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STRONG SEMICLASSICAL LIMITS FROM HARTREE AND HARTREE–FOCK TO VLASOV–POISSON EQUATIONS

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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 any fixed time interval.

1. Introduction

The Vlasov equation is 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. The problem of deriving this equation 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 1980s (see [Narnhofer and Sewell 1981; Spohn 1981]).

We study here the semiclassical limit from the Hartree and Hartree-Fock equations towards the Vlasov equation, i.e., the limit corresponding to a regime in which the Planck constant h becomes negligible. For any fixed time interval, we obtain quantitative Schatten norm estimates between the solutions of the quantum equations (Hartree and Hartree-Fock) and the Weyl quantization of the solution of the Vlasov equation. In particular, these imply the convergence of the Wigner transform of the quantum equations towards the solution of the Vlasov equation.

1A. *Context and state of the art.*

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

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

where $t \in \mathbb{R}_+$ denotes the time variable, $x \in \mathbb{R}^d$ denotes the space variable and $\xi \in \mathbb{R}^d$ denotes the momentum variable. In the above equation, $E := -\nabla K * \rho_f$ is the self-induced mean-field force field

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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

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

When K is the Green's function for the Laplace operator, (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 equation. In this case, in dimension 3, K corresponds to the Coulomb potential

$$K(x) = \frac{1}{4\pi |x|},$$

but our method allows us to consider more general attractive and repulsive potentials. To simplify the presentation, we will look at homogeneous potentials of the form $K(x) = \pm|x|^{-a}$ or at $K(x) = \pm\ln(|x|)$, and we will then indicate how to generalize our results to a class of Sobolev spaces (see page 899).

The well-posedness of the Vlasov equation (1) is due to Dobrushin [1979] for smooth interaction potentials $K \in C_c^2(\mathbb{R}^d)$. Concerning singular interactions, the cases of Coulomb and gravitational potentials have been tackled first in [Iordanskiĭ 1961] and [Ukai and Okabe 1978] for $d = 1$ and $d = 2$, respectively. In $d = 3$, the well-posedness for small data has been proven in [Bardos and Degond 1985] and later extended to general initial data by Pfaffelmoser [1992] and by Lions and Perthame [1991]. In recent years, improvements on the conditions of propagation of momenta and on the uniqueness condition have been addressed in [Desvillettes et al. 2015; Holding and Miot 2018; Loeper 2006; Miot 2016; Pallard 2012; 2014]. The setting of this paper will be close to the setting of the paper by Lions and Perthame [1991]; that is the one that best suits the comparison with the quantum dynamics because of its Eulerian viewpoint.

The Vlasov equation (1) is supposed to emerge as a joint mean-field (weakly interacting particles at high density) and semiclassical limit from the dynamics of N interacting quantum particles. This was first proven in [Narnhofer and Sewell 1981] and [Spohn 1981] for analytic and C^2 interaction potentials, respectively, using the BBGKY approach in the fermionic setting. The case of bosons interacting through a smooth pair potential has been studied in [Graffi et al. 2003] in the mean-field limit combined with a semiclassical limit through the analysis of the dynamics of factored WKB states.

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

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

an evolution equation for the density operator $\boldsymbol{\rho} = \boldsymbol{\rho}(t)$, a nonnegative bounded operator on the space $L^2(\mathbb{R}^d)$ with $\mathrm{Tr}(\boldsymbol{\rho}) = 1$. In (2), $\hbar = \frac{h}{2\pi}$ is the reduced Planck constant, and H is the Hamiltonian

$$H = -\tfrac{1}{2}\hbar^2\Delta + K * \rho, \tag{3}$$

where Δ is the Laplace operator, K is the pair interaction potential, $\rho(x) = \boldsymbol{\rho}(x, x)$ is the diagonal of the integral kernel of the trace class operator $\boldsymbol{\rho}$ and $K * \rho$ is identified with the operator of multiplication by the function $x \mapsto K * \rho(x)$.

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

$$i\hbar\partial_t \boldsymbol{\rho} = [H_{\mathrm{HF}}, \boldsymbol{\rho}], \tag{4}$$

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

$$\mathsf{X}(x, y) = K(x - y)\boldsymbol{\rho}(x, y). \tag{5}$$

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 large numbers of particles, which typically range between 10^2 and 10^{23}, while the above equations only describe the behavior of one typical particle in a system of infinitely many particles. The mathematical literature on this subject is rather extensive. See for example [Bardos et al. 2000; 2002; Chen et al. 2011; 2018; Erdős and Yau 2001; Fröhlich et al. 2009; Golse and Paul 2017; 2019; Golse et al. 2016; 2018; Grillakis et al. 2010; Kuz 2015; Mitrouskas et al. 2019; Pickl 2011; Rodnianski and Schlein 2009] for the case of bosons, and [Bach et al. 2016; Benedikter et al. 2014; 2016a; Elgart et al. 2004; Fröhlich and Knowles 2011; Petrat 2017; Petrat and Pickl 2016; Porta et al. 2017; Saffirio 2018] for the case of fermions.

Semiclassical limit. 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 the abstract sense, without rate of convergence and in weak topologies, but including the case of singular interaction potentials, such as the Coulomb interaction (see [Figalli et al. 2012; Gasser et al. 1998; Lions and Paul 1993; Markowich and Mauser 1993]). Explicit bounds on the convergence rate in stronger topologies were established in [Amour et al. 2013a; 2013b; Athanassoulis et al. 2011; Benedikter et al. 2016b; Golse and Paul 2017; Pezzotti and Pulvirenti 2009]. They all deal with smooth interaction potentials. More recently, the case of singular interactions, including the Coulomb potential, has been considered in [Lafleche 2019; 2021], where the convergence from the Hartree to the Vlasov equation is achieved in weak topology using the 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 $a \in \left(0, \frac{1}{2}\right)$ have been proven in [Saffirio 2020b], and a proof that includes the Coulomb potential has been provided in [Saffirio 2020a] but under restrictive assumptions on the initial data.

Key novelties. 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 which are smooth as $h \to 0$, thus giving a thorough answer to the question of strong convergence of the Hartree equation to the Vlasov system for singular interactions, at least in the case of mixed states converging to smooth solutions of the Vlasov equation.

With respect to the results present in the 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 us to consider inverse power law potentials that are more singular than the Coulomb potential, and our methods easily extend to very general nonradially 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 [Saffirio 2020b]), 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 $[K(\cdot - z), \boldsymbol{\rho}]$ and a careful analysis of the propagation in time of initial conditions leading to bound the quantity

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

uniformly in $\hbar$, for $p > 3$. This requires using kinetic interpolation inequalities as in [Lafleche 2019] and an extension of the Calderón–Vaillancourt theorem for Weyl quantization.

Finally, we extend our results to the Hartree–Fock equation (4), thus proving the strong convergence of the Hartree–Fock dynamics to the Vlasov equation. 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 also subleading with respect to the direct term when the interaction potential is singular (this was proved in [Benedikter et al. 2014] in the case of smooth potentials).

Open problems. Our work gives good answers to the problem of the semiclassical limit from the Hartree and Hartree–Fock equations to the Vlasov equation with general singular potentials in the context of mixed states. However, a certain number of questions related to the derivation of the Vlasov equation from quantum dynamics remain open.

(i) To our knowledge, the mean-field limit from a system of N quantum particles interacting through a singular potential in the case of mixed states is open in both the bosonic and the fermionic settings.

