} |y|^{n} d\xi
= \iint_{\mathbb{R}^{2d}} g(u,\xi) e^{-i v\cdot\xi/\hbar} \left(\left|u+\frac{v}{2}\right|^{2}\right)^{\frac{n}{2}} d\xi
= \iint_{\mathbb{R}^{2d}} g(u,\xi) e^{-i v\cdot\xi/\hbar} \left(\sum_{i=1}^{d} \left(u_{i}^{2} + \frac{v_{i}^{2}}{4} + u_{i}v_{i}\right)\right)^{\frac{n}{2}} d\xi.$$

By the multinomial theorem, this can be written under the form

$$\kappa_{2}(x,y) = \sum_{|\alpha+\beta|=n} b_{\alpha,\beta} \iint_{\mathbb{R}^{2d}} u^{\alpha} g(u,\xi) v^{\beta} e^{-i v \cdot \xi/\hbar} d\xi
= \sum_{|\alpha+\beta|=n} b_{\alpha,\beta} \iint_{\mathbb{R}^{2d}} u^{\alpha} g(u,\xi) (i\hbar)^{|\beta|} \partial_{\xi}^{\beta} e^{-i v \cdot \xi/\hbar} d\xi
= \sum_{|\alpha+\beta|=n} b_{\alpha,\beta} (-i\hbar)^{|\beta|} \iint_{\mathbb{R}^{2d}} u^{\alpha} \partial_{\xi}^{\beta} g(u,\xi) e^{-i v \cdot \xi/\hbar} d\xi,$$

where we used $|\beta|$ times integration by parts to get the last line, and the $b_{\alpha,\beta}$ are nonnegative constants that satisfy

$$\sum_{|\alpha+\beta|=n} b_{\alpha,\beta} = \left(\frac{9d}{4}\right)^{\frac{n}{2}}.$$

In term of operators, this yields the following identity

$$\boldsymbol{\rho}_{\hbar}^{W}(g)\left|x\right|^{n} = \sum_{\left|\alpha+\beta\right|=n} b_{\alpha,\beta}\left(-i\hbar\right)^{\left|\beta\right|} \boldsymbol{\rho}_{\hbar}^{W}\!\!\left(x^{\alpha}\,\partial_{\xi}^{\beta}g\right).$$

This yields Identity (20b). To get the last identity, we combine the two first to get

$$\begin{aligned} \boldsymbol{\rho}_{\hbar}^{W}(g) \left| \boldsymbol{p} \right|^{n_{1}} \left| \boldsymbol{x} \right|^{n} &= \sum_{\left| \alpha + \beta \right| = n_{1}} a_{\alpha,\beta} \left(\frac{i\hbar}{2} \right)^{\left| \beta \right|} \boldsymbol{\rho}_{\hbar}^{W} \left(\boldsymbol{\xi}^{\alpha} \, \partial_{x}^{\beta} g \right) \left| \boldsymbol{x} \right|^{n} \\ &= \sum_{\left| \alpha + \beta \right| = n_{1}} a_{\alpha,\beta} b_{\alpha',\beta'} \left(-i\hbar \right)^{\left| \beta' \right|} \left(\frac{i\hbar}{2} \right)^{\left| \beta \right|} \boldsymbol{\rho}_{\hbar}^{W} \left(\boldsymbol{x}^{\alpha'} \, \partial_{\xi}^{\beta'} \left(\boldsymbol{\xi}^{\alpha} \, \partial_{x}^{\beta} g \right) \right). \end{aligned}$$

From this lemma, we deduce the following \mathcal{L}^2 inequalities.

Proposition 3.2. Let $n \in 2\mathbb{N}$ and g a function of the phase space, then there exists a constant C > 0 depending only on d and n such that

(21a)
$$\|\boldsymbol{\rho}_{\hbar}^{W}(g) |\boldsymbol{p}|^{n}\|_{\mathcal{L}^{2}} \leq (4d)^{n} \left(\|g|\xi|^{n}\|_{L^{2}(\mathbb{R}^{2d})} + \left(\frac{\hbar}{2}\right)^{n} \|\nabla_{x}^{n}g\|_{L^{2}(\mathbb{R}^{2d})} \right)$$

(21b)
$$\|\boldsymbol{\rho}_{\hbar}^{W}(g)|x|^{n}\|_{\mathcal{L}^{2}} \leq \left(\frac{9d}{4}\right)^{n} \left(\|g|x|^{n}\|_{L^{2}(\mathbb{R}^{2d})} + \hbar^{n} \|\nabla_{\xi}^{n}g\|_{L^{2}(\mathbb{R}^{2d})}\right)$$

$$\|\boldsymbol{\rho}_{\hbar}^{W}(g) |\boldsymbol{p}|^{n_{1}} |x|^{n} \|_{\mathcal{L}^{2}} \leq C \left(\|(1 + |x|^{n} |\xi|^{n_{1}}) g\|_{L^{2}(\mathbb{R}^{2d})} + \hbar^{n_{1}} \||x|^{n} \nabla_{x}^{n_{1}} g\|_{L^{2}(\mathbb{R}^{2d})} \right)$$

(21c)
$$+ \hbar^{n} \| |\xi|^{n_{1}} \nabla_{\xi}^{n} g \|_{L^{2}(\mathbb{R}^{2d})} + \hbar^{n+n_{1}} \| \nabla_{x}^{n_{1}} \nabla_{\xi}^{n} g \|_{L^{2}(\mathbb{R}^{2d})} \right).$$

Proof of Proposition 3.2. By Formula (20a) and the fact that for any $u \in L^2(\mathbb{R}^{2d})$, $\|\boldsymbol{\rho}_{\hbar}^W(u)\|_{\mathcal{L}^2} = \|u\|_{L^2(\mathbb{R}^{2d})}$, we obtain

(22)
$$\|\boldsymbol{\rho}_{\hbar}^{W}(g) |\boldsymbol{p}|^{n} \|_{\mathcal{L}^{2}} \leq \sum_{|\alpha+\beta|=n} a_{\alpha,\beta} \left(\frac{\hbar}{2}\right)^{|\beta|} \|\xi^{\alpha} \partial_{x}^{\beta} g\|_{L^{2}(\mathbb{R}^{2d})}.$$

Then, for any multi-index α and β such that $|\alpha + \beta| = n$, by defining $\hat{g}(y, \xi)$ as the Fourier transform of $g(x, \xi)$ with respect to the variable x, the fact that the Fourier transform is unitary in L_x^2 yields

$$\begin{split} \left(\frac{\hbar}{2}\right)^{|\beta|} \left\| \xi^{\alpha} \, \partial_{x}^{\beta} g \right\|_{L^{2}(\mathbb{R}^{2d})} &= \left(\frac{\hbar}{2}\right)^{|\beta|} \left\| \xi^{\alpha} \, y^{\beta} \, \hat{g} \right\|_{L^{2}(\mathbb{R}^{2d})} \\ &\leq \frac{|\alpha|}{n} \left\| \left| \xi \right|^{n} \, \hat{g} \right\|_{L^{2}(\mathbb{R}^{2d})} + \frac{|\beta|}{n} \, \left(\frac{\hbar}{2}\right)^{|\beta|} \left\| \left| y \right|^{n} g \right\|_{L^{2}(\mathbb{R}^{2d})} \\ &\leq \left\| \left| \xi \right|^{n} g \right\|_{L^{2}(\mathbb{R}^{2d})} + \left(\frac{\hbar}{2}\right)^{n} \left\| \nabla_{x}^{n} \hat{g} \right\|_{L^{2}(\mathbb{R}^{2d})}. \end{split}$$

Moreover, as remarked in the proof of Lemma 3.1, it holds

$$\sum_{|\alpha+\beta|=n} a_{\alpha,\beta} = (4d)^n,$$

from which we obtain Inequality (21a). Formulas (21b) and (21c) can be proved in the same way. $\hfill\Box$

Moreover, we can bound weighted \mathcal{L}^1 norms using \mathcal{L}^2 norms with bigger weights. This is the content of the following proposition where we recall the notation $\langle y \rangle = \sqrt{1 + |y|^2}$ for the weights.

Proposition 3.3. Let $(n, n_1) \in \mathbb{N}^2$ be even numbers such that n > d/2 and define $k := n + n_1$. Assume $\boldsymbol{\rho} := \boldsymbol{\rho}_h^W(g)$ is the Weyl transform of a function $g \in H_{n+k}^{n+k}(\mathbb{R}^{2d})$. Then the following inequality holds

$$\operatorname{Tr}(\left|\boldsymbol{\rho}\right|\left|\boldsymbol{p}\right|^{n_{1}}) \leq C\left(\left\|\left\langle \xi\right\rangle^{k} \left\langle x\right\rangle^{n} g\right\|_{L^{2}(\mathbb{R}^{2d})} + \hbar^{k} \left\|\left\langle x\right\rangle^{n} \nabla_{x}^{k} g\right\|_{L^{2}(\mathbb{R}^{2d})} \right.$$
$$\left. + \hbar^{n} \left\|\left\langle \xi\right\rangle^{k} \nabla_{\xi}^{n} g\right\|_{L^{2}(\mathbb{R}^{2d})} + \hbar^{k+n} \left\|\nabla_{x}^{k} \nabla_{\xi}^{n} g\right\|_{L^{2}(\mathbb{R}^{2d})}\right).$$

Proof. First remark that since the sum of eigenvalues is always smaller than the sum of singular values (see for example Formula (3.1) in [62]), it holds

$$\mathrm{Tr}(\left|\boldsymbol{\rho}\right|\left|\boldsymbol{p}\right|^{n_1}) \leq \mathrm{Tr}\left(\left|\left(\left|\boldsymbol{\rho}\right|\left|\boldsymbol{p}\right|^{n_1}\right)\right|\right),$$

and from the definition of |AB| if A and B are two operators, we see that $|AB| = (B^*A^*AB)^{\frac{1}{2}} = ||A|B|$, so that $\mathrm{Tr}(\left|\left(|\boldsymbol{\rho}||\boldsymbol{p}|^{n_1}\right)\right|) = \mathrm{Tr}(|\boldsymbol{\rho}||\boldsymbol{p}|^{n_1}|)$. Defining $\boldsymbol{m}_n := (1+|\boldsymbol{p}|^n)(1+|x|^n)$, we deduce from the Cauchy-Schwarz inequality that

(23)
$$\operatorname{Tr}(|\boldsymbol{\rho}||\boldsymbol{p}|^{n_1}) \leq \operatorname{Tr}(|\boldsymbol{\rho}||\boldsymbol{p}|^{n_1}|) \leq ||\boldsymbol{\rho}||\boldsymbol{p}|^{n_1}||\boldsymbol{m}_n||_2 ||\boldsymbol{m}_n^{-1}||_2.$$

To control the second factor in the right-hand side, we remark that it is of the form $\boldsymbol{m}_n^{-1} = w(x)\,w(-i\hbar\nabla)$ with $w(y) = (1+|y|^n)^{-1}$, so that its Hilbert-Schmidt norm can be computed exactly (see e.g. [62, Equation (4.7)])

$$\|\boldsymbol{m}_n^{-1}\|_2 = (2\pi)^{-d/2} \|\boldsymbol{w}\|_{L^2} \|\boldsymbol{w}(\hbar \cdot)\|_{L^2} = C_{d,n} h^{-d/2},$$

where $C_{d,n} = \|w\|_{L^2}^2$ is finite since n > d/2. Therefore, by definition of the \mathcal{L}^2 norm, Inequality (23) leads to

$$\operatorname{Tr}(|\boldsymbol{\rho}| |\boldsymbol{p}|^{n_1}) \leq C_{d,n} \|\boldsymbol{\rho}| |\boldsymbol{p}|^{n_1} \boldsymbol{m}_n\|_{\mathcal{L}^2} \\ \leq C_{d,n} \left(\|\boldsymbol{\rho}(|\boldsymbol{p}|^{n_1} + |\boldsymbol{p}|^{n_1} |x|^n + |\boldsymbol{p}|^{n+n_1} + |\boldsymbol{p}|^{n+n_1} |x|^n) \|_{\mathcal{L}^2} \right).$$

To get the result, we take $\rho = \rho_{\hbar}^{W}(g)$ and use Proposition 3.2 to bound the right-hand side of above inequality by weighted classical L^{2} norms of g.

We can now prove the main proposition of this section following the strategy explained at the beginning of this section.

Proof of Proposition 3.1. We use an improvement of the Calderón-Vaillancourt theorem for Weyl operators proved by Boulkhemair in [14] which states that if $g \in W^{n_0,\infty}(\mathbb{R}^{2d})$ with $n_0 = \lfloor \frac{d}{2} \rfloor + 1$, then $\rho_1^W(g)$ is a bounded operator on L^2 , so that its operator norm is bounded by

(24)
$$\| \boldsymbol{\rho}_{1}^{W}(g) \|_{\mathscr{B}(L^{2})} \leq C \| g \|_{W^{n_{0},\infty}(\mathbb{R}^{2d})}.$$

Since $\rho_h^W(g) = h^d \rho_1^W(g(\cdot, h \cdot))$, and that for $h \leq 1$

$$\|g(\,\cdot,h\,\cdot)\|_{W^{n_0,\infty}(\mathbb{R}^{2d})} \le \|g\|_{W^{n_0,\infty}(\mathbb{R}^{2d})}\,,$$

by taking $g = \nabla_{\xi} f$, we deduce from Inequality (24) and the definition of the \mathcal{L}^{∞} norm that

$$\left\| \nabla_{\xi} \boldsymbol{\rho}_{\hbar}^{W}(f) \right\|_{\mathcal{L}^{\infty}} \leq C \left\| \nabla_{\xi} f \right\|_{W^{n_0,\infty}(\mathbb{R}^{2d})},$$

uniformly in \hbar . Moreover, taking $g = \nabla_{\varepsilon} f$ in Proposition 3.3 yields

$$\operatorname{Tr}(\left|\nabla_{\xi} \boldsymbol{\rho}_{\hbar}^{W}(f)\right| \left|\boldsymbol{p}\right|^{n_{1}}) \leq C \left\|\nabla_{\xi} f\right\|_{H_{\sigma}(\mathbb{R}^{2d})}.$$

The result then follows by combining these two inequalities to bound the right-hand-side of the interpolation inequality (19).

4. Proof of Theorem 1 and Theorem 2

In this section, we will start by proving a stability estimate similar to the one of the classical case and then use the results of Section 3 and the propagation of regularity for the Vlasov equation to get the proof of Theorem 1 and then the proof of Theorem 2. The conditional result is stated in the following proposition.