(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 $\mathcal{L}^2$ are optimal, and thus for the L^2 convergence of the associated Wigner functions, is open. The exact same question can be asked about the bounds in Theorem 1.6 for the convergence of the Hartree–Fock equation to the Vlasov equation. In both cases, we believe the bounds we get are not optimal and there is room for improvement.

Structure of the paper. The paper is structured as follows:

- We state our main result in Section 1B and include additional comments and generalizations in Section 1C.

- In Section 2 we explain our strategy. We introduce a semiclassical notion of regularity (Section 2A) and then explain our method to get the semiclassical limit by making a comparison with the classical Vlasov dynamics, finding a new stability estimate for the Vlasov system (Section 2B).
- Section 3 contains the main results concerning the regularity of the Weyl transform of a solution to the Vlasov equation, which will be crucial to prove the theorems stated in Section 1B.
- Section 4 is devoted to proving Theorems 1.1 and 1.4, dealing with the semiclassical limit from the Hartree equation under the assumption that the regularity proved in Section 3 holds.
- In Section 5 we present the proof of Theorem 1.6 about the semiclassical limit from the Hartree–Fock equation, based on additional estimates on the exchange term.
- Two appendices on the propagation of regularity for the Vlasov equation and on basic operator identities complement the paper.

1B. ***Main results.***

Operators and function spaces. We denote by $L^p = L^p(\mathbb{R}^d)$ the classical Lebesgue spaces and by $L^{p,q} = L^{p,q}(\mathbb{R}^d)$ the classical Lorentz spaces for $(p,q) \in [1,\infty]^2$; see for example [Bergh and Löfström 1976]. In particular, $L^{p,p} = L^p$. We define the space of positive and trace class operators by

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

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

$$\|\boldsymbol{\rho}\|_{\mathcal{L}^p} := h^{-d/p'} \|\boldsymbol{\rho}\|_p = h^{-d/p'} (\mathrm{Tr}(|\boldsymbol{\rho}|^p))^{1/p},$$

where $\|\boldsymbol{\rho}\|_p$ denotes the usual Schatten norm (i.e., without dependency in h) and $p' = p/(p-1)$ denotes the conjugate exponent.

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 write the following for smooth polynomial weight functions,

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

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

$$\|f\|_{W^{\sigma,p}_k(\mathbb{R}^{2d})} := \|\langle z\rangle^k f(z)\|_{L^p(\mathbb{R}^{2d})} + \|\langle z\rangle^k \nabla^\sigma_z f(z)\|_{L^p(\mathbb{R}^{2d})},$$

where $z = (x,\xi)$ with $\langle z\rangle^2 = 1 + |x|^2 + |\xi|^2$. We also use the standard notation when $\sigma = 0$ or $p = 2$:

$$L^p_k(\mathbb{R}^{2d}) := W^{0,p}_k(\mathbb{R}^{2d}), \qquad H^\sigma_k(\mathbb{R}^{2d}) := W^{\sigma,2}_k(\mathbb{R}^{2d}).$$

When $\mathbb{R}^{2d}$ is replaced by $\mathbb{R}^d$, as for Lebesgue spaces, we will use shortcut notation and write H^n instead of $H^n(\mathbb{R}^d)$, for example, and C^∞_c for the space of smooth compactly supported functions on $\mathbb{R}^d$.

Wigner and Weyl transforms. We can associate to each density operator $\boldsymbol{\rho}$ a function of the phase space called the Wigner transform, which is defined (for $h = 1$) by

$$w(\boldsymbol{\rho})(x,\xi) := \int_{\mathbb{R}^d} e^{-2i\pi y\cdot\xi} \boldsymbol{\rho}\big(x + \tfrac{1}{2}y, x - \tfrac{1}{2}y\big)\,\mathrm{d}y = \mathcal{F}(\tilde{\boldsymbol{\rho}}_x)(\xi),$$

where $\tilde{\boldsymbol{\rho}}_x(y) = \boldsymbol{\rho}\big(x + \tfrac{1}{2}y, x - \tfrac{1}{2}y\big)$ and we used the following convention for the Fourier transform:

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

This function of the phase space is not a probability distribution, however, since it is generally not nonnegative. We refer to [Lions and Paul 1993] for more properties of the Wigner transform. Given $\boldsymbol{\rho}$, we will write its semiclassical Wigner transform as

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

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 $\boldsymbol{\rho}^W_\hbar(g)$ such that for any $\varphi \in C^\infty_c$,

$$\boldsymbol{\rho}^W_\hbar(g)\varphi := \iint_{\mathbb{R}^{2d}} g\big(\tfrac{1}{2}(x+y),\xi\big) e^{-i(y-x)\cdot\xi/\hbar}\varphi(y)\,\mathrm{d}y\,\mathrm{d}\xi.$$

Theorems. We state our theorems, starting with our main result.

Theorem 1.1. *Let $d \in \{2,3\}$, $a \in \big(\max\big\{\tfrac{1}{2}d - 2, -1\big\}, d-2\big]$ and K be given by either*

$$K(x) = \frac{\pm 1}{|x|^a} \quad \text{or} \quad K(x) = \pm\ln(|x|). \tag{6}$$

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

$$f^{\mathrm{in}} \in W^{\sigma+1,\infty}_m(\mathbb{R}^{2d}) \cap H^{\sigma+1}_\sigma(\mathbb{R}^{2d}), \tag{7}$$

$$\boldsymbol{\rho}^{\mathrm{in}} \in \mathcal{L}^1, \tag{8}$$

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

$$\mathrm{Tr}(|\boldsymbol{\rho} - \boldsymbol{\rho}_f|) \leq (\mathrm{Tr}(|\boldsymbol{\rho}^{\mathrm{in}} - \boldsymbol{\rho}^{\mathrm{in}}_f|) + C_f(t)\hbar)e^{\lambda_f(t)}, \tag{9}$$

where $\boldsymbol{\rho}_f = \boldsymbol{\rho}^W_\hbar(f)$ and $\boldsymbol{\rho}^{\mathrm{in}}_f = \boldsymbol{\rho}_{f^{\mathrm{in}}}$. Upper bounds for the functions λ_f and C_f are given by

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

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

where $\nu = \big(\tfrac{1}{2}m + a + 2 - d\big)_+$ and $n_0 = 2\big\lfloor \tfrac{1}{2}d\big\rfloor + 2$, and remain bounded at any time $t \geq 0$.

Remark 1.2. Condition (6) includes in particular the Coulomb or Newton potential in dimensions $d=3$ and $d=2$. In these cases, the conditions of regularity (7) of the initial data of the Vlasov equation become $f^{\mathrm{in}} \in W_4^{13,\infty}(\mathbb{R}^{2d}) \cap H_{12}^{13}(\mathbb{R}^{2d})$ when $d=3$ and $a=1$, and $f^{\mathrm{in}} \in W_4^{9,\infty}(\mathbb{R}^{2d}) \cap H_8^{9}(\mathbb{R}^{2d})$ when $d=2$ and $a=0$. These conditions are of course not optimal: for example, we ask that $m/2$ and σ be even numbers to simplify some computations.

Remark 1.3. To see more explicitly that (9) gives a good semiclassical approximation estimate, one can take $\boldsymbol{\rho}^{\mathrm{in}}$ and $\boldsymbol{\rho}_f^{\mathrm{in}}$ such that $\mathrm{Tr}(|\boldsymbol{\rho}^{\mathrm{in}} - \boldsymbol{\rho}_f^{\mathrm{in}}|) \leq C\hbar$ and fix some $T>0$, which yields the existence of a constant $C_T>0$ such that for any $t \in [0,T]$,

$$\mathrm{Tr}(|\boldsymbol{\rho} - \boldsymbol{\rho}_f|) \lesssim C_T \hbar. \tag{10}$$

The theorem also implies the convergence of the spatial density of particles $\rho \to \rho_f$ in L^1. Indeed, by duality we have

$$\|\rho - \rho_f\|_{L^1} = \sup_{\substack{O \in L^\infty(\mathbb{R}^d) \\ \|O\|_{L^\infty} \leq 1}} \left| \int O(x)(\rho(x) - \rho_f(x))\,\mathrm{d}x \right| \leq \mathrm{Tr}(|\boldsymbol{\rho} - \boldsymbol{\rho}_f|), \tag{11}$$

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

From the bound in Theorem 1.1 we obtain estimates in other semiclassical Lebesgue spaces.

Theorem 1.4. *Take the same assumptions and notations as in Theorem 1.1, define $\mathfrak{b} = d/(a+1)$ and assume moreover that*

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

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

$$\|\boldsymbol{\rho} - \boldsymbol{\rho}_f\|_{\mathcal{L}^p} \leq \|\boldsymbol{\rho}^{\mathrm{in}} - \boldsymbol{\rho}_f^{\mathrm{in}}\|_{\mathcal{L}^p} + (\mathrm{Tr}(|\boldsymbol{\rho}^{\mathrm{in}} - \boldsymbol{\rho}_f^{\mathrm{in}}|) + c(t)\hbar)e^{\lambda(t)}, \tag{12}$$

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 estimate

$$\|\boldsymbol{\rho} - \boldsymbol{\rho}_f\|_{\mathcal{L}^q} \leq c_2(t)(\|\boldsymbol{\rho}^{\mathrm{in}} - \boldsymbol{\rho}_f^{\mathrm{in}}\|_{\mathcal{L}^p}^{p/q} + \mathrm{Tr}(|\boldsymbol{\rho}^{\mathrm{in}} - \boldsymbol{\rho}_f^{\mathrm{in}}|)^{p/q} + \hbar^{p/q})e^{(p/q)\lambda(t)}, \tag{13}$$

where $\boldsymbol{\rho}_f = \boldsymbol{\rho}_\hbar^W(f)$, $\boldsymbol{\rho}_f^{\mathrm{in}} = \boldsymbol{\rho}_{f^{\mathrm{in}}}$ and $c_2 \in C^0(\mathbb{R}_+, \mathbb{R}_+)$ can be computed explicitly and depend on the initial conditions.

Remark 1.5. In particular, if we assume $\boldsymbol{\rho}^{\mathrm{in}} = \boldsymbol{\rho}_f^{\mathrm{in}}$, or more generally

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

then we have a rate of the form $\hbar^{\mathfrak{b}/2-\varepsilon}$ with $\varepsilon > 0$ arbitrarily small. For the Coulomb potential in dimension $d=3$, the estimate reads

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

for any $t \in [0,T]$ for some fixed $T>0$, where $f_{\boldsymbol{\rho}} = w_\hbar(\boldsymbol{\rho})$ is the Wigner transform of $\boldsymbol{\rho}$. Notice that Theorem 1.1 does not imply convergence of the operators but is only a quantitative estimate, where both $\boldsymbol{\rho}$ and $\boldsymbol{\rho}_\hbar^W(f)$ depend on $\hbar$. As operators, they both for instance converge to 0 in operator norm since by hypothesis $\|\boldsymbol{\rho}\|_\infty \sim Ch^d$. On the contrary, the above equation is both a quantitative estimate and a convergence result since f is a fixed element which does not depend on $\hbar$. Thus it implies the convergence of $f_{\boldsymbol{\rho}}$ to f in $L^\infty_{\mathrm{loc}}(\mathbb{R}_+, L^2(\mathbb{R}^{2d}))$.

With the same assumptions in the case $d = 2$, the Coulomb kernel is of the form $K(x) = C\ln(|x|)$ and $\mathfrak{b} = 2$, implying that (12) holds for any $p \in [1, 2)$ and that we almost get the conjectured optimal rate of convergence for $p = 2$,

$$\|f_{\boldsymbol{\rho}} - f\|_{L^2(\mathbb{R}^{2d})} \leq C_T \hbar^{1-\varepsilon}.$$

Our third result concerns the Hartree–Fock equation. In this case, we combine $p = 1$ and $p > 1$ in one theorem.

Theorem 1.6. *Let $\boldsymbol{\rho}$ be a solution of the Hartree–Fock equation (4) and f be a solution of the Vlasov equation (1) which satisfy the same initial conditions as in Theorem 1.1, and if $p > 1$, the same initial conditions as in Theorem 1.4. If $a > 0$, we also assume 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 exist functions $c \in C^0(\mathbb{R}_+, \mathbb{R}_+)$ and $\lambda \in C^0(\mathbb{R}_+, \mathbb{R}_+)$ depending on d, a, p and f^{in} such that

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

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

$$\|\boldsymbol{\rho} - \boldsymbol{\rho}_f\|_{\mathcal{L}^q} \leq c_2(t)(\|\boldsymbol{\rho}^{\mathrm{in}} - \boldsymbol{\rho}_f^{\mathrm{in}}\|_{\mathcal{L}^p}^{p/q} + \operatorname{Tr}(|\boldsymbol{\rho}^{\mathrm{in}} - \boldsymbol{\rho}_f^{\mathrm{in}}|)^{p/q} + \hbar^{(p/q)\min\{1,\tilde{s}-1\}})e^{(p/q)\lambda(t)},$$

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

1C. *Discussion.*

Higher singularities. 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 1.1 and Theorem 1.4 are still satisfied. More precisely, if $d = 3$, such conditional results hold for any $a \in (1, 2)$. As for Theorem 1.6, a conditional result is still true. However, due to the need to control the exchange term X, we can only address a smaller class of potentials. In particular, in dimension $d = 3$ we have $a \in \left(1, \frac{3}{2}\right)$. Our results in dimensions 2 and 3 can be summarized as follows:

settings:	$d=2$, $a \in (-1, 0]$	$d=2$, $a \in (0, 1)$	$d=3$, $a \in \left(-\frac{1}{2}, 1\right]$	$d=3$, $a \in \left(1, \frac{3}{2}\right)$	$d=3$, $a \in \left[\frac{3}{2}, 2\right)$
Hartree	global	conditional	global	conditional	conditional
Hartree–Fock	global	conditional	global	conditional	no results

General class of potentials. All our results generalize to more general nonradial pair interactions. For $s \in (0, d)$, define the weak Sobolev space $\dot{H}^{s,1}_w$ as the completion of C^∞_c with respect to the norm

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

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

$$u(x) = \int_{\mathbb{R}^d} \frac{1}{|x-w|^{d-s}} \mu(\mathrm{d}w), \tag{14}$$

for some measure $\mu \in \mathcal{M}$.

Notice that this space contains the interaction kernel

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

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

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

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 $\|\Delta^{s/2} u\|_{L^1}$. When $n \in \mathbb{N}$, then $\dot{H}^{n,1} = \dot{W}^{n,1}$ is a classical homogeneous Sobolev space.