Proposition 4.1. Let $K = \frac{1}{|x|^a}$ with $a \in \left(\left(\frac{d}{2} - 2\right)_+, d - 1\right)$ and assume ρ is a solution of the Hartree equation (2) with initial condition $\rho^{\text{in}} \in \mathcal{L}^1_+$ and $f \geq 0$ is a solution of the Vlasov equation verifying

$$(25a) f \in L^{\infty}_{loc}(\mathbb{R}_+, W^{n_0+1,\infty}(\mathbb{R}^{2d}) \cap H^{\sigma+1}_{\sigma}(\mathbb{R}^{2d}))$$

(25b)
$$\rho_f \in L^{\infty}_{loc}(\mathbb{R}_+, L^1 \cap H^{\nu}),$$

where $n_0 = \lfloor d/2 \rfloor + 1$, $(n, n_1) \in (2\mathbb{N})^2$ are such that n > d/2 and $n_1 \ge \frac{d}{\mathfrak{b}-1}$ and we used the notations $\sigma = 2n + n_1$ and $\nu = (n + a + 2 - d)_+$ and $\mathfrak{b} = \frac{d}{a+1}$. Then the following inequality holds

$$\operatorname{Tr}(|\boldsymbol{\rho} - \boldsymbol{\rho}_f|) \le (\operatorname{Tr}(|\boldsymbol{\rho}^{\text{in}} - \boldsymbol{\rho}_f^{\text{in}}|) + C_f(t) \hbar) e^{\lambda_f(t)},$$

where

$$\lambda_f(t) = C_{d,n_1,a} \int_0^t \|\nabla_{\xi} f\|_{W^{n_0,\infty}(\mathbb{R}^{2d}) \cap H^{\sigma}_{\sigma}(\mathbb{R}^{2d})} \, \mathrm{d}s$$

$$C_f(t) = C_{d,n_1,a} \int_0^t \|\rho_f(s)\|_{L^1 \cap H^{\nu}} \|\nabla_{\xi}^2 f(s)\|_{H^{2n}_{2n}(\mathbb{R}^{2d})} e^{-\lambda_f(s)} \, \mathrm{d}s.$$

In analogy with the classical case (cf. proof of Proposition 2.2), we introduce the two-parameter semigroup $\mathcal{U}_{t,s}$ such that $\mathcal{U}_{s,s} = 1$ and defined for t > s by

$$i \,\hbar \,\partial_t \,\mathcal{U}_{t,s} = H(t) \,\mathcal{U}_{t,s}$$
,

where H is the Hartree Hamiltonian (3). We consider the quantity

$$i \,\hbar \,\partial_t \left(\mathcal{U}_{t,s}^* \left(\boldsymbol{\rho}(t) - \boldsymbol{\rho}_f(t) \right) \mathcal{U}_{t,s} \right) = \mathcal{U}_{t,s}^* \left[K * \left(\rho(t) - \rho_f(t) \right), \boldsymbol{\rho}_f(t) \right] \mathcal{U}_{t,s} + \mathcal{U}_{t,s}^* \,\partial_t \,\mathcal{U}_{t,s} \,,$$

where B_t is an operator defined through its kernel

$$B_t(x,y) = \left((K * \rho_f)(x) - (K * \rho_f)(y) - (\nabla K * \rho_f) \left(\frac{x+y}{2} \right) \cdot (x-y) \right) \boldsymbol{\rho}_f(x,y).$$

Using Duhamel's formula and taking the Schatten p norm (recall that $\mathcal{U}_{t,s}$ is a unitary operator), we get

(26)
$$\|\boldsymbol{\rho}(t) - \boldsymbol{\rho}_{f}(t)\|_{p} \leq \|\boldsymbol{\rho}^{\text{in}} - \boldsymbol{\rho}_{f}^{\text{in}}\|_{p} + \frac{1}{\hbar} \int_{0}^{t} \|B_{t}\|_{p} ds + \frac{1}{\hbar} \int_{0}^{t} \int |\rho(s, z) - \rho_{f}(s, z)| \|[K(\cdot - z), \boldsymbol{\rho}_{f}(s)]\|_{p} dz ds.$$

We now take p=1, i.e. the trace norm, and we have to bound each term on the right-hand side of Inequality (26) in order to obtain a Grönwall type inequality which will prove Proposition 4.1. Remark that we will then use again Inequality (26) with p>1 together with Theorem 1 to prove Theorem 2.

4.1. The commutator inequality. Generalizing [57, Lemma 3.1], we obtain the quantum equivalent of Inequality (17), which is is the following inequality for the trace norm of the commutator of K and a trace class operator ρ .

Theorem 4. Let $a \in (-1, d-1)$, $K(x) = \frac{1}{|x|^a}$ or $K(x) = \ln(|x|)$ when a = 0 and let $\mathfrak{b} := \mathfrak{b}_a = \frac{d}{a+1}$ so that $\nabla K \in L^{\mathfrak{b},\infty}$. Let \mathfrak{b}' be the conjugated Hölder exponent of \mathfrak{b} . Then for any $\varepsilon \in (0, \mathfrak{b}' - 1]$, there exists a constant C > 0 such that

$$\operatorname{Tr}(|[K(\cdot - z), \boldsymbol{\rho}]|) \leq C h \|\operatorname{diag}(|\nabla_{\xi} \boldsymbol{\rho}|)\|_{L^{\mathfrak{b}' - \varepsilon}}^{\frac{1}{2} + \tilde{\varepsilon}} \|\operatorname{diag}(|\nabla_{\xi} \boldsymbol{\rho}|)\|_{L^{\mathfrak{b}' + \varepsilon}}^{\frac{1}{2} - \tilde{\varepsilon}},$$

for any $\tilde{\varepsilon} \in (0, \frac{\varepsilon}{2\mathfrak{b}'})$ and with the additional assumption $\varepsilon < \mathfrak{b}_3' - \mathfrak{b}'$ if $d \geq 4$.

Remark 4.1. In the case of Coulomb interaction and d=3, we have $K(x)=\frac{1}{|x|}$, $\mathfrak{b}=\mathfrak{b}_1=\frac{3}{2}$ and $\nabla K\in L^{\frac{3}{2},\infty}$. Thus for any $\varepsilon\in(0,2]$, there exists a constant C>0 such that

$$\mathrm{Tr}(|[K(\cdot-z),\boldsymbol{\rho}]|) \leq C\,h\,\|\mathrm{diag}(|\boldsymbol{\nabla}_{\!\boldsymbol{\xi}}\boldsymbol{\rho}|)\|_{L^{3-\varepsilon}}^{\frac{1}{2}+\tilde{\varepsilon}}\,\|\mathrm{diag}(|\boldsymbol{\nabla}_{\!\boldsymbol{\xi}}\boldsymbol{\rho}|)\|_{L^{3+\varepsilon}}^{\frac{1}{2}-\tilde{\varepsilon}}$$

for any $\tilde{\varepsilon} \in (0, \frac{\varepsilon}{6})$

This theorem is a corollary of the slightly more precise following proposition.

Proposition 4.2. For any $\delta \in \left(\left(\frac{1}{\mathfrak{b}'_1} - \frac{1}{\mathfrak{b}'}\right)_+, 1 - \frac{1}{\mathfrak{b}'}\right)$ and $q \in \left(\frac{\mathfrak{b}'}{1 - \delta \mathfrak{b}'}, \infty\right]$, there exists a constant C > 0 such that

(27)
$$\operatorname{Tr}(|[K(\cdot - z), \boldsymbol{\rho}]|) \leq C h \|\operatorname{diag}(|\nabla_{\xi} \boldsymbol{\rho}|)\|_{L^{p}}^{\theta} \|\operatorname{diag}(|\nabla_{\xi} \boldsymbol{\rho}|)\|_{L^{q}}^{1-\theta},$$

where $\theta = \delta / \left(\frac{1}{p} - \frac{1}{q}\right)$ and $\frac{1}{p} = \frac{1}{b'} + \delta$ and with the additional assumption that $q < b'_3$ if $d \ge 4$.

Proof of Theorem 4. To prove our result, we will decompose the potential as a combination of Gaussian functions (see e.g. [42, 5.9 (3)]). By using the definition of the Gamma function and a simple change of variable, when a>0, one obtains the following formula for any r>0

(28)
$$\frac{1}{\omega_a r^{a/2}} = \frac{1}{2} \int_0^\infty t^{\frac{a}{2} - 1} e^{-\pi r t} dt,$$

where $\omega_a = \frac{2 \pi^{a/2}}{\Gamma(a/2)}$. Taking $r = |x|^2$ directly leads to the following decomposition

$$\frac{1}{\omega_a |x|^a} = \frac{1}{2} \int_0^\infty t^{\frac{a}{2} - 1} e^{-\pi |x|^2 t} \, \mathrm{d}t.$$

Now when $a \in (-2,0)$, take Equation (28) with a+2 instead of a, integrate it with respect to r, exchange the integrals and then replace again r by $|x|^2$. This yields a similar decomposition under the form

$$\frac{1}{\omega_a \left| x \right|^a} = \frac{1}{2} \int_0^\infty t^{\frac{a}{2} - 1} \left(e^{-\pi |x|^2 t} - 1 \right) \, \mathrm{d}t.$$

In order to treat the case of the logarithm, do the same steps with a=0 to obtain

$$-\ln(|x|) = \frac{1}{2} \int_0^\infty t^{\frac{a}{2}-1} \left(e^{-\pi|x|^2 t} - e^{-\pi t} \right) dt.$$

In any of these case, defining $\omega_0 := 1$, we get the following identity

$$\frac{1}{\omega_a} \left(K(x) - K(y) \right) = \frac{1}{2} \int_0^\infty t^{\frac{a}{2} - 1} \left(e^{-\pi |x|^2 t} - e^{-\pi |y|^2 t} \right) dt.$$

Trying to follow the idea of [57] but with this new decomposition, we write

$$\frac{1}{\omega_a} \left(K(x) - K(y) \right) = \frac{1}{2} \int_0^\infty t^{\frac{a}{2} - 1} \int_0^1 \frac{\mathrm{d}}{\mathrm{d}\theta} \left(e^{-\pi\theta |x|^2 t} e^{-\pi(1-\theta)|y|^2 t} \right) \mathrm{d}\theta \, \mathrm{d}t
= -\pi \int_0^\infty t^{\frac{a}{2}} \int_0^1 \left(x - y \right) \cdot (x + y) e^{-\pi\theta |x|^2 t} e^{-\pi(1-\theta)|y|^2 t} \mathrm{d}\theta \, \mathrm{d}t,$$

from which we get

$$\frac{K(x-z) - K(y-z)}{-\pi \omega_a} = \int_0^1 \int_0^\infty t^{\frac{a}{2}} (x-y) \cdot (\phi_{\theta}(x)\varphi_{1-\theta}(y) + \varphi_{\theta}(x)\phi_{1-\theta}(y)) dt d\theta,$$

where we defined $\varphi_k(x) := e^{-k\pi|x-z|^2t}$ and $\phi_k(x) = (x-z)\,\varphi_k(x)$. Thus, since the kernel of $\nabla_{\xi}\boldsymbol{\rho}$ is $\frac{x-y}{i\hbar}\boldsymbol{\rho}(x,y)$ and exchanging θ by $1-\theta$ in the second term of the integral, we obtain

$$\frac{1}{i\pi\hbar\omega_a}\left[K(\cdot-z),\boldsymbol{\rho}\right] = \int_0^1 \int_0^\infty t^{\frac{a}{2}} \left(\phi_\theta \cdot \nabla_{\xi}\boldsymbol{\rho}\,\varphi_{1-\theta} + \varphi_{1-\theta}\,\nabla_{\xi}\boldsymbol{\rho}\cdot\phi_\theta\right) dt d\theta.$$

Remarking that $(\phi_{\theta} \cdot \nabla_{\xi} \boldsymbol{\rho} \varphi_{1-\theta})^* = \varphi_{1-\theta} \nabla_{\xi} \boldsymbol{\rho} \cdot \phi_{\theta}$, we can now estimate the trace norm by

(29)
$$\frac{1}{h|\omega_a|} \|[K(\cdot - z), \boldsymbol{\rho}]\|_1 \le \int_0^1 \int_0^\infty t^{\frac{a}{2}} \|\phi_\theta \cdot \nabla_{\xi} \boldsymbol{\rho} \varphi_{1-\theta}\|_1 dt d\theta.$$

Then, by decomposing the self-adjoint operator $\nabla_{\xi} \boldsymbol{\rho}$ on an orthogonal basis $(\psi_j)_{j \in J}$, we can write $\nabla_{\xi} \boldsymbol{\rho} = \sum_{j \in J} \lambda_j |\psi_j\rangle \langle \psi_j|$ and we get

$$\begin{split} \left\| \phi_{\theta} \cdot \nabla_{\xi} \boldsymbol{\rho} \, \varphi_{1-\theta} \right\|_{1} &\leq \sum_{j \in J} \left| \lambda_{j} \right| \left\| \left| \phi_{\theta} \psi_{j} \right\rangle \left\langle \psi_{j} \varphi_{1-\theta} \right| \right\|_{1} \\ &\leq \sum_{j \in J} \left| \lambda_{j} \right| \left\| \phi_{\theta} \psi_{j} \right\|_{L^{2}} \left\| \psi_{j} \varphi_{1-\theta} \right\|_{L^{2}}, \end{split}$$

where we used the fact that $||u\rangle\langle v||_1 = ||u||_{L^2} ||v||_{L^2}$. Thus, by the inequality of Cauchy-Schwarz for series

$$\|\phi_{\theta} \cdot \nabla_{\xi} \boldsymbol{\rho} \varphi_{1-\theta}\|_{1} \leq \left(\sum_{j \in J} |\lambda_{j}| \|\phi_{\theta} \psi_{j}\|_{L^{2}}^{2} \right)^{\frac{1}{2}} \left(\sum_{j \in J} |\lambda_{j}| \|\psi_{j} \varphi_{1-\theta}\|_{L^{2}}^{2} \right)^{\frac{1}{2}}$$
$$\leq \left(\int_{\mathbb{R}^{d}} |\phi_{\theta}|^{2} \rho_{1} \right)^{\frac{1}{2}} \left(\int_{\mathbb{R}^{d}} |\varphi_{1-\theta}|^{2} \rho_{1} \right)^{\frac{1}{2}},$$

with the notation $\rho_1 = \operatorname{diag}(|\nabla_{\xi} \boldsymbol{\rho}|) = \sum_{j \in J} |\lambda_j| |\psi_j|^2$. By the integral Hölder's inequality, this yields