The proof for more general potentials follows mainly from the fact that the equation and most of our estimates depend linearly on K. As an example, Proposition 5.1 is proved with this class of potentials. Hence, all our results also hold with the assumption $K \in \dot{H}^{d-a}_w$ instead of $K(x) = |x|^{-a}$ when $a > 0$, except Theorem 1.6, 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 $K \in \dot{H}^{d-a}_w$ and $K^2 \in \dot{H}^{d-2a}_w$ when $a \geq 0$.

From Hartree to Hartree–Fock. Notice that Theorem 1.4 and Theorem 1.6 give a semiclassical estimate between the solutions of the Hartree equation (2) and the solutions of the Hartree–Fock equation (4). Indeed, let $\boldsymbol{\rho}_{\mathrm{H}}$ and $\boldsymbol{\rho}_{\mathrm{HF}}$ be solutions to the Hartree equation and the Hartree–Fock equation, respectively, and let $\boldsymbol{\rho}_f$ be a solution to the Weyl transformed Vlasov equation. Then, for $p \in [1, \infty)$, we have

$$\|\boldsymbol{\rho}_H - \boldsymbol{\rho}_{\mathrm{HF}}\|_{\mathcal{L}^p} \leq \|\boldsymbol{\rho}_H - \boldsymbol{\rho}_f\|_{\mathcal{L}^p} + \|\boldsymbol{\rho}_{\mathrm{HF}} - \boldsymbol{\rho}_f\|_{\mathcal{L}^p},$$

where the first term on the right-hand side is bounded by Theorem 1.4 and the second term on the right-hand side can be estimated by Theorem 1.6.

Well-posedness. One of the strengths of the method is that our strong regularity assumptions that must be independent of $\hbar$ only concern the solutions of the Vlasov equation. Our assumptions on the solution of the Hartree equation imply the global well-posedness of solutions, as proved in [Castella 1997], where the trace norm corresponds to the $L^2(\lambda)$-norm; see also [Ginibre and Velo 1980; 1985; Lions and Paul 1993]. Even if these assumptions are weak, observe however that the operator $\boldsymbol{\rho}^{\mathrm{in}}$ has to be at a finite trace norm distance from the operator $\boldsymbol{\rho}^{\mathrm{in}}$ which by construction is bounded in higher Sobolev spaces (as can be deduced from Proposition 3.3). The additional moment bound when $a \leq 0$ ensures that the energy is finite, which allows us to propagate the space moments; see e.g., [Lafleche 2019, Remark 3.1]. This is sufficient to give a meaning to the pair interaction potential which is growing at infinity in this case.

2. Strategy

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

$$\boldsymbol{p} := -i\hbar\nabla,$$

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 $H = \frac{1}{2}|\boldsymbol{p}|^2 + V(x)$.

2A. ***Quantum gradients of the phase space.*** Since our method 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:

$$\begin{aligned} \boldsymbol{\nabla}_x\boldsymbol{\rho} &:= [\nabla, \boldsymbol{\rho}] = \left[\frac{\boldsymbol{p}}{i\hbar}, \boldsymbol{\rho}\right], \\ \boldsymbol{\nabla}_\xi\boldsymbol{\rho} &:= \left[\frac{x}{i\hbar}, \boldsymbol{\rho}\right]. \end{aligned}$$

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 observe that they are Weyl quantizations, since we have

$$\begin{aligned} \boldsymbol{\nabla}_x\boldsymbol{\rho} &= \boldsymbol{\rho}_\hbar^W(\nabla_x w_\hbar(\boldsymbol{\rho})), \\ \boldsymbol{\nabla}_\xi\boldsymbol{\rho} &= \boldsymbol{\rho}_\hbar^W(\nabla_\xi w_\hbar(\boldsymbol{\rho})). \end{aligned}$$

One should not confuse $\nabla \in \mathcal{L}(L^2)$ with $\boldsymbol{\nabla}_x \in \mathcal{L}(\mathcal{L}(L^2))$. In Section 3, we prove that if a function on the phase space is sufficiently smooth in the classical sense, then its Weyl quantization also has some smoothness in the semiclassical sense.

2B. ***The classical case: L^1 weak-strong stability.*** In the classical case, the method we use to prove the semiclassical limit, which is the content of Sections 4 and 5 can be seen as an equivalent of the following L^1 weak-strong stability estimate for the Vlasov equation, which says that we need to have control of the gradient of only one of the solutions to get a bound on the integral of their difference.

We use the shortcut notation $L^p_x L^{q,r}_\xi = L^p(\mathbb{R}^d, L^{q,r}(\mathbb{R}^d))$ for functions on the phase space of the form $f = f(x,\xi)$. The next proposition can be seen as the classical equivalent of Theorem 1.1.

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*

$$\nabla_\xi f_2 \in L^1([0,T], L^{\mathfrak{b}',1}_x L^1_\xi), \tag{15}$$

one has the stability estimate

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

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

Remark 2.2. In the case of the Coulomb interaction and $\mathfrak{b} = \frac{3}{2}$, 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 if

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

for some $\varepsilon \in (0, 2]$. In particular, the case $\varepsilon = 2$ yields $(3-\varepsilon, 3+\varepsilon) = (1, 5)$, which corresponds to the classical equivalent of the hypotheses required on the solutions in [Saffirio 2020a]. A quantum version of this hypothesis can also be found in [Porta et al. 2017].

Remark 2.3. 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 (15) 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 A. If the potential is more singular than the Coulomb potential, then it is not clear that there are cases such that condition (15) is satisfied.

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

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

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

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

where the notation $\dot{*}$ indicates that we perform the dot product of vectors inside the convolution. We conclude by noticing that by Hölder's inequality for Lorentz spaces (see for example [Hunt 1966, (2.7)]), for any $g \in L^{\mathfrak{b}',1}$,

$$\|\nabla K * g\|_{L^\infty} \le \sup_{z \in \mathbb{R}^d} \int_{\mathbb{R}^d} |\nabla K(z - \cdot) g| \le \|\nabla K\|_{L^{\mathfrak{b},\infty}} \|g\|_{L^{\mathfrak{b}',1}}, \tag{16}$$

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

The next proposition is the classical equivalent of the first part of Theorem 1.4.

Proposition 2.4. *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 $\nabla_\xi f_2 \in L^1([0,T], L^{q,1}_x L^p_\xi)$,*

$$\|f_1 - f_2\|_{L^p(\mathbb{R}^{2d})} \leq \|f_1^{\mathrm{in}} - f_2^{\mathrm{in}}\|_{L^p(\mathbb{R}^{2d})} + C\|f_1^{\mathrm{in}} - f_2^{\mathrm{in}}\|_{L^1(\mathbb{R}^{2d})} \int_0^t \|\nabla_\xi f_2\|_{L^{q,1}_x L^p_\xi} \,\mathrm{d}t \exp\left(C \int_0^T \|\nabla_\xi f_2\|_{L^{\mathfrak{b}',1}_x L^1_\xi} \,\mathrm{d}t\right),$$

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

$$\frac{1}{q} = \frac{1}{p} - \frac{1}{\mathfrak{b}}. \tag{17}$$

Remark 2.5. Formula (17) 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-parameter semigroup $S_{t,s}$ such that $S_{s,s} = 1$ and

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

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

$$\tilde{\Lambda}_t := -\xi \cdot \nabla_x - E_2(t) \cdot \nabla_\xi$$

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

$$\begin{aligned}\partial_s S_{t,s}(f_1 - f_2)(s) &= -S_{t,s}\Lambda_s(f_1 - f_2)(s) + S_{t,s}\Lambda_s f_1(s) - S_{t,s}\tilde{\Lambda}_s f_2(s) \\ &= S_{t,s}(\Lambda_s - \tilde{\Lambda}_s) f_2(s) = S_{t,s}((E_2(s) - E_1(s)) \cdot \nabla_\xi f_2(s)),\end{aligned}$$

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

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

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

$$\|f(t)\|_{L^p_{x,\xi}} \leq \|f^{\mathrm{in}}\|_{L^p_{x,\xi}} + \int_0^t \|E(s) \cdot \nabla_\xi f_2(s)\|_{L^p_{x,\xi}}\,\mathrm{d}s.$$

To bound the expression inside the time integral we write

$$\begin{aligned}\|E(s) \cdot \nabla_\xi f_2(s)\|_{L^p_{x,\xi}} = \|(\rho * \nabla K) \cdot \nabla_\xi f_2(s)\|_{L^p_{x,\xi}} &\leq \int_{\mathbb{R}^d} |\rho(z)| \, \|\nabla K(\cdot - z) \cdot \nabla_\xi f_2(s)\|_{L^p_{x,\xi}}\,\mathrm{d}z \\ &\leq \int_{\mathbb{R}^d} |\rho(z)| \, \Big\| |\nabla K(\cdot - z)| \|\nabla_\xi f_2(s)\|_{L^p_\xi} \Big\|_{L^p_x}\,\mathrm{d}z \\ &\leq \|\rho\|_{L^1} \|\nabla K\|_{L^{\mathfrak{b},\infty}} \|\nabla_\xi f_2(s)\|_{L^{q,1}_x L^p_\xi},\end{aligned}$$

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

3. Regularity of the Weyl transform

In this section, we 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 terms of the Weyl transform of f.

Proposition 3.1. *Let $n, n_1 \in \mathbb{N}$ be even numbers such that $n > \frac{1}{2}d$, and define $\sigma := 2n + n_1$ and $n_0 = 2\lfloor \frac{1}{2}d \rfloor + 2$. 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 $C_{d,n_1} > 0$ depending only on d and n_1 such that*

$$\|\mathrm{diag}(|\nabla_\xi \boldsymbol{\rho}^W_\hbar(f)|)\|_{L^p} \leq C_{d,n_1} \|\nabla_\xi f\|_{W^{n_0,\infty}(\mathbb{R}^{2d}) \cap H^\sigma_\sigma(\mathbb{R}^{2d})}$$

for any $p \in [1, 1+n_1/d]$.

The strategy is to use a special case of the quantum kinetic interpolation inequality proved in Theorem 6 of [Lafleche 2019]. For the operator $|\nabla_\xi \boldsymbol{\rho}|$, this special case reads

$$\|\mathrm{diag}(|\nabla_\xi \boldsymbol{\rho}|)\|_{L^p} \leq C(\mathrm{Tr}(|\nabla_\xi \boldsymbol{\rho}|\,|\boldsymbol{p}|^{n_1}))^\theta \|\nabla_\xi \boldsymbol{\rho}\|^{1-\theta}_{\mathcal{L}^\infty}, \tag{18}$$

where $p = 1 + n_1/d$ and $\theta = 1/p$. The corresponding kinetic inequality is

$$\|\nabla_\xi f\|_{L^p_x(L^1_\xi)} \leq C\left(\iint_{\mathbb{R}^{2d}} |\nabla_\xi f|\,|\xi|^{n_1}\,\mathrm{d}x\,\mathrm{d}\xi\right)^\theta \|\nabla_\xi f\|^{1-\theta}_{L^\infty_{x,\xi}}.$$

To do this, we will need to compare the multiplication of the Weyl transform of a phase space function g by $|\boldsymbol{p}|^n$ and $|x|^n$, with the Weyl transform of the multiplication of g by $|\xi|^n$ and $|x|^n$. This makes error terms appear involving derivatives of g. For example, in the case $n = 2$,

$$\boldsymbol{\rho}^W_\hbar(g)|\boldsymbol{p}|^2 = \boldsymbol{\rho}^W_\hbar\big(|\xi|^2 g + \tfrac{1}{2} i\hbar\xi\cdot\nabla_x g - \tfrac{1}{4}\hbar^2\Delta_x g\big) \quad \text{and} \quad \boldsymbol{\rho}^W_\hbar(g)|x|^2 = \boldsymbol{\rho}^W_\hbar\big(|x|^2 g + i\hbar\xi\cdot\nabla_\xi g + \tfrac{1}{4}\hbar^2\Delta_\xi g\big).$$

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

$$\alpha := (\alpha_{\mathrm{i}})_{\mathrm{i}\in[\![1,d]\!]} \in \mathbb{N}^d, \qquad |\alpha| := \sum_{\mathrm{i}=1}^d \alpha_{\mathrm{i}}, \qquad \alpha! := \alpha_1!\,\alpha_2!\cdots\alpha_d!,$$

$$x^\alpha := x_1^{\alpha_1} x_2^{\alpha_2}\cdots x_d^{\alpha_d}, \qquad \partial_x^\alpha := \partial_{x_1}^{\alpha_1}\partial_{x_2}^{\alpha_2}\cdots\partial_{x_d}^{\alpha_d}, \qquad \alpha \leq \beta \iff \forall \mathrm{i} \in [\![1,d]\!], \alpha_{\mathrm{i}} \leq \beta_{\mathrm{i}}.$$

We then obtain the following set of identities.

Lemma 3.2. *For any $n \in 2\mathbb{N}$ and any tempered distribution g of the phase space,*

$$\boldsymbol{\rho}^W_\hbar(g)|\boldsymbol{p}|^n = \sum_{|\alpha+\beta|=n} a_{\alpha,\beta}\big(\tfrac{1}{2}i\hbar\big)^{|\beta|}\boldsymbol{\rho}^W_\hbar(\xi^\alpha\partial_x^\beta g), \tag{19a}$$

$$\boldsymbol{\rho}^W_\hbar(g)|x|^n = \sum_{|\alpha+\beta|=n} b_{\alpha,\beta}(-i\hbar)^{|\beta|}\boldsymbol{\rho}^W_\hbar(x^\alpha\partial_\xi^\beta g), \tag{19b}$$

$$\boldsymbol{\rho}^W_\hbar(g)|\boldsymbol{p}|^{n_1}|x|^n = \sum_{\substack{|\alpha+\beta|=n_1\\|\alpha'+\beta'|=n}} a_{\alpha,\beta}b_{\alpha',\beta'}(-i\hbar)^{|\beta'|}\big(\tfrac{1}{2}i\hbar\big)^{|\beta|}\boldsymbol{\rho}^W_\hbar(x^{\alpha'}\partial_\xi^{\beta'}(\xi^\alpha\partial_x^\beta g)), \tag{19c}$$

where the coefficients $a_{\alpha,\beta}$ and $b_{\alpha,\beta}$ are nonnegative and do not depend on $\hbar$.