(30)
$$\|\phi_{\theta} \cdot \nabla_{\xi} \boldsymbol{\rho} \varphi_{1-\theta}\|_{1} \leq \|\phi_{\theta}\|_{L^{2p'}} \|\varphi_{1-\theta}\|_{L^{2q'}} \|\rho_{1}\|_{L^{p}}^{\frac{1}{2}} \|\rho_{1}\|_{L^{q}}^{\frac{1}{2}},$$

where $(p,q) \in [1,\infty]^2$ can depend on the parameter t, which will help us to obtain the convergence of the integral in Inequality (29). We can now compute explicitly

the integrals of the functions ϕ and φ . It holds

$$\|\phi_{\theta}\|_{L^{2p'}}^{2p'} = \int_{\mathbb{R}^d} |x - z|^{2p'} e^{-2\pi\theta|x - z|^2 p' t} dx = \frac{\omega_d}{\omega_{d+2p'}} \frac{1}{(2\theta p' t)^{\frac{d+2p'}{2}}}$$
$$\|\varphi_{1-\theta}\|_{L^{2q'}}^{2q'} = \int_{\mathbb{R}^d} e^{-2\pi(1-\theta)|x - z|^2 q' t} dx = \frac{1}{(2(1-\theta)q' t)^{\frac{d}{2}}}.$$

Combining these two formulas with inequalities (29) and (30) leads to

$$\|[K(\cdot - z), \boldsymbol{\rho}]\|_{1} \le h \int_{0}^{\infty} \frac{C_{d,a,p'} \|\rho_{1}\|_{L^{p}}^{\frac{1}{2}} \|\rho_{1}\|_{L^{q}}^{\frac{1}{2}}}{t^{\frac{1}{2}\left(\frac{d}{2p'} + \frac{d}{2q'} + 1 - a\right)}} \int_{0}^{1} \frac{\mathrm{d}\theta}{\theta^{\frac{d+2p'}{4p'}} (1 - \theta)^{\frac{d}{4q'}}} \, \mathrm{d}t.$$

with $C_{d,a,p'} = |\omega_a| \left(\frac{\omega_d}{\omega_{d+2p'}}\right)^{\frac{1}{2p'}} (2p')^{-\frac{d+2p'}{4p'}} (2q')^{-\frac{d}{4q'}}$. We remark that the integral on θ is converging as soon as

(31)
$$\frac{1}{p'} < \frac{2}{d} = \frac{1}{\mathfrak{b}_1} \text{ and } \frac{1}{q'} < \frac{4}{d} = \frac{1}{\mathfrak{b}_3}.$$

Now, in order to get a finite integral of the variable t, we can cut the integral in two parts. The first one for $t \in (0, R)$ and the second one for $t \in (R, \infty)$ for a given R > 0. Then we have to choose p and q such that

$$\frac{1}{2} \left(\frac{d}{2p'} + \frac{d}{2q'} + 1 - a \right) < 1 \text{ for } t \in (0, R)$$

$$\frac{1}{2} \left(\frac{d}{2p'} + \frac{d}{2q'} + 1 - a \right) > 1 \text{ for } t \ge R,$$

or equivalently since $\mathfrak{b} = \frac{d}{a+1}$

$$\frac{1}{2} \left(\frac{1}{p'} + \frac{1}{q'} \right) < \frac{1}{\mathfrak{b}} \text{ for } t \in (0, R)$$

$$\frac{1}{2} \left(\frac{1}{p'} + \frac{1}{q'} \right) > \frac{1}{\mathfrak{b}} \text{ for } t \ge R.$$

However, this has to be compatible with the constraint (31). Therefore, when $t \in (0, R)$, we can in particular take $q = p_0$ with $p_0 < \min(\mathfrak{b}', \mathfrak{b}'_1)$. When $t \ge R$, then we can also take for example $p = p_0 > \frac{\mathfrak{b}'}{2}$ and then any q such that

(32)
$$\frac{2}{\mathfrak{b}} - \frac{1}{p_0'} < \frac{1}{q'} < \frac{4}{d} \text{ and } \frac{1}{q'} \le 1.$$

Remark that the condition $\frac{1}{q'} < \frac{4}{d}$ is only used when $d \geq 4$ and can be rewritten $q \leq \mathfrak{b}_3'$. Such a pair (p_0,q) exists as long as $a \leq \frac{d}{2}$ and a < 2. By defining $\delta := \frac{1}{p_0} - \frac{1}{\mathfrak{b}'}$, then these conditions are equivalent to

$$\begin{split} \left(\frac{1}{\mathfrak{b}_1'} - \frac{1}{\mathfrak{b}'}\right)_+ &< \delta < 1 - \frac{1}{\mathfrak{b}'} \\ \frac{1}{p_0} &= \frac{1}{\mathfrak{b}'} + \delta \\ \frac{1}{q} &< \frac{1}{\mathfrak{b}'} - \delta. \end{split}$$

With these p and q, we therefore deduce that there exists a constant C depending on d, a, p_0 and q such that

$$\|[K(\cdot-z),\boldsymbol{\rho}]\|_{1} \leq C h \left(R^{\frac{d}{2}\left(\frac{1}{b} - \frac{1}{p_{0}'}\right)} \|\rho_{1}\|_{L^{p_{0}}} + R^{\frac{d}{2}\left(\frac{1}{b} - \frac{1}{2p_{0}'} - \frac{1}{2q'}\right)} \|\rho_{1}\|_{L^{p_{0}}}^{\frac{1}{2}} \|\rho_{1}\|_{L^{q}}^{\frac{1}{2}} \right).$$

Optimizing with respect to R yields

(33)
$$\operatorname{Tr}(|[K(\cdot - z), \boldsymbol{\rho}]|) \leq C h \|\rho_1\|_{L^{p_0}}^{\theta_0} \|\rho_1\|_{L^q}^{1-\theta_0}$$

where $\theta_0 = \frac{1/p_0 - 1/\mathfrak{b}'}{1/p_0 - 1/q}$. In order to arrive to an equation on the form (27), we can define $\varepsilon := q - \mathfrak{b}'$, which is positive by Equation (32) and the fact that $p_0 < \mathfrak{b}'$. The condition $q \leq \mathfrak{b}'_3$ when $d \geq 4$ then reads $\varepsilon \leq \mathfrak{b}'_3 - \mathfrak{b}'$. We can also define $p := \mathfrak{b}' - \varepsilon \geq 1$. Then by a direct computation and using again (32), we obtain

$$p_0 - p = p_0 + q - 2\mathfrak{b}' > 0,$$

so that $p < p_0 < \mathfrak{b}' < q$ and by interpolation of Lebesgue spaces,

$$\|\rho_1\|_{L^{p_0}} \le \|\rho_1\|_{L^p}^{\theta_1} \|\rho_1\|_{L^q}^{1-\theta_1}$$

where $\theta_1 = \frac{1/p_0 - 1/q}{1/p - 1/q}$. Remarking that $\theta_0 \theta_1 = \frac{1/p_0 - 1/b'}{1/p - 1/q}$ and that we can take $\frac{1}{p_0}$ as close as we want from $\frac{1}{p}$, there exists ε_1 such that we can choose p_0 such that $\theta_0 \theta_1 + \varepsilon_1 = \frac{1/p - 1/b'}{1/p - 1/q} = \frac{1}{2} + \frac{\varepsilon}{2b'}$. Therefore, the last inequality combined with Inequality (33) leads to Formula (27).

The following Proposition is an extension of Theorem 4 to \mathcal{L}^p spaces, for $p < \mathfrak{b}$. Remark however that the right-side here is expressed in terms of weighted quantum Lebesgue norms, which makes the inequality weaker than the one in Theorem 4.

Proposition 4.3. Let $d \ge 2$, $a \in \left(-1, \min\left(2, \frac{d}{2}\right)\right)$, $1 \le p < \mathfrak{b} := \frac{d}{a+1}$. Then for any $\varepsilon \in (0, q-1)$ and n > a+1, there exists a constant C > 0 such that

$$\|[K(\cdot - z), \boldsymbol{\rho}]\|_{\mathcal{L}^{p}} \leq C h \|\nabla_{\xi} \boldsymbol{\rho} \, \boldsymbol{m}_{n}\|_{\mathcal{L}^{q+\varepsilon}}^{\frac{1}{2} + \tilde{\varepsilon}} \|\nabla_{\xi} \boldsymbol{\rho} \, \boldsymbol{m}_{n}\|_{\mathcal{L}^{q-\varepsilon}}^{\frac{1}{2} - \tilde{\varepsilon}},$$

where $\tilde{\varepsilon} = \varepsilon/q$, $\boldsymbol{m}_n = 1 + |\boldsymbol{p}|^n$ and with

$$\frac{1}{p} = \frac{1}{q} + \frac{1}{\mathfrak{b}}.$$

Proof. First we do the same decomposition as for the \mathcal{L}^1 case but then take a \mathcal{L}^p norm in (29). This yields

(34)
$$\frac{1}{h|\omega_a|} \|[K(\cdot - z), \boldsymbol{\rho}]\|_p \le \int_0^\infty \int_0^1 t^{\frac{a}{2}} \|\phi_\theta \cdot \nabla_{\xi} \boldsymbol{\rho} \varphi_{1-\theta}\|_p d\theta dt.$$

In order to bound this integral, we will cut it into two parts corresponding to $t \in (0,R)$ and when $t \geq R$, and we take $\frac{1}{q} > \frac{1}{p} - \frac{1}{\mathfrak{b}}$ when t is small, and $\frac{1}{q} < \frac{1}{p} - \frac{1}{\mathfrak{b}}$ in the second case. Using the hypotheses, we can find $(\alpha,\beta) \in [2,\infty)^2$ and $(n_{\alpha},n_{\beta}) \in (\frac{d}{\alpha},\infty) \times (\frac{d}{\beta},\infty)$ such that $\alpha > d$, $\beta > d/2$, $n_{\alpha} + n_{\beta} = n$ and $\frac{1}{\alpha} + \frac{1}{\beta} = \frac{1}{p} - \frac{1}{q}$. Then we define $\mathbf{m}_k := 1 + |\mathbf{p}|^k$ and multiply and divide by $\mathbf{m}_{n_{\alpha}}$

and m_{n_β} . This yields

$$\begin{aligned} \left\| \phi_{\theta} \cdot \nabla_{\xi} \boldsymbol{\rho} \, \varphi_{1-\theta} \right\|_{p} &= \left\| \left(\phi_{\theta} \, \boldsymbol{m}_{n_{\alpha}}^{-1} \right) \cdot \boldsymbol{m}_{n_{\alpha}} \nabla_{\xi} \boldsymbol{\rho} \, \boldsymbol{m}_{n_{\beta}} \, \boldsymbol{m}_{n_{\beta}}^{-1} \varphi_{1-\theta} \right\|_{p} \\ &\leq \left\| \phi_{\theta} \, \boldsymbol{m}_{n_{\alpha}}^{-1} \right\|_{\alpha} \left\| \boldsymbol{m}_{n_{\beta}}^{-1} \varphi_{1-\theta} \right\|_{\beta} \left\| \boldsymbol{m}_{n_{\alpha}} \nabla_{\xi} \boldsymbol{\rho} \, \boldsymbol{m}_{n_{\beta}} \right\|_{q}, \end{aligned}$$

where we used twice Holder's inequality for operators to get from the second to the third line. We remark that $\phi_{\theta} m_{n_{\alpha}}^{-1}$ is of the form $g(-i\nabla) f(x)$, so that since $\alpha \geq 2$, by the Kato-Seiler-Simon inequality (see e.g. [62, Thm 4.1]), it holds

$$\left\|\phi_{\theta} \, \boldsymbol{m}_{n_{\alpha}}^{-1}\right\|_{\alpha} \leq (2\pi)^{-\frac{d}{\alpha}} \left\|\phi_{\theta}\right\|_{L^{\alpha}} \left\|m_{n_{\alpha}}^{-1}(\hbar \cdot)\right\|_{L^{\alpha}},$$

with $m_{n_{\alpha}}^{-1}(\hbar x)=(1+|\hbar x|^{n_{\alpha}})^{-1}$. By the change of variable $y=\hbar\,x$ in the last integral, and using the fact that $C_{d,n_{\alpha},\alpha}:=\left\|m_{n_{\alpha}}^{-1}\right\|_{L^{\alpha}}<\infty$, this yields

$$\|\phi_{\theta} \, \boldsymbol{m}_{n_{\alpha}}^{-1}\|_{\alpha} \leq C_{d,n_{\alpha},\alpha} \, h^{-\frac{d}{\alpha}} \|\phi_{\theta}\|_{L^{\alpha}}.$$

Then a direct computation of the integral of ϕ_{θ} yields

$$\left\|\phi_{\theta} \, \boldsymbol{m}_{n_{\alpha}}^{-1}\right\|_{\alpha} \leq C_{d,n_{\alpha},\alpha} \, h^{-\frac{d}{\alpha}} \left(\frac{\omega_{d}}{\omega_{d+\alpha}}\right)^{\frac{1}{\alpha}} \frac{1}{\left(\alpha\theta t\right)^{\frac{d+\alpha}{2\alpha}}}.$$

By the same proof but replacing ϕ_{θ} by $\varphi_{1-\theta}$, if $\beta \geq 2$, we have

$$\left\|\boldsymbol{m}_{n_{\beta}}^{-1}\varphi_{1-\theta}\right\|_{\beta} \leq C_{d,n_{\beta},\beta} h^{-\frac{d}{\beta}} \frac{1}{(\beta(1-\theta)t)^{\frac{d}{2\beta}}}.$$

Therefore, (34) leads to

$$\begin{aligned} \|[K(\cdot - z), \boldsymbol{\rho}]\|_{p} &\leq \int_{0}^{\infty} \frac{C_{\boldsymbol{\rho}} h^{1 - d\left(\frac{1}{\alpha} + \frac{1}{\beta}\right)}}{t^{\frac{1}{2}\left(\frac{d}{\alpha} + \frac{d}{\beta} + 1 - a\right)}} \left(\int_{0}^{1} \frac{\mathrm{d}\theta}{\theta^{\frac{d + \alpha}{2\alpha}} \left(1 - \theta\right)^{\frac{d}{2\beta}}} \right) \mathrm{d}t \\ &\leq \int_{0}^{\infty} \frac{C_{\boldsymbol{\rho}} h^{1 + \frac{d}{p'} - \frac{d}{q'}}}{t^{\frac{d}{2}\left(\frac{1}{p} - \frac{1}{q} - \frac{1}{b}\right) + 1}} \left(\int_{0}^{1} \frac{\mathrm{d}\theta}{\theta^{\frac{d + \alpha}{2\alpha}} \left(1 - \theta\right)^{\frac{d}{2\beta}}} \right) \mathrm{d}t, \end{aligned}$$

where $C_{\rho} = \left(\frac{\omega_d}{\omega_{d+\alpha}}\right)^{\frac{1}{\alpha}} \frac{C_{d,n_{\alpha},\alpha}C_{d,n_{\beta},\beta}}{\beta^{\frac{d}{2}\beta}\alpha^{\frac{d+\alpha}{2}\alpha}} \|\boldsymbol{m}_{n_{\alpha}}\nabla_{\xi}\rho\,\boldsymbol{m}_{n_{\beta}}\|_{q}$. The integrals in θ and t converge since

$$\begin{split} \alpha > d & \text{ and } \beta > \frac{d}{2} \\ \frac{1}{p} - \frac{1}{q} < \frac{1}{\mathfrak{b}} & \text{if } t \in [0, R] \\ \frac{1}{p} - \frac{1}{a} > \frac{1}{\mathfrak{b}} & \text{if } t \in (R, \infty). \end{split}$$

Then remark that as proved in appendix (Inequality (56)), it holds

$$\left\|oldsymbol{m}_{n_{lpha}}oldsymbol{
abla}_{\xi}oldsymbol{
ho}\,oldsymbol{m}_{n_{eta}}
ight\|_{q} \leq \left\|oldsymbol{
abla}_{\xi}oldsymbol{
ho}\,oldsymbol{m}_{n_{eta}}oldsymbol{m}_{n_{lpha}}
ight\|_{q} = \left\|oldsymbol{
abla}_{\xi}oldsymbol{
ho}\,oldsymbol{m}_{n_{eta}}
ight\|_{q},$$

and we can conclude by taking the optimal R as in the proof of Theorem 4. \square

4.2. Bound for the error term.

Proposition 4.4. Under the hypotheses of Theorem 1, if $p \in [1,2]$ and $n \in 2\mathbb{N}$ with n > d/2, then

$$||B_t||_{\mathcal{L}^p} \le C \,\hbar^2 \,||\rho_f||_{L^1 \cap H^{\nu}} \,||\nabla_{\xi}^2 f||_{H^{2n}_{\sigma}(\mathbb{R}^{2d})},$$

where $\nu = (n + a + 2 - d)_+$ and C is independent from \hbar .

Proof. As in [61, 60], we decompose B_t as follow

$$\frac{1}{i\hbar}B_t(x,y) = \int_0^1 E((1-\theta)x + \theta y) - E\left(\frac{x+y}{2}\right) d\theta \cdot \nabla_{\xi} \boldsymbol{\rho}_f(x,y)$$

$$= i\hbar \int_0^1 \int_0^1 \left(\theta - \frac{1}{2}\right) \nabla E\left(((1-\theta)x + \theta y)\theta' + \frac{x+y}{2}(1-\theta')\right) d\theta d\theta' : \nabla_{\xi}^2 \boldsymbol{\rho}_f(x,y)$$

$$= i\hbar \int_0^1 \int_0^1 \left(\theta - \frac{1}{2}\right) \nabla E\left(a_{\theta,\theta'}x + b_{\theta,\theta'}y\right) d\theta d\theta' : \nabla_{\xi}^2 \boldsymbol{\rho}_f(x,y)$$

where $a_{\theta,\theta'} = \frac{\theta'+1}{2} - \theta\theta'$ and $b_{\theta,\theta'} = \frac{1-\theta'}{2} + \theta\theta'$. In term of the Fourier transform of ∇E , this yields

$$\frac{1}{i\hbar}B_t(x,y) = i\hbar \int_0^1\!\int_0^1\int_{\mathbb{R}^d} \left(\theta - \frac{1}{2}\right)e^{2i\pi z\cdot(a_{\theta,\theta'}x + b_{\theta,\theta'}y)}\,\widehat{\nabla E}\left(z\right)\mathrm{d}\theta\,\mathrm{d}\theta'\,\mathrm{d}z: \boldsymbol{\nabla}_{\xi}^2\boldsymbol{\rho}_f(x,y).$$

Defining e_{ω} as the operator of multiplication by the function $e^{2i\pi\omega}$, we obtain

$$\frac{1}{i\hbar}B_t = i\hbar \int_0^1 \int_0^1 \int_{\mathbb{R}^d} \left(\theta - \frac{1}{2}\right) \widehat{\nabla E}(z) : e_{a_{\theta,\theta'}} \left(\nabla_{\xi}^2 \rho_f\right) e_{b_{\theta,\theta'}} d\theta d\theta' dz,$$

and since e_{ω} is a bounded (unitary) operator, taking the quantum Lebesgue norms yields

$$\frac{1}{\hbar} \|B_t\|_{\mathcal{L}^p} \leq \hbar \int_0^1 \int_0^1 \int_{\mathbb{R}^d} \left| \theta - \frac{1}{2} \right| \left| \widehat{\nabla E}(z) \right| \left\| e_{a_{\theta,\theta'}} \left(\nabla_{\xi}^2 \rho_f \right) e_{b_{\theta,\theta'}} \right\|_{\mathcal{L}^p} d\theta d\theta' dz$$

$$\leq \frac{\hbar}{2} \|\nabla E\|_{\mathcal{F}(L^1)} \|\nabla_{\xi}^2 \rho_f\|_{\mathcal{L}^p}.$$

• Now to bound $\|\nabla E\|_{\mathcal{F}(L^1)}$, we can use the fact that for any n > d/2, $H^n \subset \mathcal{F}(L^1)$ to get

$$\left\|\nabla E\right\|_{\mathcal{F}(L^1)} \le C_{d,n} \left\|\nabla^2 K * \rho_f\right\|_{H^n}.$$

If a = d - 2, then by continuity of $\nabla^2 K * \cdot$ in H^n , we get $\|\nabla E\|_{\mathcal{F}(L^1)} \leq C \|\rho_f\|_{H^n}$. Else if $a \in \left(\frac{d}{2} - 2, d\right) \setminus \{2\}$

$$\|\nabla E\|_{\mathcal{F}(L^{1})} \leq C_{d,n,a} \|(1+|x|^{n})|x|^{a+2-d} \widehat{\rho_{f}}\|_{L^{2}} \leq C_{d,n,a} \|\rho_{f}\|_{\dot{H}^{a+2-d} \cap \dot{H}^{n+a+2-d}}$$
$$\leq C_{d,n,a} \|\rho_{f}\|_{L^{1} \cap \dot{H}^{(n+a+2-d)+}}$$

where we used the fact that if $\alpha \in (-\frac{d}{2}, 0)$, then by Sobolev's inequalities $L^{p^*} \subset \dot{H}^{\alpha}$ with $\frac{1}{p^*} = \frac{1}{2} - \frac{\alpha}{d}$, and then $L^2 \cap L^1 \subset L^{p^*}$ since $p^* \in [1, 2]$.

• Finally, to bound $\|\nabla_{\xi}^2 \rho_f\|_{\mathcal{L}^p}$, we interpolate it between the \mathcal{L}^1 and the \mathcal{L}^2 norms to get

(35)
$$\|\nabla_{\xi}^{2} \rho_{f}\|_{\mathcal{L}^{p}} \leq \|\nabla_{\xi}^{2} \rho_{f}\|_{\mathcal{L}^{2}}^{\theta} \|\nabla_{\xi}^{2} \rho_{f}\|_{\mathcal{L}^{1}}^{1-\theta} = \|\nabla_{\xi}^{2} f\|_{L^{2}(\mathbb{R}^{2d})}^{\theta} \|\nabla_{\xi}^{2} \rho_{f}\|_{\mathcal{L}^{1}}^{1-\theta}$$

where $\theta = 2/p'$. Then using the fact that $\nabla_{\xi}^2 \rho_f = \rho_{\hbar}^W (\nabla_{\xi}^2 f)$, we can use Proposition 3.3 with $g = \nabla_{\xi}^2 f$, $n_1 = 0$ and n > d/2 to get

$$\left\| \nabla_{\xi}^{2} \rho_{f} \right\|_{\mathcal{L}^{1}} \leq C \left\| \nabla_{\xi}^{2} f \right\|_{H_{s}^{2n}(\mathbb{R}^{2d})},$$

which using Inequality (35) implies that $\|\nabla_{\xi}^{2} \rho_{f}\|_{\mathcal{L}^{p}} \leq C \|\nabla_{\xi}^{2} f\|_{H_{s}^{2n}(\mathbb{R}^{2d})}$.

4.3. **Proof of Proposition 4.1.** We can now use the bounds on the commutator and the error terms proved in previous sections to prove the stability estimate of Proposition 4.1.

Proof of Proposition 4.1. For p = 1, Equation (26) yields

$$\begin{split} \operatorname{Tr} \left(\left| \boldsymbol{\rho}(t) - \boldsymbol{\rho}_f(t) \right| \right) &\leq \operatorname{Tr} \left(\left| \boldsymbol{\rho}^{\text{in}} - \boldsymbol{\rho}_f^{\text{in}} \right| \right) + \frac{1}{\hbar} \int_0^t \operatorname{Tr} (|B_s|) \, \mathrm{d}s \\ &+ \frac{1}{\hbar} \int_0^t \int \left| \rho(s, z) - \rho_f(s, z) \right| \, \operatorname{Tr} \left(\left| \left[K(\cdot - z), \boldsymbol{\rho}_f(s) \right] \right| \right) \, \mathrm{d}z \, \mathrm{d}s. \end{split}$$

Proposition 4.4 gives a bound on the second term on the right-hand side, whereas Theorem 4 allows us to bound the last term on the right-hand side uniformly in z. Moreover, because of (12) we have

$$\|\rho - \rho_f\|_{L^1} \le \operatorname{Tr}(|\boldsymbol{\rho} - \boldsymbol{\rho}_f|)$$
.

Altogether, we obtain for some small $\varepsilon > 0$ to be chosen later

$$\begin{split} \operatorname{Tr} \left(\left| \boldsymbol{\rho} - \boldsymbol{\rho}_f \right| \right) &\leq \operatorname{Tr} \left(\left| \boldsymbol{\rho}^{\text{in}} - \boldsymbol{\rho}_f^{\text{in}} \right| \right) \\ &+ C \, \hbar \int_0^t \left\| \rho_f(s) \right\|_{L^1 \cap H^{(n+a+2-d)_+}} \left\| \nabla_\xi^2 f(s) \right\|_{H^{2n}_{2n}(\mathbb{R}^{2d})} \mathrm{d}s \\ &+ C \int_0^t \operatorname{Tr} \left(\left| \boldsymbol{\rho}(s) - \boldsymbol{\rho}_f(s) \right| \right) \left\| \operatorname{diag} \left(\left| \boldsymbol{\nabla}_\xi \boldsymbol{\rho}_f(s) \right| \right) \right\|_{L^{\mathfrak{b}' + \varepsilon} \cap L^{\mathfrak{b}' - \varepsilon}} \mathrm{d}s \end{split}$$

where $\mathfrak{b}' = \frac{d}{d-a+1}$. We then use Proposition 3.1 to bound the L^p norm of the diagonal for $p = \mathfrak{b}' + \varepsilon$ and $p = \mathfrak{b}' - \varepsilon$

$$\left\|\operatorname{diag}(\left|\nabla_{\xi}\boldsymbol{\rho}_{f}\right|)\right\|_{L^{p}} \leq \mathcal{C}_{d,n_{1}} \left\|\nabla_{\xi}f\right\|_{W^{n_{0},\infty}(\mathbb{R}^{2d})\cap H_{2n+n_{1}}^{2n+n_{1}}(\mathbb{R}^{2d})},$$

where since $n_1 > \frac{d}{\mathfrak{b}-1} = d(\mathfrak{b}'-1)$ we can choose ε such that $\mathfrak{b}' + \varepsilon \leq 1 + \frac{n_1}{d}$. We conclude by Grönwall's Lemma.

4.4. End of the Proof of Theorem 1.

Proof of Theorem 1. To prove this theorem, it just remains to prove that the assumptions (25a) and (25b) are satisfied with our choice of initial conditions, which will imply the result by Proposition 4.1. But these bounds are only about the solution of the classical Vlasov equation for which the long time existence of regular solutions is known. More precisely, we prove the regularity we need in our case in Proposition A.1 in appendix. With our assumptions on the initial data, we have $f^{\rm in} \in W^{\sigma+1,\infty}_m(\mathbb{R}^{2d})$ with m>d. Moreover, since $f^{\rm in} \in H^{\sigma+1}_\sigma(\mathbb{R}^{2d})$ with $\sigma>m+\frac{d}{\mathfrak{b}-1}$, by Hölder's inequality we deduce in particular that $f^{\rm in} \in L^2_\sigma(\mathbb{R}^{2d})$ which by Hölder's inequality yields

$$\iint_{\mathbb{R}^{2d}} f^{\mathrm{in}} |\xi|^{n_1} \, \mathrm{d}x \, \mathrm{d}\xi < \infty$$

for some $n_1 > \frac{d}{b-1}$. Therefore, Proposition A.1 indeed lead to

$$f \in L^{\infty}_{\mathrm{loc}}(\mathbb{R}_+, W^{\sigma+1,\infty}_m(\mathbb{R}^{2d}) \cap H^{\sigma+1}_{\sigma}(\mathbb{R}^{2d})).$$

where we remark that $\sigma > n_0 := \left\lfloor \frac{d}{2} \right\rfloor + 1$. Finally, the H^{ν} bound for ρ also follows from Hölder's inequality since $\sigma > d/2$ so that

$$\left\| \nabla^{\lceil \nu \rceil} \rho \right\|_{L^2} \le \left\| \int_{\mathbb{R}^d} \left| \nabla_x^{\lceil \nu \rceil} f \right| d\xi \right\|_{L^2} \le C_{d,\sigma} \left\| \langle \xi \rangle^{\sigma} \nabla_x^{\lceil \nu \rceil} f \right\|_{L^2(\mathbb{R}^{2d})} \le C \left\| f \right\|_{H^{\sigma+1}_{\sigma}(\mathbb{R}^{2d})},$$

where the last inequality follows from the fact that $\lceil \nu \rceil \leq \sigma + 1$.

4.5. **Proof of Theorem 2.** We now prove Theorem 2 using also the results of Propositions 4.3 and 4.4.