Proof. By definition of the Weyl transform, we deduce that for any $\varphi \in C_c^\infty$,

$$\begin{aligned}\boldsymbol{\rho}_\hbar^W(g)|\boldsymbol{p}|^n\varphi &= (i\hbar)^n \iint_{\mathbb{R}^{2d}} g\big(\tfrac{1}{2}(x+y),\xi\big)e^{-i(y-x)\cdot\xi/\hbar}\Delta^{n/2}\varphi(y)\,\mathrm{d}y\,\mathrm{d}\xi \\ &= (i\hbar)^n \iint_{\mathbb{R}^{2d}} \Delta_y^{n/2}\big(g\big(\tfrac{1}{2}(x+y),\xi\big)e^{-i(y-x)\cdot\xi/\hbar}\big)\varphi(y)\,\mathrm{d}y\,\mathrm{d}\xi.\end{aligned}$$

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

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

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

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

Thus we deduce that the integral kernel κ of the operator $\boldsymbol{\rho}_\hbar^W(g)|\boldsymbol{p}|^n$ is given by

$$\kappa(x,y) = \sum_{|\alpha+\beta|=n} a_{\alpha,\beta}(i\hbar)^{n-|\alpha|}\int_{\mathbb{R}^d} 2^{-|\beta|}\partial_x^\beta g\big(\tfrac{1}{2}(x+y),\xi\big)\xi^\alpha e^{-i(y-x)\cdot\xi/\hbar}\,\mathrm{d}\xi,$$

which yields

$$\boldsymbol{\rho}_\hbar^W(g)|\boldsymbol{p}|^n = \sum_{|\alpha+\beta|=n} a_{\alpha,\beta}\big(\tfrac{1}{2}i\hbar\big)^{|\beta|}\boldsymbol{\rho}_\hbar^W(\xi^\alpha\partial_x^\beta g).$$

This proves (19a). To prove the second identity, we write $u := \frac{1}{2}(x+y)$ and $v := y-x$, so that the integral kernel κ_2 of the operator $\boldsymbol{\rho}_\hbar^W(g)|x|^2$ is given by

$$\begin{aligned}\kappa_2(x,y) &= \iint_{\mathbb{R}^{2d}} g\big(\tfrac{1}{2}(x+y),\xi\big)e^{-i(y-x)\cdot\xi/\hbar}|y|^n\,\mathrm{d}\xi \\ &= \iint_{\mathbb{R}^{2d}} g(u,\xi)e^{-iv\cdot\xi/\hbar}\big(\big|u+\tfrac{1}{2}v\big|^2\big)^{n/2}\,\mathrm{d}\xi \\ &= \iint_{\mathbb{R}^{2d}} g(u,\xi)e^{-iv\cdot\xi/\hbar}\bigg(\sum_{\mathrm{i}=1}^d\big(u_\mathrm{i}^2+\tfrac{1}{4}v_\mathrm{i}^2+u_\mathrm{i}v_\mathrm{i}\big)\bigg)^{n/2}\,\mathrm{d}\xi.\end{aligned}$$

By the multinomial theorem, this can be written as

$$\begin{aligned}\kappa_2(x,y) &= \sum_{|\alpha+\beta|=n} b_{\alpha,\beta}\iint_{\mathbb{R}^{2d}} u^\alpha g(u,\xi)v^\beta e^{-iv\cdot\xi/\hbar}\,\mathrm{d}\xi \\ &= \sum_{|\alpha+\beta|=n} b_{\alpha,\beta}\iint_{\mathbb{R}^{2d}} u^\alpha g(u,\xi)(i\hbar)^{|\beta|}\partial_\xi^\beta e^{-iv\cdot\xi/\hbar}\,\mathrm{d}\xi \\ &= \sum_{|\alpha+\beta|=n} b_{\alpha,\beta}(-i\hbar)^{|\beta|}\iint_{\mathbb{R}^{2d}} u^\alpha\partial_\xi^\beta g(u,\xi)e^{-iv\cdot\xi/\hbar}\,\mathrm{d}\xi,\end{aligned}$$

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

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

In term of operators, this leads to

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

which is (19b). To get the last identity, we combine the first two to get

$$\begin{aligned}\boldsymbol{\rho}_\hbar^W(g)|\boldsymbol{p}|^{n_1}|x|^n &= \sum_{|\alpha+\beta|=n_1} a_{\alpha,\beta}\left(\tfrac{1}{2}i\hbar\right)^{|\beta|}\boldsymbol{\rho}_\hbar^W(\xi^\alpha\partial_x^\beta g)|x|^n \\ &= \sum_{\substack{|\alpha+\beta|=n_1\\|\alpha'+\beta'|=n}} a_{\alpha,\beta}b_{\alpha',\beta'}(-i\hbar)^{|\beta'|}\left(\tfrac{1}{2}i\hbar\right)^{|\beta|}\boldsymbol{\rho}_\hbar^W(x^{\alpha'}\partial_\xi^{\beta'}(\xi^\alpha\partial_x^\beta g)).\end{aligned}$$ □

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

Proposition 3.3. *Let $n\in 2\mathbb{N}$, and let g be a function of the phase space. Then there exists a constant $C>0$ depending only on d and n such that*

$$\|\boldsymbol{\rho}_\hbar^W(g)|\boldsymbol{p}|^n\|_{\mathcal{L}^2} \le (4d)^n\left(\|g|\xi|^n\|_{L^2(\mathbb{R}^{2d})} + \left(\tfrac{1}{2}\hbar\right)^n\|\nabla_x^n g\|_{L^2(\mathbb{R}^{2d})}\right), \tag{20a}$$

$$\|\boldsymbol{\rho}_\hbar^W(g)|x|^n\|_{\mathcal{L}^2} \le \left(\tfrac{9}{4}d\right)^n(\|g|x|^n\|_{L^2(\mathbb{R}^{2d})} + \hbar^n\|\nabla_\xi^n g\|_{L^2(\mathbb{R}^{2d})}), \tag{20b}$$

$$\begin{aligned}\|\boldsymbol{\rho}_\hbar^W(g)|\boldsymbol{p}|^{n_1}|x|^n\|_{\mathcal{L}^2} \le C\big(&\|(1+|x|^n|\xi|^{n_1})g\|_{L^2(\mathbb{R}^{2d})} + \hbar^{n_1}\||x|^n\nabla_x^{n_1}g\|_{L^2(\mathbb{R}^{2d})} \\ &+ \hbar^n\||\xi|^{n_1}\nabla_\xi^n g\|_{L^2(\mathbb{R}^{2d})} + \hbar^{n+n_1}\|\nabla_x^{n_1}\nabla_\xi^n g\|_{L^2(\mathbb{R}^{2d})}\big).\end{aligned} \tag{20c}$$

Proof. By (19a) and the fact that $\|\boldsymbol{\rho}_\hbar^W(u)\|_{\mathcal{L}^2} = \|u\|_{L^2(\mathbb{R}^{2d})}$ for any $u\in L^2(\mathbb{R}^{2d})$, we obtain

$$\|\boldsymbol{\rho}_\hbar^W(g)|\boldsymbol{p}|^n\|_{\mathcal{L}^2} \le \sum_{|\alpha+\beta|=n} a_{\alpha,\beta}\left(\tfrac{1}{2}\hbar\right)^{|\beta|}\|\xi^\alpha\partial_x^\beta g\|_{L^2(\mathbb{R}^{2d})}. \tag{21}$$