Proof of Theorem 2. Recall Equation (26). The bound (12) yields

$$\begin{aligned} \left\| \boldsymbol{\rho} - \boldsymbol{\rho}_f \right\|_{\mathcal{L}^p} &\leq \left\| \boldsymbol{\rho}^{\text{in}} - \boldsymbol{\rho}_f^{\text{in}} \right\|_{\mathcal{L}^p} + \frac{1}{\hbar} \int_0^t \left\| B_t \right\|_{\mathcal{L}^p} \mathrm{d}s \\ &+ \frac{1}{\hbar} \int_0^t \mathrm{Tr} \left(\left| \boldsymbol{\rho} - \boldsymbol{\rho}_f \right| \right) \sup_z \left\| \left[K(\cdot - z), \boldsymbol{\rho}_f \right] \right\|_{\mathcal{L}^p} \mathrm{d}s. \end{aligned}$$

The second term on the right-hand side can be estimated thanks to Proposition 4.4 and can then be bounded as in the case p=1. The last term on the right-hand side is bounded by Proposition 4.3 by terms of the form $\|\nabla_{\xi} \boldsymbol{\rho}_f \boldsymbol{m}_n\|_{\mathcal{L}^q}$ with $\boldsymbol{m}_n = 1 + |\boldsymbol{p}|^n$, $n > a + 1 = \frac{d}{\mathfrak{b}}$ and $\frac{1}{q}$ close to $\frac{1}{p} - \frac{1}{\mathfrak{b}}$. When $a < \frac{d-2}{2}$, then $q \leq 2$ and we can bound them by interpolating them between \mathcal{L}^1 and \mathcal{L}^2 weighted norms, yielding

$$\left\|\boldsymbol{\nabla}_{\!\boldsymbol{\xi}}\boldsymbol{\rho}_{\!f}\,\boldsymbol{m}_{\!n}\right\|_{\mathcal{L}^{q}}\leq\left\|\boldsymbol{\nabla}_{\!\boldsymbol{\xi}}\boldsymbol{\rho}_{\!f}\,\boldsymbol{m}_{\!n}\right\|_{\mathcal{L}^{2}}^{2/q'}\left\|\boldsymbol{\nabla}_{\!\boldsymbol{\xi}}\boldsymbol{\rho}_{\!f}\,\boldsymbol{m}_{\!n}\right\|_{\mathcal{L}^{1}}^{1-2/q'},$$

and we can bound these terms by Proposition 3.2 and Proposition 3.3. When q>2, this strategy is no more possible, but remark that by the property of the Weyl transform and Calderón-Vaillancourt-Boulkhemair inequality (24), we know that

$$\left\| \boldsymbol{\rho}_{\hbar}^{W}(g) \right\|_{\mathcal{L}^{2}} = \left\| g \right\|_{L^{2}(\mathbb{R}^{2d})}$$
$$\left\| \boldsymbol{\rho}_{\hbar}^{W}(g) \right\|_{\mathcal{L}^{\infty}} \leq C_{d} \left\| g \right\|_{W^{n_{0},\infty}(\mathbb{R}^{2d})},$$

where $n_0 = \left| \frac{d}{2} \right| + 1$. Therefore, we get

(36)
$$\|\boldsymbol{\rho}_{\hbar}^{W}(g)\|_{\mathcal{L}^{q}} \leq C_{d}^{\theta} \|\boldsymbol{\rho}_{\hbar}^{W}(g)\|_{\mathcal{L}^{\infty}}^{\theta} \|\boldsymbol{\rho}_{\hbar}^{W}(g)\|_{\mathcal{L}^{2}}^{1-\theta}$$
$$\leq C_{d}^{\theta} \|g\|_{W^{n_{0},\infty}(\mathbb{R}^{2d})}^{\theta} \|g\|_{L^{2}(\mathbb{R}^{2d})}^{1-\theta},$$

where $\theta=1-\frac{2}{q}$ is close to $\frac{2}{p'}-\frac{1}{\mathfrak{b}'}\pm\varepsilon$, and the second inequality comes again from complex interpolation. Using Lemma 3.1, we see that $\nabla_{\xi}\rho_{f}m_{n}$ can be written as a linear combination of terms of the form $\rho_{\hbar}^{W}(\xi^{\alpha}\partial_{x}^{\beta}\nabla_{\xi}f)=:\rho_{\hbar}^{W}(g_{\alpha,\beta})$ where α and β are multi-indices verifying $|\alpha+\beta|\leq n$. Therefore, taking $g=g_{\alpha,\beta}$ in inequality (36) for each $g_{\alpha,\beta}$, we obtain a control in terms of weighted Sobolev norms of the solution f of the classical solution of the Vlasov equation (1) of the form $\|f\|_{W_{\sigma}^{\sigma+1,\infty}(\mathbb{R}^{2d})\cap H_{\sigma}^{\sigma+1}(\mathbb{R}^{2d})}$ with $\sigma>n_0+d/\mathfrak{b}$, which can be controlled as in the proof of Theorem 1. We can therefore conclude by Grönwall's Lemma that Inequality (13) holds.

Now we prove Formula (14). Consider Equation (13) and the following bound:

(37)
$$\|\boldsymbol{\rho} - \boldsymbol{\rho}_f\|_{\mathcal{L}^{\infty}} \leq \|\boldsymbol{\rho}\|_{\mathcal{L}^{\infty}} + \|\boldsymbol{\rho}_f\|_{\mathcal{L}^{\infty}}.$$

As for the first term in the right-hand side, we know that all \mathcal{L}^p norms are propagated by the Hartree equation, therefore $\|\boldsymbol{\rho}\|_{\mathcal{L}^{\infty}} = \|\boldsymbol{\rho}^{\text{in}}\|_{\mathcal{L}^{\infty}}$, that is bounded by assumption. In the second term in the right-hand side we use again the Calderón-Vaillancourt-Boulkhemair inequality (24). Hence, if $f \in W^{n_0,\infty}(\mathbb{R}^{2d})$ and $\boldsymbol{\rho}^{\text{in}} \in \mathcal{L}^{\infty}$, the \mathcal{L}^{∞} norm of the difference $\boldsymbol{\rho} - \boldsymbol{\rho}_f$ is bounded uniformly in \hbar . To conclude, we use the complex interpolation theorem between \mathcal{L}^{∞} and \mathcal{L}^p , with $p = \mathfrak{b} - \varepsilon$, for $\varepsilon > 0$ small enough, and get

$$\left\|oldsymbol{
ho} - oldsymbol{
ho}_f
ight\|_{\mathcal{L}^q} \leq \left\|oldsymbol{
ho} - oldsymbol{
ho}_f
ight\|_{\mathcal{L}^\infty}^{rac{p}{q}} \left\|oldsymbol{
ho} - oldsymbol{
ho}_f
ight\|_{\mathcal{L}^\infty}^{1-rac{p}{q}},$$

since $q \in (p, \infty)$. Then Formula (13) yields

$$\left\|\boldsymbol{\rho} - \boldsymbol{\rho}_f\right\|_{\mathcal{L}^q} \le C(t) \left(\left\|\boldsymbol{\rho}^{\text{in}} - \boldsymbol{\rho}_f^{\text{in}}\right\|_{\mathcal{L}^p}^{\frac{p}{q}} + \text{Tr}\left(\left|\boldsymbol{\rho}^{\text{in}} - \boldsymbol{\rho}_f^{\text{in}}\right|\right)^{\frac{p}{q}} + \hbar^{\frac{p}{q}}\right) e^{\lambda(t)},$$

where C is a constant which depends on the dimension of the space d, on $\|\boldsymbol{\rho}^{\text{in}}\|_{\mathcal{L}^{\infty}}$ and on f^{in} .

5. Proof of Theorem 3

We recall that $X = X_{\rho}$ is the operator of time dependent kernel $X_{\rho}(x,y) = K(x-y) \rho(x,y)$, where ρ is the kernel of the operator ρ . Under the conditions of Theorem 3, the associated energy is bounded and we have the following inequalities

Proposition 5.1. Let $a \in [0, d)$, s := d - a and ρ be a positive trace class operator. Then if $K \in \dot{H}^{s,1}_w$, it holds

(38)
$$\operatorname{Tr}(\mathsf{X}\boldsymbol{\rho}) \leq C h^{s} \|K\|_{\dot{H}_{w}^{s,1}} \left\| |\boldsymbol{p}|^{\frac{a}{2}} \boldsymbol{\rho} \right\|_{\mathcal{L}^{2}}^{2}.$$

Moreover, if $a \in [0, \frac{d}{2})$ and $K^2 \in \dot{H}_w^{2s-d,1}$, then for any $p \in [1, 2]$ and $q = \frac{2p}{2-p} \in [2, \infty]$ there exists a constant such that for any operator ρ_2

(39a)
$$\|X_{\rho} \rho_{2}\|_{\mathcal{L}^{p}} \leq C h^{s} \|K^{2}\|_{\dot{H}_{w}^{2s-d,1}}^{\frac{1}{2}} \||p|^{\frac{a}{2}} \rho\|_{\mathcal{L}^{2}} \|\rho_{2}\|_{\mathcal{L}^{q}}.$$

When $p \in [2, \infty]$ then we still have

(39b)
$$\|X_{\rho} \rho_{2}\|_{\mathcal{L}^{p}} \leq C h^{s+d\left(\frac{1}{p}-\frac{1}{2}\right)} \|K^{2}\|_{\dot{H}^{2s-d,1}}^{\frac{1}{2}} \||p|^{\frac{a}{2}} \rho\|_{c_{2}} \|\rho_{2}\|_{\mathcal{L}^{\infty}},$$

where in both (39a) and (39b) the constants C depend only on s and d.

Remark 5.1. We can control the weighted \mathcal{L}^2 norms by the following inequality

(40)
$$\left\| |\boldsymbol{p}|^{\frac{a}{2}} \boldsymbol{\rho} \right\|_{\mathcal{L}^{2}}^{2} \leq \|\boldsymbol{\rho}\|_{\mathcal{L}^{\infty}} \operatorname{Tr}(|\boldsymbol{p}|^{a} \boldsymbol{\rho}).$$

Remark that we cannot deduce it immediately by Hölder's inequality for the Schatten norms because it would give us $\operatorname{Tr}(||\boldsymbol{p}|^a\boldsymbol{\rho}|)$ instead of $\operatorname{Tr}(|\boldsymbol{p}|^a\boldsymbol{\rho})$ in the right-hand side. However, by definition of the absolute value for operators and by cyclicity of the trace, we get

$$\left\| \left| \boldsymbol{p} \right|^{\frac{a}{2}} \boldsymbol{\rho} \, \right\|_2^2 = \mathrm{Tr}(\boldsymbol{\rho} \, |\boldsymbol{p}|^a \, \boldsymbol{\rho}) = \mathrm{Tr}\Big(\boldsymbol{\rho} \, \boldsymbol{\rho}^{\frac{1}{2}} \, |\boldsymbol{p}|^a \, \boldsymbol{\rho}^{\frac{1}{2}} \Big) = \mathrm{Tr}\bigg(\boldsymbol{\rho} \, \left| \left| \boldsymbol{p} \right|^{\frac{a}{2}} \boldsymbol{\rho}^{\frac{1}{2}} \right|^2 \bigg) \, .$$

Now, Hölder's inequality gives

$$\operatorname{Tr}\left(oldsymbol{
ho}\left\|oldsymbol{p}
ight\|_{2}^{rac{a}{2}}oldsymbol{
ho}^{rac{1}{2}}
ight)\leq\left\|oldsymbol{
ho}
ight\|_{\infty}\operatorname{Tr}\left(\left\|oldsymbol{p}
ight\|_{2}^{rac{a}{2}}oldsymbol{
ho}^{rac{1}{2}}
ight)^{2}
ight)=\left\|oldsymbol{
ho}
ight\|_{\infty}\operatorname{Tr}\left(\left\|oldsymbol{p}
ight\|^{a}oldsymbol{
ho}
ight),$$

which leads to (40) by the definition of \mathcal{L}^2 and \mathcal{L}^{∞} .

Proof of Proposition 5.1. We first prove Inequality (38) and then use it to show formulas (39a) and (39b).

• Proof of Inequality (38). Let a := d - s and use Formula (15) to get that

$$\iint_{\mathbb{R}^{2d}} K(x-y) \left| \boldsymbol{\rho}(x,y) \right|^2 dx dy = c_{d,a} \int_{\mathbb{R}^d} \left(\iint_{\mathbb{R}^{2d}} \frac{\left| \boldsymbol{\rho}(x,y) \right|^2}{\left| x - y - w \right|^a} dx dy \right) Q(dw),$$

for some measure Q such that $||Q||_{\text{TV}} = ||K||_{\dot{H}^{s,1}_{w}}$. This leads to

$$\mathcal{E}_{\mathsf{X}} \le c_{d,a} \sup_{w \in \mathbb{R}^d} \left(\iint_{\mathbb{R}^{2d}} \frac{|\boldsymbol{\rho}(x,y)|^2}{|x - y - w|^a} \, \mathrm{d}x \, \mathrm{d}y \right) \|Q\|_{\mathsf{TV}}.$$

Now we concentrate on bounding the double integral. First we remark that by the change of variable z = x - y - w, it holds

$$\mathcal{E}_a := \iint_{\mathbb{R}^{2d}} \frac{|\rho(x,y)|^2}{|x-y-w|^a} dx dy = \iint_{\mathbb{R}^{2d}} \frac{1}{|z|^a} |\rho(z+y+w,y)|^2 dz dy.$$

Then, by the Hardy-Rellich inequality (see e.g. [65]), since $a \in [0, d)$, for any $\varphi \in H^{\frac{a}{2}}$, it holds

$$\int_{\mathbb{R}^d} \frac{|\varphi(z)|^2}{|z|^a} \, \mathrm{d}z \le \mathcal{C}_{d,a} \int_{\mathbb{R}^d} \left| \Delta^{\frac{a}{4}} \varphi(z) \right|^2 \, \mathrm{d}z.$$

Therefore, taking $\varphi(z) = \rho(z+y+w,y)$ in the above inequality and integrating with respect to y yields

$$\mathcal{E}_a \leq \mathcal{C}_{d,a} \iint_{\mathbb{R}^{2d}} \left| \Delta_z^{\frac{a}{4}} \boldsymbol{\rho}(z+y+w,y) \right|^2 dz dy = \mathcal{C}_{d,a} \iint_{\mathbb{R}^{2d}} \left| \Delta_x^{\frac{a}{4}} \boldsymbol{\rho}(x,y) \right|^2 dx dy.$$

Remarking that $\Delta_x^{\frac{a}{4}} \rho(x, y)$ is nothing but the kernel of the operator $\hbar^{-\frac{a}{2}} |p|^{\frac{a}{2}} \rho$ and using the definition of the \mathcal{L}^2 norm, we obtain

$$\mathcal{E}_a \leq C_{d,a} h^{d-a} \left\| |\boldsymbol{p}|^{\frac{a}{2}} \boldsymbol{\rho} \right\|_{\mathcal{L}^2}^2,$$

where $C_{d,a} = (2\pi)^a \mathcal{C}_{d,a}$.

• Proof of Inequality (39a). Since X_{ρ} is a positive operator, it holds $X_{\rho}^2 = |X_{\rho}|^2$. Moreover, denoting \tilde{X}_{ρ} the exchange operator associated to the kernel K^2 , the following interesting property holds

$$\operatorname{Tr}(\mathsf{X}_{\boldsymbol{\rho}}^2) = \iint_{\mathbb{R}^{2d}} K(x-y)^2 \left| \boldsymbol{\rho}(x,y) \right|^2 \mathrm{d}x \, \mathrm{d}y = \operatorname{Tr}(\tilde{\mathsf{X}}_{\boldsymbol{\rho}} \, \boldsymbol{\rho}).$$

From this and Hölder's inequality for operators, we deduce that if $K^2 \in \dot{H}_w^{2s-d,1}$ with $s \in \left(\frac{d}{2}, d\right]$, then the following inequality holds

$$\left\| \mathsf{X}_{\boldsymbol{\rho}} \, \boldsymbol{\rho}_{2} \right\|_{p} \leq \left\| \boldsymbol{\rho}_{2} \right\|_{q} \left\| \mathsf{X}_{\boldsymbol{\rho}} \right\|_{2} \leq h^{\frac{d}{q'}} \left\| \boldsymbol{\rho}_{2} \right\|_{\mathcal{L}^{q}} \mathrm{Tr} \big(\tilde{\mathsf{X}}_{\boldsymbol{\rho}} \, \boldsymbol{\rho} \big)^{\frac{1}{2}} \,,$$

which by Formula (38) for K^2 leads exactly to (39a).

• Proof of Inequality (39b). We use the fact that $\|X_{\rho} \rho_2\|_p \leq \|X_{\rho} \rho_2\|_2$ for any $p \geq 2$ and then we use (39a) for p = 2 to get

$$\|\mathsf{X}_{\rho}\,\rho_{2}\|_{\mathcal{L}^{p}} \leq h^{\left(\frac{d}{2} - \frac{d}{p'}\right)} \, \|\mathsf{X}_{\rho}\,\rho_{2}\|_{\mathcal{L}^{2}} \leq C \, h^{s + d\left(\frac{1}{p} - \frac{1}{2}\right)} \, \|K^{2}\|_{\dot{H}^{2s - d, 1}_{w}}^{\frac{1}{2}} \, \||p|^{\frac{a}{2}} \, \rho \, \|_{\mathcal{L}^{2}} \, \|\rho\|_{\mathcal{L}^{\infty}} \, .$$

The use of the non-semiclassical inequality $\|X_{\rho} \rho_2\|_p \le \|X_{\rho} \rho_2\|_2$ explains the deterioration of the rate, which might not be optimal.

When a < 0, we have similar bounds but using moments in x instead of moments in p.

Proposition 5.2. Let a < 0 and $K(x) = |x|^{|a|}$, then for any positive operator ρ

(41)
$$\operatorname{Tr}(\mathsf{X}\boldsymbol{\rho}) \le C h^d \left\| |x|^{\frac{|a|}{2}} \boldsymbol{\rho} \right\|_{\mathcal{L}^2}^2.$$

Moreover, for any $p \in [1, \infty]$, there exists a constant C > 0 such that for any operator ρ_2

(42a)
$$\|X_{\rho} \rho_2\|_{\mathcal{L}^p} \le C h^d \||x|^{\frac{|a|}{2}} \rho\|_{\mathcal{L}^2} \|\rho_2\|_{\mathcal{L}^q}$$
 when $p \in [1, 2)$

where $q = \frac{2p}{2-p} \in [2,\infty)$ when p < 2 and the constants C depend only on a and d.

Proof. The proof of (41) follows simply by writing

$$\iint_{\mathbb{R}^{2d}} K(x-y) \left| \boldsymbol{\rho}(x,y) \right|^2 dx dy \le C \iint_{\mathbb{R}^{2d}} \left(\left| x \right|^{|a|} + \left| y \right|^{|a|} \right) \left| \boldsymbol{\rho}(x,y) \right|^2 dx dy$$

and remarking that the right-hand side is exactly the right-hand side of inequality (41). The two other inequalities follow by taking K^2 instead of K and Hölder's inequality as in the proof of Proposition 5.2.

Proof of Theorem 3. We proceed as in the proof of Theorem 1 and consider the one-parameter group of unitary transformations \mathcal{U}_t generated by the Hartree-Fock Hamiltonian, i.e.

$$i \hbar \partial_t \mathcal{U}_t = H_{HF}(t) \mathcal{U}_t$$
,

and compute

$$i \,\hbar \,\partial_t \left(\mathcal{U}_t^* \left(\boldsymbol{\rho} - \boldsymbol{\rho}_{\hbar}^W(f) \right) \mathcal{U}_t \right) = \mathcal{U}_t^* \left[K * (\rho - \rho_f), \boldsymbol{\rho}_{\hbar}^W(f) \right] \mathcal{U}_t$$
$$+ \mathcal{U}_t^* B_t \,\mathcal{U}_t - \mathcal{U}_t^* \left[\mathsf{X}_{\boldsymbol{\rho}}, \left(\boldsymbol{\rho} - \boldsymbol{\rho}_{\hbar}^W(f) \right) \right] \mathcal{U}_t.$$

Using Duhamel formula and taking the \mathcal{L}^p norm using that \mathcal{U}_t is a unitary operator, we obtain

(43)
$$\| \boldsymbol{\rho} - \boldsymbol{\rho}_{\hbar}^{W}(f) \|_{\mathcal{L}^{p}} \leq \| \boldsymbol{\rho}^{\text{in}} - \boldsymbol{\rho}_{f}^{\text{in}} \|_{\mathcal{L}^{p}} + \frac{1}{\hbar} \int_{0}^{t} \| [K * (\rho - \rho_{f}), \boldsymbol{\rho}_{\hbar}^{W}(f)] \|_{\mathcal{L}^{p}} \, ds$$

 $+ \frac{1}{\hbar} \int_{0}^{t} \| B_{s} \|_{\mathcal{L}^{p}} \, ds + \frac{1}{\hbar} \int_{0}^{t} \| [X_{\boldsymbol{\rho}}, (\boldsymbol{\rho} - \boldsymbol{\rho}_{\hbar}^{W}(f))] \|_{\mathcal{L}^{p}} \, ds.$

The second and third terms on the right-hand side in (43) can be bounded as in Theorem 1. As for the fourth term, we use Proposition 5.1. More precisely, if

 $a \in [0, d/2)$, using (39a) or (39b)

$$\begin{split} \frac{1}{\hbar} \left\| \left[\mathsf{X}_{\boldsymbol{\rho}}, (\boldsymbol{\rho} - \boldsymbol{\rho}_{\hbar}^{W}(f)) \right] \right\|_{\mathcal{L}^{p}} &\leq C \, h^{\tilde{s}-1} \, \left\| K^{2} \right\|_{\dot{H}_{w}^{d-2a,1}}^{\frac{1}{2}} \, \left\| |\boldsymbol{p}|^{\frac{a}{2}} \, \boldsymbol{\rho} \, \right\|_{\mathcal{L}^{2}} \left\| \boldsymbol{\rho} - \boldsymbol{\rho}_{\hbar}^{W}(f) \right\|_{\mathcal{L}^{p}} \\ &\leq C \, h^{\tilde{s}-1} \, \left\| K^{2} \right\|_{\dot{H}_{w}^{d-2a,1}}^{\frac{1}{2}} \, \left\| |\boldsymbol{p}|^{\frac{a}{2}} \, \boldsymbol{\rho} \, \right\|_{\mathcal{L}^{2}} \left(\|\boldsymbol{\rho}\|_{\mathcal{L}^{p}} + \left\| \boldsymbol{\rho}_{\hbar}^{W}(f) \right\|_{\mathcal{L}^{p}} \right), \end{split}$$

with $\tilde{s}=d-a-d\left(\frac{1}{2}-\frac{1}{p}\right)_+$. When $\tilde{s}\geq 2$, this does not change the order of the rate of convergence O(h). When it is not the case (for high values of a and of p), the contribution of the exchange term becomes bigger than the one of the second term in the right-hand side of Inequality (43), thus leading to a rate of convergence of the order $O(h^{\tilde{s}-1})$. If $a\in (-1,0)$, then we use inequalities (42a) or (39b) to get bounds in terms of $\left\||x|^{\frac{|a|}{2}}\rho\right\|_{\mathcal{L}^2}$ instead of $\left\||x|^{\frac{|a|}{2}}\rho\right\|_{\mathcal{L}^2}$. When $K(x)=\pm\ln(|x|)$, we write that $K(x)\leq C_{\varepsilon}\left(|x|^{\varepsilon}+|x|^{-\varepsilon}\right)$ and use both type of inequalities to get bounds with $\left\|\left(|x|^{\frac{\varepsilon}{2}}+|p|^{\frac{\varepsilon}{2}}\right)\rho\right\|_{\mathcal{L}^2}$ instead. When p=1, we can therefore conclude that

(44)
$$\| \boldsymbol{\rho} - \boldsymbol{\rho}_{\hbar}^{W}(f) \|_{\mathcal{L}^{1}} \le \left(\| \boldsymbol{\rho}^{\text{in}} - \boldsymbol{\rho}_{f}^{\text{in}} \|_{\mathcal{L}^{1}} + C_{0}(t) \, \hbar + C_{1}(t) \, \hbar^{s-1} \right) e^{\lambda(t)}.$$

When $p \in (1, \mathfrak{b})$, we proceed as in the proof of Formula (13) (the Hartree case) and use Inequality (44) to get

$$(45) \quad \left\| \boldsymbol{\rho} - \boldsymbol{\rho}_{\hbar}^{W}(f) \right\|_{\mathcal{L}^{p}} \leq \left\| \boldsymbol{\rho}^{\text{in}} - \boldsymbol{\rho}_{f}^{\text{in}} \right\|_{\mathcal{L}^{p}} + C(t) \left(\left\| \boldsymbol{\rho}^{\text{in}} - \boldsymbol{\rho}_{f}^{\text{in}} \right\|_{\mathcal{L}^{1}} + \hbar + \hbar^{\tilde{s}-1} \right) e^{\lambda(t)}.$$

Moreover, when $p \in [\mathfrak{b}, \infty)$, again as in the Hartree case, we proceed as in the proof of (14). Following the exact same argument, $\|\boldsymbol{\rho} - \boldsymbol{\rho}_{\hbar}^W(f)\|_{\mathcal{L}^{\infty}}$ is bounded uniformly in \hbar as soon as $\boldsymbol{\rho}^{\text{in}} \in \mathcal{L}^{\infty}$ and $f \in W^{\left[\frac{d}{2}\right]+1,\infty}$. Whence,

$$\left\|\boldsymbol{\rho} - \boldsymbol{\rho}_{\hbar}^{W}(f)\right\|_{\mathcal{L}^{p}} \leq C(t) \left(\left\|\boldsymbol{\rho}^{\mathrm{in}} - \boldsymbol{\rho}_{f}^{\mathrm{in}}\right\|_{1}^{1-\theta} + C_{0} \, \hbar^{\frac{p}{q}} + C_{1} \, \hbar^{(\tilde{s}-1)\frac{p}{q}}\right) e^{\lambda(t)}.$$

In particular, if $\|\boldsymbol{\rho}^{\text{in}} - \boldsymbol{\rho}_f^{\text{in}}\|_1 \leq C \hbar$, we get for the Hilbert-Schmidt norm (p=2) a convergence rate $\hbar^{\left(\frac{3}{4}-\varepsilon\right)\min\{1,s-1\}}$.

Appendix A. Propagation of weighted Sobolev norms for Vlasov Equation

The existence of global smooth solutions and the propagation of regularity is a classical result for the Vlasov-Poisson equation. It can be deduced starting from the works of Pfaffelmoser [55] or Lions and Perthame [44], which imply the boundedness of the force field, so that any solution with compact support in the phase space will remain compactly supported at any time. Other general results concerning the propagation of regularity can be found in the more recent work [35] by Han-Kwan or in Appendix A in the work [61] by the second author. In our case, we need the boundedness of the solutions of the Vlasov equation in weighted Sobolev norms and we will see that we can propagate norms of the form $W_n^{\sigma,\infty}(\mathbb{R}^{2d})$. Remark that we prefer to work in the framework of [44] which allows to have non compactly supported solutions which are very interesting physically, since they include for example Gaussian distributions of velocities. Moreover compactly supported solutions are perhaps less pertinent in the context of quantum mechanics. Furthermore, the

proof here follows a completely Eulerian point of view. The result of this section is the following.

Proposition A.1. Let $K = \frac{1}{|x|^a}$ with $a \in (-1, d-2]$ and let $(n, \sigma, n_1) \in \mathbb{N}^3$ be such that n > d and $n_1 > \frac{d}{\mathfrak{b}-1}$ with $\mathfrak{b} = \frac{d}{a+1}$. Let $f \geq 0$ be solution of the Vlasov equation (1) with initial data $f^{\text{in}} \in W_n^{\sigma,\infty}(\mathbb{R}^{2d})$ satisfying

$$\iint_{\mathbb{R}^{2d}} f^{\mathrm{in}} \left| \xi \right|^{n_1} \, \mathrm{d}x \, \mathrm{d}\xi < \infty.$$

Then the following regularity estimates hold

$$(46a) f \in L^{\infty}_{loc}(\mathbb{R}_+, W^{\sigma, \infty}_n(\mathbb{R}^{2d}))$$

(46b)
$$\nabla^{\sigma} \rho_f \in L^{\infty}_{loc}(\mathbb{R}_+, L^{\infty}).$$

If in addition $f^{\text{in}} \in H_{\nu}^{\sigma}(\mathbb{R}^{2d})$ for some $k \in \mathbb{R}_{+}$, then

$$f \in L^{\infty}_{loc}(\mathbb{R}_+, H^{\sigma}_k(\mathbb{R}^{2d})).$$

The proof works in two steps. We first explain in the next lemma how to get a control of the regularity as soon as ρ_f is uniformly bounded. Then we finish the proof of the theorem by proving that this assumption on ρ_f holds.

Lemma A.1. Let f be a solution of the Vlasov equation (1) as in Proposition A.1 with $\sigma > 1$ and assume moreover that

(47)
$$\rho_f \in L^{\infty}_{loc}(\mathbb{R}_+, L^{\infty} \cap L^1).$$

Then the regularity estimates (46a) and (46b) hold.