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

$$\begin{aligned}\left(\tfrac{1}{2}\hbar\right)^{|\beta|}\|\xi^\alpha\partial_x^\beta g\|_{L^2(\mathbb{R}^{2d})} = \left(\tfrac{1}{2}h\right)^{|\beta|}\|\xi^\alpha y^\beta\hat{g}\|_{L^2(\mathbb{R}^{2d})} &\le \frac{|\alpha|}{n}\||\xi|^n\hat{g}\|_{L^2(\mathbb{R}^{2d})} + \frac{|\beta|}{n}\left(\tfrac{1}{2}h\right)^{|\beta|}\||y|^n g\|_{L^2(\mathbb{R}^{2d})} \\ &\le \||\xi|^n g\|_{L^2(\mathbb{R}^{2d})} + \left(\tfrac{1}{2}\hbar\right)^n\|\nabla_x^n\hat{g}\|_{L^2(\mathbb{R}^{2d})}.\end{aligned}$$

Moreover, as remarked in the proof of Lemma 3.2,

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

from which we obtain (20a). Formulas (20b) and (20c) can be proved in the same way. □

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 3.4. *Let n, $n_1 \in \mathbb{N}$ be even numbers such that $n > \frac{1}{2}d$, and define $k := n + n_1$. Assume $\boldsymbol{\rho} := \boldsymbol{\rho}_\hbar^W(g)$ is the Weyl transform of a function $g \in H^{n+k}_{n+k}(\mathbb{R}^{2d})$. Then the following inequality holds*:

$$\mathrm{Tr}(|\boldsymbol{\rho}|\,|\boldsymbol{p}|^{n_1}) \leq C(\|\langle\xi\rangle^k\langle x\rangle^n g\|_{L^2(\mathbb{R}^{2d})} + \hbar^k\|\langle x\rangle^n\nabla_x^k g\|_{L^2(\mathbb{R}^{2d})} + \hbar^n\|\langle\xi\rangle^k\nabla_\xi^n g\|_{L^2(\mathbb{R}^{2d})} + \hbar^{k+n}\|\nabla_x^k\nabla_\xi^n g\|_{L^2(\mathbb{R}^{2d})}).$$

Proof. First notice that since the sum of eigenvalues is always smaller than the sum of singular values (see for example [Simon 2005, (3.1)]), we have that

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

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

$$\mathrm{Tr}(|\boldsymbol{\rho}|\,|\boldsymbol{p}|^{n_1}) \leq \mathrm{Tr}(|\boldsymbol{\rho}|\boldsymbol{p}|^{n_1}|) \leq \|\boldsymbol{\rho}|\boldsymbol{p}|^{n_1}\boldsymbol{m}_n\|_2\|\boldsymbol{m}_n^{-1}\|_2. \tag{22}$$

To control the second factor on the right-hand side, we observe that it is of the form $\boldsymbol{m}_n^{-1} = w(x)w(-i\hbar\nabla)$ with $w(y) = (1+|y|^n)^{-1}$, so its Hilbert–Schmidt norm can be computed (see e.g., [Simon 2005, (4.7)]) as

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

where $C_{d,n} = \|w\|_{L^2}^2$ is finite since $n > \frac{1}{2}d$. Therefore, by the definition of the $\mathcal{L}^2$-norm, (22) leads to

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

To get the result, we take $\boldsymbol{\rho} = \boldsymbol{\rho}_\hbar^W(g)$ and use Proposition 3.3 to bound the right-hand side of the 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 [1999] which states that if $g \in W^{n_0,\infty}(\mathbb{R}^{2d})$ with $n_0 = 2\lfloor\frac{1}{2}d\rfloor + 2$, then $\boldsymbol{\rho}_1^W(g)$ is a bounded operator on L^2 and its operator norm is bounded by

$$\|\boldsymbol{\rho}_1^W(g)\|_{\mathscr{B}(L^2)} \leq C\|g\|_{W^{n_0,\infty}(\mathbb{R}^{2d})}. \tag{23}$$

Since $\boldsymbol{\rho}_\hbar^W(g) = h^d\boldsymbol{\rho}_1^W(g(\,\cdot\,, h\,\cdot\,))$, and, for $h \leq 1$,

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

by taking $g = \nabla_\xi f$ we deduce from (23) and the definition of the $\mathcal{L}^\infty$-norm that

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

uniformly in $\hbar$. Moreover, taking $g = \nabla_\xi f$ in Proposition 3.4 yields

$$\mathrm{Tr}(|\boldsymbol{\nabla}_\xi\boldsymbol{\rho}_\hbar^W(f)|\,|\boldsymbol{p}|^{n_1}) \leq C\|\nabla_\xi f\|_{H^\sigma_\sigma(\mathbb{R}^{2d})}.$$

The result then follows by combining these two inequalities to bound the right-hand side of the interpolation inequality (18). □

4. Proof of Theorems 1.1 and 1.4

We start this section by proving a stability estimate similar to the inequality used in 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 1.1 and then the proof of Theorem 1.4. The conditional result is stated here.

Proposition 4.1. *Let $K = 1/|x|^a$ with $a \in \big((\frac{1}{2}d-2)_+, d-1\big)$, and assume $\boldsymbol{\rho}$ is a solution of the Hartree equation (2) with initial condition $\boldsymbol{\rho}^{\mathrm{in}} \in \mathcal{L}^1_+$ and $f \geq 0$ is a solution of the Vlasov equation satisfying*

$$f \in L^\infty_{\mathrm{loc}}(\mathbb{R}_+, W^{n_0+1,\infty}(\mathbb{R}^{2d}) \cap H^{\sigma+1}_\sigma(\mathbb{R}^{2d})), \tag{24a}$$

$$\rho_f \in L^\infty_{\mathrm{loc}}(\mathbb{R}_+, L^1 \cap H^\nu), \tag{24b}$$

where $n_0 = 2\lfloor\frac{1}{2}d\rfloor + 2$ and $n,\ n_1 \in 2\mathbb{N}$ are such that $n > \frac{1}{2}d$ and $n_1 \geq d/(\mathfrak{b}-1)$, and we use the notation $\sigma = 2n + n_1,\ \nu = (n+a+2-d)_+$ and $\mathfrak{b} = d/(a+1)$. Then

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

where

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

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

Remark 4.2. It is actually sufficient to assume that $f \geq 0$ when $t = 0$ since this implies that it holds at any time $t \geq 0$.

In analogy with the classical case (see the proof of Proposition 2.4), 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

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

where B_t is an operator defined through its integral kernel by

$$B_t(x,y) = \big((K * \rho_f)(x) - (K * \rho_f)(y) - (\nabla K * \rho_f)\big(\tfrac{1}{2}(x+y)\big) \cdot (x-y)\big)\boldsymbol{\rho}_f(x,y). \tag{25}$$

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

$$\begin{aligned}\|\boldsymbol{\rho}(t) - \boldsymbol{\rho}_f(t)\|_p&\\ \leq \|\boldsymbol{\rho}^{\mathrm{in}} - \boldsymbol{\rho}^{\mathrm{in}}_f\|_p + \frac{1}{\hbar}\int_0^t \|B_t\|_p\,\mathrm{d}s + \frac{1}{\hbar}\int_0^t\!\!\int |\rho(s,z) - \rho_f(s,z)|\,\|[K(\cdot - z), \boldsymbol{\rho}_f(s)]\|_p\,\mathrm{d}z\,\mathrm{d}s.&\end{aligned} \tag{26}$$

We now take $p = 1$, i.e., the trace norm, and we have to bound each term on the right-hand side of (26) in order to obtain a Grönwall type inequality which will prove Proposition 4.1. Note that we will then again use (26) with $p > 1$ together with Theorem 1.1 to prove Theorem 1.4.