Proof. For clarity, we first start with the case $\sigma=1$ for which we will do a detailed proof, and we will then explain how to modify the proof to get higher regularity estimates. We follow the strategy explained in the course notes [28].

Step 1. Case $\sigma = 1$. We have, by denoting $T := \xi \cdot \nabla_x + E \cdot \nabla_\xi$

(48a)
$$\partial_t(\nabla_x f) = -\mathsf{T}\nabla_x f - \nabla E \cdot \nabla_\xi f$$

(48b)
$$\partial_t(\nabla_{\xi} f) = -\mathsf{T}\nabla_{\xi} f - \nabla_x f.$$

To simplify the computations, recall that the transport operator verifies $\mathsf{T}^* = -\mathsf{T}$ and $\mathsf{T}(uv) = u\mathsf{T}(v) + \mathsf{T}(u)v$, so that by writing $m_n := 1 + |\xi|^{np} + |x|^{np}$ and using the notation $u^p := |u|^{p-1}u$, it holds

(49)
$$\iint_{\mathbb{R}^{2d}} \mathsf{T}(u) \cdot u^{p-1} \, m_n = -\iint_{\mathbb{R}^{2d}} u \cdot \mathsf{T}(u^{p-1}) \, m_n + |u|^p \, \mathsf{T}(m_n).$$

However remarking that

$$\begin{split} u\cdot (\mathsf{T}(u^{p-1})) &= u\cdot \left(|u|^{p-2}\mathsf{T}(u) + (p-2)\left(\mathsf{T}(u)\cdot u\right)u^{p-3}\right) \\ &= u^{p-1}\cdot \mathsf{T}(u) + (p-2)\left(\mathsf{T}(u)\cdot u\right)|u|^{p-2} \\ &= (p-1)\,u^{p-1}\cdot \mathsf{T}(u). \end{split}$$

we can simplify Equation (49) into

(50)
$$-p \iint_{\mathbb{R}^{2d}} \mathsf{T}(u) \cdot u^{p-1} m_n = \iint_{\mathbb{R}^{2d}} |u|^p \, \mathsf{T}(m_n).$$

Now define

$$M_x := \iint_{\mathbb{R}^{2d}} \left| \nabla_x f \right|^p m_n \text{ and } M_\xi := \iint_{\mathbb{R}^{2d}} \left| \nabla_\xi f \right|^p m_n.$$

Then using (48a) and Formula (50) for $u = \nabla_x f$ leads to

$$\frac{\mathrm{d}M_x}{\mathrm{d}t} = -p \iint_{\mathbb{R}^{2d}} (\nabla_x f)^{p-1} \cdot (\mathsf{T}\nabla_x f + \nabla E \cdot \nabla_\xi f) \, m_n$$

$$\leq \iint_{\mathbb{R}^{2d}} |\nabla_x f|^p \, \mathsf{T}(m_n) + \|\nabla E\|_{L^{\infty}} \left(M_\xi + (p-1)M_x\right)$$

where we used the multiplicative Young's inequality $p \, a \, b^{p-1} \leq a^p + (p-1) \, b^p$ to get the second term. In the same way, using (48b) and taking $u = \nabla_{\xi} f$ yields

$$\frac{\mathrm{d}M_{\xi}}{\mathrm{d}t} \le \iint_{\mathbb{R}^{2d}} \left| \nabla_{\xi} f \right|^p \mathsf{T}(m_n) + (M_x + (p-1)M_{\xi})$$

Then again by the multiplicative Young's inequality

$$\mathsf{T}(m_n) = np \left(E \cdot \xi^{np-1} + \xi \cdot x^{np-1} \right) \le np \left(||E||_{L^{\infty}} + 1 \right) m_n$$

Thus, for $M_{x,\xi} := M_x + M_\xi$, we obtain

$$\frac{\mathrm{d}}{\mathrm{d}t} M_{x,\xi} \le p \left(n \|E\|_{L^{\infty}} + 1 + \|\nabla E\|_{L^{\infty}} \right) M_{x,\xi}$$

However, since we know that $\rho_f \in L^{\infty}_{loc}(\mathbb{R}_+, L^{\infty} \cap L^1)$ by assumption, we also get the following control on $||E||_{L^{\infty}}$

$$||E||_{L^{\infty}} \le C (||\rho_f||_{L^{\infty}} + ||\rho_f||_{L^1}) \le C_t$$

for some function of time C_t locally bounded on \mathbb{R}_+ . To control ∇E , we can use the integral Young's inequality if ∇K is less singular than the Coulomb potential (i.e. if a < d-2), and if a = 1, then we use a singular integral estimate in the spirit of the one in [9] which can be found in the course notes [28] and can be written

$$\|\nabla E\|_{L^{\infty}} \le C \left(1 + M_0 + \|\rho_f\|_{L^{\infty}} \ln(1 + \|\nabla \rho_f\|_{L^{\infty}}) \right)$$

$$\le C_t \left(1 + \ln(1 + \|\nabla \rho_f\|_{L^{\infty}}) \right) =: J(t),$$

since $p \geq 1$, combining these bounds we arrive at $\frac{d}{dt}M_{x,\xi} \leq p(1+n)J(t)M_{x,\xi}$ which by Grönwall's Lemma implies

$$M_{x,\mathcal{E}}^{\frac{1}{p}}(t) \le M_{x,\mathcal{E}}^{\frac{1}{p}}(0) e^{(1+n)\int_0^t J}.$$

Now, since $M_{x,\xi}^{\frac{1}{p}} \simeq \|f\|_{W_n^{1,p}(\mathbb{R}^{2d})}$ (i.e. each one is bounded by above by the other up to a multiplicative constant), letting $p \to \infty$, we obtain

(51)
$$||f||_{W_n^{1,\infty}(\mathbb{R}^{2d})} \le ||f^{\text{in}}||_{W_n^{1,\infty}(\mathbb{R}^{2d})} e^{(1+n) \int_0^t J}.$$

However, since n > d, we have

(52)
$$|\nabla \rho_f| \le \int_{\mathbb{R}^d} |\nabla_x f| \, \mathrm{d}\xi \le C_{d,n} \, ||f||_{W_n^{1,\infty}(\mathbb{R}^{2d})}$$

where $C_{d,n} = \int_{\mathbb{R}^d} \langle \xi \rangle^{-n} d\xi < \infty$. Combining the two inequalities (51) and (52) and the fact that $e^{J(t)} \geq 1$, we deduce

$$J(t) \leq C_t + C_t \ln\left(\left(1 + C_{d,n} \|f^{\text{in}}\|_{W_n^{1,\infty}(\mathbb{R}^{2d})}\right) e^{(1+n)\int_0^t J}\right)$$

$$\leq C_t + C_t \ln\left(1 + C_{d,n} \|f^{\text{in}}\|_{W_n^{1,\infty}(\mathbb{R}^{2d})}\right) + C_t (1+n) \int_0^t J.$$

Hence, by Grönwall's Lemma

$$J(t) \le J(0) + \frac{1 + \ln\left(1 + C_{d,n} \left\| f^{\text{in}} \right\|_{W_n^{1,\infty}(\mathbb{R}^{2d})}\right)}{n+1} \frac{e^{C_t(1+n)t}}{1+n}.$$

We then deduce the bounds on $||f||_{W_n^{1,\infty}(\mathbb{R}^{2d})}$ and $\nabla \rho_f$ by inequalities (51) and (52). **Step 2.** Case $\sigma > 1$. We give details for $\sigma = 2$. The generalization to $\sigma \geq 2$ follows in the same way. In the case $\sigma = 2$, Formulas (48b) and (48a) become

$$\begin{split} &\partial_t(\nabla_\xi^2 f) + \mathsf{T} \nabla_\xi^2 f = -2 \, \nabla_x \nabla_\xi f \\ &\partial_t(\nabla_x^2 f) + \mathsf{T} \nabla_x^2 f = -2 \, \nabla E \cdot \nabla_\xi \nabla_x f - \nabla^2 E \cdot \nabla_\xi f \,. \end{split}$$

Moreover, the mixed derivative of order two solves

$$\partial_t (\nabla_x \nabla_\xi f) + \mathsf{T} \nabla_x \nabla_\xi f = -\nabla_x^2 f - \nabla E \cdot \nabla_\xi^2 f \,.$$

We define the quantities

$$M_{xx} := \iint_{\mathbb{R}^{2d}} |\nabla_x^2 f|^p m_n \, dx \, d\xi;$$

$$M_{\xi\xi} := \iint_{\mathbb{R}^{2d}} |\nabla_\xi^2 f|^p m_n \, dx \, d\xi;$$

$$M_{x\xi} := \iint_{\mathbb{R}^{2d}} |\nabla_x \nabla_\xi f|^p m_n \, dx \, d\xi;$$

and compute their time derivatives, using the multiplicative Young's inequality, the bound on $T(m_n)$ as in Step 1 and the fact that p > 1:

$$\frac{\mathrm{d} M_{\xi\xi}}{\mathrm{d} t} \le p (n \|E\|_{L^{\infty}} + n + 2) M_{\xi\xi} + 2 p M_{x\xi},$$

$$\frac{\mathrm{d}M_{x\xi}}{\mathrm{d}t} \le p \left(n \|E\|_{L^{\infty}} + n + 1 + \|\nabla E\|_{L^{\infty}} \right) M_{x\xi} + p M_{xx} + p \|\nabla E\|_{L^{\infty}} M_{\xi\xi} ,$$

$$\frac{dM_{xx}}{dt} \le p \left(n \|E\|_{L^{\infty}} + n + 2 \|\nabla E\|_{L^{\infty}} + \|\nabla^2 E\|_{L^{\infty}} \right) M_{xx} + 2 p \|\nabla E\|_{L^{\infty}} M_{x\xi} + p \|\nabla^2 E\|_{L^{\infty}} M_{\xi},$$

where M_{ξ} is defined and bounded as in Step 1. Thus, for $M_2 := M_{xx} + M_{x\xi} + M_{\xi\xi}$, we obtain

$$\frac{\mathrm{d}}{\mathrm{d}t} M_2 \le C p \left(n \left\| E \right\|_{L^{\infty}} + n + 2 + 2 \left\| \nabla E \right\|_{L^{\infty}} + \left\| \nabla^2 E \right\|_{L^{\infty}} \right) M_2$$

We proved in Step 1 that $||E||_{L^{\infty}}$ and $||\nabla E||_{L^{\infty}}$ are bounded. To control $\nabla^2 E$, we proceed analogously to Step 1. More generally, we can bound $\nabla^{\sigma} E$ by $\nabla_x^{\sigma} f$. This leads, by Grönwall's Lemma, to

$$M_2^{\frac{1}{p}}(t) \leq M_2^{\frac{1}{p}}(0) \, e^{C_t},$$

for some positive time dependent constant $C_t > 0$. Now, since $M_2^{\frac{1}{p}} \simeq ||f||_{W_n^{2,p}(\mathbb{R}^{2d})}$ (with the exact same meaning given in Step 1), letting $p \to \infty$, we obtain

$$||f||_{W_n^{2,\infty}(\mathbb{R}^{2d})} \le ||f^{\text{in}}||_{W_n^{2,\infty}(\mathbb{R}^{2d})} e^{C_t}.$$

The general case $\sigma > 1$ can be handled analogously by defining

$$M_{\sigma} := \iint |\nabla^{\sigma} f|^p \, m_n \, \mathrm{d}x \, \mathrm{d}\xi \,,$$

where $\sigma = |\sigma|$ stands for the length of the multi-index $\sigma = (\sigma_1, \sigma_2, \dots)$.

Proof of Proposition A.1. It just remains to prove that Assumption (47) holds. First remark that the method used in [44, Theorem 1] actually works for any $a \in (-1, d-2]$ since the Coulomb potential is decomposed in two parts of the form $\nabla K \in L^{3/2,\infty} \cap L^1 + W^{2,\infty}$. This proves that the n_1 moments can be propagated, which implies that $\rho_f \in L^p$ for $p = 1 + \frac{n_1}{d}$ by the kinetic interpolation inequality. Then, by Young's inequality, since $n_1 > \frac{d}{b-1}$, we deduce that

$$E \in L^{\infty}_{loc}(\mathbb{R}_+, L^{\infty}).$$

Finally, as proved in [41, Corollary 5.1], this bound combined with the initial assumption $f \in L^{\infty}(1+|\xi|^n)$ is sufficient to control $\|\rho_f\|_{L^{\infty}}$ and gives

$$\|\rho_f(t)\|_{L^{\infty}} \le C \left(1 + \int_0^t \|E(s)\|_{L^{\infty}} ds\right),$$

which implies (47) so that we can apply the lemma. Then once we know the $W_n^{s,\infty}(\mathbb{R}^{2d})$ norm is bounded at any time, if the $H_k^{\sigma}(\mathbb{R}^{2d})$ is also initially bounded, we can use again Formula (53) but with p=2 and then bound the terms involving E and $\nabla_x f$ by the $W_n^{\sigma,\infty}(\mathbb{R}^{2d})$ norm. And we then conclude again by Grönwall's Lemma.

APPENDIX B. OPERATORS IDENTITIES

We list here some formulas for operators, which are used in this paper. First, let us indicate the two following basic properties. If A and B are two operators, then

$$|A|B| = |AB|$$

which first one follows from the definition of $|AB| = (B^*A^*AB)^{\frac{1}{2}}$, and if A and B are self-adjoint

$$||AB||_p = ||BA||_p$$

which follows from the fact that the singular values are the same for an operator and its adjoint [62, Formula 1.3]. Then we shall remember Hölder's inequality for operators [62, Theorem 2.8] which tells that for any bounded operator A and B and any $(p,q,r) \in [1,\infty]^3$ such that $\frac{1}{p} = \frac{1}{q} + \frac{1}{r}$, it holds

$$\left\|AB\right\|_{p} \leq \left\|A\right\|_{q} \left\|B\right\|_{r}.$$

The second important inequality is the Araki-Lieb-Thirring inequality [3, Theorem 1] which states that for any operator $A, B \geq 0$ and any $(q, r) \in [1, \infty) \times \mathbb{R}_+$, the following inequality is true

$$\operatorname{Tr}((BAB)^{qr}) < \operatorname{Tr}((B^q A^q B^q)^r)$$
.

Replacing A by A^2 and remarking that $|AB|^2 = BA^2B$, this can be rewritten

$$||AB||_{qr}^q \le ||A^q B^q||_r.$$

These inequalities show that regrouping operators together in Schatten norms increases the value of the norm, while *mixing* them will lower the value. In the same spirit, for any $A, B \ge 0$, $p \ge 1$ and $r \ge 0$, the following mixing inequality holds

Proof of Inequality (56). By Hölder's inequality, we have

$$\|B^r A B\|_p \le \|B^r A^{\frac{r}{r+1}}\|_{\frac{r+1}{r}p} \|A^{\frac{1}{r+1}} B\|_{(r+1)p}.$$

Now, by the cyclicity property (54) and by Inequality (55), we get

$$\left\| B^r A^{\frac{r}{r+1}} \right\|_{\frac{r+1}{r}p} \le \left\| A B^{r+1} \right\|_{p}^{\frac{r}{r+1}}$$
$$\left\| A^{\frac{1}{r+1}} B \right\|_{(r+1)p} \le \left\| A B^{r+1} \right\|_{p}^{\frac{1}{r+1}},$$

which yields the result.

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References

- [1] L. Amour, M. Khodja, and J. Nourrigat. The classical limit of the Heisenberg and time-dependent Hartree–Fock equations: the Wick symbol of the solution. *Mathematical Research Letters*, 20(1):119–139, Jan. 2013.
- [2] L. Amour, M. Khodja, and J. Nourrigat. The Semiclassical Limit of the Time Dependent Hartree– Fock Equation: the Weyl Symbol of the Solution. Analysis & PDE, 6(7):1649–1674, 2013
- [3] H. Araki. On an inequality of Lieb and Thirring. Letters in Mathematical Physics, 19(2):167–170, 1990.
- [4] A. Athanassoulis and T. Paul. Strong and Weak Semiclassical Limit for some Rough Hamiltonians. Mathematical Models and Methods in Applied Sciences, 22(12):1250038, 2011.
- [5] V. Bach, S. Breteaux, S. Petrat, P. Pickl, and T. Tzaneteas. Kinetic Energy Estimates for the Accuracy of the Time-Dependent Hartree-Fock Approximation with Coulomb Interaction. *Journal de Mathématiques Pures et Appliquées*, 105(1):1–30, Jan. 2016.
- [6] C. Bardos and P. Degond. Global Existence for the Vlasov-Poisson Equation in 3 Space Variables with Small Initial Data. Annales de l'Institut Henri Poincaré. Analyse Non Linéaire, 2(2):101–118, 1985.
- [7] C. Bardos, L. Erdös, F. Golse, N. J. Mauser, and H.-T. Yau. Derivation of the Schrödinger-Poisson Equation from the Quantum N-body Problem. Comptes Rendus Mathematique, 334(6):515–520, Jan. 2002.
- [8] C. Bardos, F. Golse, and N. J. Mauser. Weak Coupling Limit of the N-particle Schrödinger Equation. Methods and Applications of Analysis, 7(2):275-294, 2000.
- [9] J. T. Beale, T. Kato, and A. Majda. Remarks on the breakdown of smooth solutions for the 3-D Euler equations. Communications in Mathematical Physics, 94(1):61-66, Mar. 1984.
- [10] N. Benedikter, V. Jaksic, M. Porta, C. Saffirio, and B. Schlein. Mean-Field Evolution of Fermionic Mixed States. Communications on Pure and Applied Mathematics, 69(12):2250– 2303, 2016.
- [11] N. Benedikter, M. Porta, C. Saffirio, and B. Schlein. From the Hartree Dynamics to the Vlasov Equation. Archive for Rational Mechanics and Analysis, 221(1):273–334, 2016.
- [12] N. Benedikter, M. Porta, and B. Schlein. Mean-field Evolution of Fermionic Systems. Communications in Mathematical Physics, 331(3):1087–1131, Nov. 2014.
- [13] J. Bergh and J. Löfström. Interpolation spaces. An introduction, volume 223 of Grundlehren der Mathematischen Wissenschaften. Springer Berlin Heidelberg, Berlin, Heidelberg, 1976.

- [14] A. Boulkhemair. L2 Estimates for Weyl Quantization. Journal of Functional Analysis, 165(1):173–204, June 1999.
- [15] F. Castella. L2 Solutions to the Schrödinger-Poisson System: Existence, Uniqueness, Time Behaviour, and Smoothing Effects. Mathematical Models and Methods in Applied Sciences, 7(08):1051-1083, 1997.
- [16] L. Chen, J. O. Lee, and J. Lee. Rate of Convergence towards Hartree Dynamics with Singular Interaction Potential. *Journal of Mathematical Physics*, 59(3):031902, 2018. arXiv: 1708.07278.
- [17] L. Chen, J. O. Lee, and B. Schlein. Rate of Convergence Towards Hartree Dynamics. *Journal of Statistical Physics*, 144(4):872–903, 2011. arXiv: 1103.0948.
- [18] L. Desvillettes, E. Miot, and C. Saffirio. Polynomial propagation of moments and global existence for a Vlasov-Poisson system with a point charge. Ann. Inst. H. Poincaré (C) Anal. Non Linéaire, 32(2):373–400, 2015.
- [19] R. L. Dobrushin. Vlasov equations. Functional Analysis and Its Applications, 13(2):115–123, 1979.
- [20] A. Elgart, L. Erdős, B. Schlein, and H.-T. Yau. Nonlinear Hartree equation as the mean field limit of weakly coupled fermions. *Journal de Mathématiques Pures et Appliquées*, 83(10):1241–1273, Oct. 2004. arXiv: math-ph/0311043.
- [21] L. Erdös and H.-T. Yau. Derivation of the Nonlinear Schrödinger Equation from a Many Body Coulomb System. Advances in Theoretical and Mathematical Physics, 5(6):1169–1205, 2001.
- [22] A. Figalli, M. Ligabò, and T. Paul. Semiclassical Limit for Mixed States with Singular and Rough Potentials. *Indiana University Mathematics Journal*, 61(1):193–222, 2012. arXiv: 1012.2483.
- [23] J. Fröhlich and A. Knowles. A Microscopic Derivation of the Time-Dependent Hartree-Fock Equation with Coulomb Two-Body Interaction. *Journal of Statistical Physics*, 145(1):23, Oct. 2011. arXiv: 0810.4282.
- [24] J. Fröhlich, A. Knowles, and S. Schwarz. On the Mean-Field Limit of Bosons with Coulomb Two-Body Interaction. *Communications in Mathematical Physics*, 288(3):1023–1059, June 2009. arXiv: 0805.4299.
- [25] I. Gasser, R. Illner, P. A. Markowich, and C. Schmeiser. Semiclassical, asymptotics and dispersive effects for Hartree-Fock systems. ESAIM: Mathematical Modelling and Numerical Analysis, 32(6):699–713, 1998.
- [26] J. Ginibre and G. Velo. On a Class of non Linear Schrödinger Equations with non Local Interaction. Mathematische Zeitschrift, 170(2):109–136, 1980.
- [27] J. Ginibre and G. Velo. The Global Cauchy Problem for the non Linear Schrödinger Equation Revisited. Annales de l'Institut Henri Poincare (C) Non Linear Analysis, 2(4):309–327, July 1985.
- [28] F. Golse. Mean Field Kinetic Equations. Course Notes, Ecole Polytechnique, 2013.
- [29] F. Golse, C. Mouhot, and T. Paul. On the Mean Field and Classical Limits of Quantum Mechanics. Communications in Mathematical Physics, 343(1):165–205, 2016. arXiv: 1502.06143.
- [30] F. Golse and T. Paul. The Schrödinger Equation in the Mean-Field and Semiclassical Regime. Archive for Rational Mechanics and Analysis, 223(1):57–94, 2017.
- [31] F. Golse and T. Paul. Empirical Measures and Quantum Mechanics: Applications to the Mean-Field Limit. Communications in Mathematical Physics, 1711:arXiv:1711.08350, Mar. 2019.
- [32] F. Golse, T. Paul, and M. Pulvirenti. On the Derivation of the Hartree Equation from the N-Body Schrödinger Equation: Uniformity in the Planck Constant. *Journal of Functional Analysis*, 275(7):1603–1649, Oct. 2018.
- [33] S. Graffi, A. Martinez, and M. Pulvirenti. Mean-Field Approximation of Quantum Systems and Classical Limit. Mathematical Models and Methods in Applied Sciences, 13(01):59-73, Jan. 2003. arXiv: math-ph/0205033.
- [34] M. G. Grillakis, M. Machedon, and D. Margetis. Second-order corrections to mean field evolution for weakly interacting Bosons. I. Communications in Mathematical Physics, 294(1):273–301, Feb. 2010. arXiv: 0904.0158.
- [35] D. Han-Kwan. On propagation of higher space regularity for nonlinear Vlasov equations. Analysis & PDE, 12(1):189–244, 2019.

- [36] T. Holding and E. Miot. Uniqueness and stability for the Vlasov-Poisson system with spatial density in Orlicz spaces. In Contemporary Mathematics, Mathematical Analysis in Fluid Mechanics: Selected Results, volume 710 of Contemp. Math., pages 145–162. Amer. Math. Soc., Providence, RI, 2018.
- [37] R. A. Hunt. On L(p, q) spaces. L'Enseignement Math, 12:249–276, 1966.
- [38] S. V. Iordanskij. The Cauchy problem for the kinetic equation of plasma. Trudy Matematicheskogo Instituta Imeni V. A. Steklova, 60:181–194, 1961.
- [39] E. Kuz. Rate of Convergence to Mean Field for Interacting Bosons. Communications in Partial Differential Equations, 40(10):1831–1854, Oct. 2015.
- [40] L. Lafleche. Global Semiclassical Limit from Hartree to Vlasov Equation for Concentrated Initial Data. arXiv:1902.08520, Feb. 2019.
- [41] L. Lafleche. Propagation of Moments and Semiclassical Limit from Hartree to Vlasov Equation. Journal of Statistical Physics, 177(1):20–60, July 2019.
- [42] E. H. Lieb and M. Loss. Analysis. Graduate Studies in Mathematics. American Mathematical Society, Providence, RI, 2 edition edition, 2001.
- [43] P.-L. Lions and T. Paul. Sur les mesures de Wigner. Revista Matemática Iberoamericana, 9(3):553-618, 1993.
- [44] P.-L. Lions and B. Perthame. Propagation of moments and regularity for the 3-dimensional Vlasov-Poisson system. *Inventiones Mathematicae*, 105(2):415–430, 1991.
- [45] G. Loeper. Uniqueness of the solution to the Vlasov-Poisson system with bounded density. Journal de Mathématiques Pures et Appliquées, 86(1):68-79, July 2006.
- [46] P. A. Markowich and N. J. Mauser. The Classical Limit of a Self-Consistent Quantum Vlasov Equation. Mathematical Models and Methods in Applied Sciences, 3(01):109–124, Feb. 1993.
- [47] E. Miot. A Uniqueness Criterion for Unbounded Solutions to the Vlasov-Poisson System. Communications in Mathematical Physics, 346(2):469–482, Sept. 2016.
- [48] D. Mitrouskas, S. Petrat, and P. Pickl. Bogoliubov corrections and trace norm convergence for the Hartree dynamics. Reviews in Mathematical Physics, page 1950024, Feb. 2019. arXiv: 1609.06264.
- [49] H. Narnhofer and G. L. Sewell. Vlasov hydrodynamics of a quantum mechanical model. Communications in Mathematical Physics, 79(1):9–24, Mar. 1981.
- [50] C. Pallard. Moment Propagation for Weak Solutions to the Vlasov-Poisson System. Communications in Partial Differential Equations, 37(7):1273-1285, July 2012.
- [51] C. Pallard. Space Moments of the Vlasov-Poisson System: Propagation and Regularity. SIAM Journal on Mathematical Analysis, 46(3):1754–1770, Jan. 2014.
- [52] S. Petrat. Hartree Corrections in a Mean-field Limit for Fermions with Coulomb Interaction. Journal of Physics A: Mathematical and Theoretical, 50(24):244004, 2017.
- [53] S. Petrat and P. Pickl. A New Method and a New Scaling for Deriving Fermionic Mean-Field Dynamics. *Mathematical Physics, Analysis and Geometry*, 19(1):3, Mar. 2016.
- [54] F. Pezzotti and M. Pulvirenti. Mean-field limit and Semiclassical Expansion of a Quantum Particle System. Ann. H. Poincaré, 10(1):145–187, 2009.
- [55] K. Pfaffelmoser. Global classical solutions of the Vlasov-Poisson system in three dimensions for general initial data. *Journal of Differential Equations*, 95(2):281–303, Feb. 1992.
- [56] P. Pickl. A Simple Derivation of Mean Field Limits for Quantum Systems. Letters in Mathematical Physics, 97(2):151–164, Aug. 2011.
- [57] M. Porta, S. Rademacher, C. Saffirio, and B. Schlein. Mean Field Evolution of Fermions with Coulomb Interaction. *Journal of Statistical Physics*, 166(6):1345–1364, 2017.
- [58] I. Rodnianski and B. Schlein. Quantum Fluctuations and Rate of Convergence Towards Mean Field Dynamics. Communications in Mathematical Physics, 291(1):31–61, Oct. 2009. arXiv: 0711.3087.
- [59] C. Saffirio. Mean-Field Evolution of Fermions with Singular Interaction. In D. Cadamuro, M. Duell, W. Dybalski, and S. Simonella, editors, *Macroscopic Limits of Quantum Systems*, Springer Proceedings in Mathematics & Statistics, pages 81–99, Cham, 2018. Springer International Publishing. arXiv: 1801.02883.
- [60] C. Saffirio. From the Hartree equation to the Vlasov-Poisson system: strong convergence for a class of mixed states. arXiv:1903.06013 [math-ph], Mar. 2019. arXiv: 1903.06013.
- [61] C. Saffirio. Semiclassical Limit to the Vlasov Equation with Inverse Power Law Potentials. Communications in Mathematical Physics, 373(2):571–619, Mar. 2019. arXiv: 1903.06001.

- [62] B. Simon. Trace Ideals and Their Applications: Second Edition, volume 120 of Mathematical Surveys and Monographs. American Mathematical Society, 2 edition edition, 2005.
- [63] H. Spohn and H. Neunzert. On the Vlasov hierarchy. Mathematical Methods in the Applied Sciences, 3(1):445–455, 1981.
- [64] S. Ukai and T. Okabe. On classical solutions in the large in time of two-dimensional Vlasov's equation. Osaka Journal of Mathematics, 15(2):245–261, 1978.
- [65] D. Yafaev. Sharp Constants in the Hardy–Rellich Inequalities. Journal of Functional Analysis, 168(1):121–144, Oct. 1999.