4A. ***The commutator inequality.*** Generalizing [Porta et al. 2017, Lemma 3.1], we obtain the quantum equivalent of (16), which is the following inequality for the trace norm of the commutator of K and a trace class operator $\boldsymbol{\rho}$.

Theorem 4.3. *Let $a \in (-1, d-1)$ and $K(x) = 1/|x|^a$ or $K(x) = \ln(|x|)$ when $a = 0$. Then*

$$\nabla K \in L^{\mathfrak{b},\infty} \quad \text{with } \mathfrak{b} = \mathfrak{b}_a := \frac{d}{a+1}.$$

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

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

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

Remark 4.4. In the case of the Coulomb interaction and $d = 3$, we have $K(x) = 1/|x|$, $\mathfrak{b} = \mathfrak{b}_1 = \frac{3}{2}$ and $\nabla K \in L^{3/2,\infty}$. Thus for any $\varepsilon \in (0, 2]$, there exists a constant $C > 0$ such that

$$\operatorname{Tr}(|[K(\cdot - z), \boldsymbol{\rho}]|) \le Ch \|\operatorname{diag}(|\nabla_\xi \boldsymbol{\rho}|)\|_{L^{3-\varepsilon}}^{1/2+\tilde{\varepsilon}} \|\operatorname{diag}(|\nabla_\xi \boldsymbol{\rho}|)\|_{L^{3+\varepsilon}}^{1/2-\tilde{\varepsilon}},$$

for any $\tilde{\varepsilon} \in \left(0, \frac{1}{6}\varepsilon\right)$.

Theorem 4.3 is a corollary of the slightly more precise proposition that follows.

Proposition 4.5. *For any $\delta \in ((1/\mathfrak{b}'_1 - 1/\mathfrak{b}')_+, 1 - 1/\mathfrak{b}')$ and $q \in (\mathfrak{b}'/(1-\delta\mathfrak{b}'), \infty]$, there exists a constant $C > 0$ such that*

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

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

Proof of Theorem 4.3. We will decompose the potential as a combination of Gaussian functions (see e.g., [Lieb and Loss 2001, 5.9 (3)]). By using the definition of the gamma function and a simple change of variable, when $a > 0$ one obtains, for any $r > 0$,

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

where $\omega_a = 2\pi^{a/2}/\left(\Gamma\left(\frac{1}{2}a\right)\right)$. Taking $r = |x|^2$ leads directly to the decomposition

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

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

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

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

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

In all these cases, defining $\omega_0 := 1$, we get the identity

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

Following the idea of [Porta et al. 2017] but using this new decomposition, we write

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

from which we get

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

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

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

Noticing 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

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

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 get

$$\begin{aligned}\|\phi_\theta\cdot\nabla_\xi\boldsymbol{\rho}\varphi_{1-\theta}\|_1 &\le \sum_{j\in J}|\lambda_j|\,\||\phi_\theta\psi_j\rangle\langle\psi_j\varphi_{1-\theta}|\|_1 \\ &\le \sum_{j\in J}|\lambda_j|\,\|\phi_\theta\psi_j\|_{L^2}\|\psi_j\varphi_{1-\theta}\|_{L^2},\end{aligned}$$

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

$$\begin{aligned}\|\phi_\theta\cdot\nabla_\xi\boldsymbol{\rho}\varphi_{1-\theta}\|_1 &\le \Big(\sum_{j\in J}|\lambda_j|\,\|\phi_\theta\psi_j\|_{L^2}^2\Big)^{1/2}\Big(\sum_{j\in J}|\lambda_j|\,\|\psi_j\varphi_{1-\theta}\|_{L^2}^2\Big)^{1/2} \\ &\le \Big(\int_{\mathbb{R}^d}|\phi_\theta|^2\rho_1\Big)^{1/2}\Big(\int_{\mathbb{R}^d}|\varphi_{1-\theta}|^2\rho_1\Big)^{1/2},\end{aligned}$$

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

$$\|\phi_\theta\cdot\nabla_\xi\boldsymbol{\rho}\varphi_{1-\theta}\|_1 \le \|\phi_\theta\|_{L^{2p'}}\|\varphi_{1-\theta}\|_{L^{2q'}}\|\rho_1\|_{L^p}^{1/2}\|\rho_1\|_{L^q}^{1/2}, \tag{30}$$

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 (29). We can now compute explicitly the integrals of the functions ϕ and φ:

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

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

$$\|[K(\cdot-z),\boldsymbol{\rho}]\|_1 \leq h\int_0^\infty \frac{C_{d,a,p'}\|\rho_1\|_{L^p}^{1/2}\|\rho_1\|_{L^q}^{1/2}}{t^{(1/2)(d/(2p')+d/(2q')+1-a)}}\int_0^1 \frac{\mathrm{d}\theta}{\theta^{(d+2p')/(4p')}(1-\theta)^{d/(4q')}}\,\mathrm{d}t,$$

with

$$C_{d,a,p'} = |\omega_a|\left(\frac{\omega_d}{\omega_{d+2p'}}\right)^{1/(2p')}(2p')^{-(d+2p')/(4p')}(2q')^{-d/(4q')}.$$

We observe that the integral over θ is converging as soon as

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

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

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

or equivalently, since $\mathfrak{b}=d/(a+1)$,

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

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 $t\geq R$, then we can also take for example $p=p_0>\frac{1}{2}\mathfrak{b}'$ and then any q such that

$$\frac{2}{\mathfrak{b}} - \frac{1}{p_0'} < \frac{1}{q'} < \frac{4}{d} \qquad \text{and} \qquad \frac{1}{q'} \leq 1. \tag{32}$$

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

$$\left(\frac{1}{\mathfrak{b}_1'}-\frac{1}{\mathfrak{b}'}\right)_+ < \delta < 1-\frac{1}{\mathfrak{b}'}, \qquad \frac{1}{p_0} = \frac{1}{\mathfrak{b}'}+\delta, \qquad \frac{1}{q} < \frac{1}{\mathfrak{b}'}-\delta.$$

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

$$\|[K(\cdot-z),\boldsymbol{\rho}]\|_1 \leq Ch(R^{(d/2)(1/\mathfrak{b}-1/p_0')}\|\rho_1\|_{L^{p_0}} + R^{(d/2)(1/\mathfrak{b}-1/(2p_0')-1/(2q'))}\|\rho_1\|_{L^{p_0}}^{1/2}\|\rho_1\|_{L^q}^{1/2}).$$

Optimizing with respect to R yields

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

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

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

where $\theta_1 = (1/p_0 - 1/q)/(1/p - 1/q)$. Noticing that $\theta_0\theta_1 = (1/p_0 - 1/\mathfrak{b}')/(1/p - 1/q)$ and that we can take $1/p_0$ as close as we want to $1/p$, there exists ε_1 such that we can choose p_0 such that

$$\theta_0\theta_1 + \varepsilon_1 = \frac{1/p - 1/\mathfrak{b}'}{1/p - 1/q} = \frac{1}{2} + \frac{\varepsilon}{2\mathfrak{b}'}.$$

Therefore, the last inequality combined with (33) leads to (27). □

The following proposition is an extension of Theorem 4.3 to $\mathcal{L}^p$ spaces, for $p < \mathfrak{b}$. Notice however that the right-hand side here is expressed in terms of weighted quantum Lebesgue norms, which makes the inequality weaker than the one in Theorem 4.3.

Proposition 4.6. *Let $d \geq 2$, $a \in \left(-1, \min\left(2, \frac{1}{2}d\right)\right)$ and $1 \leq p < \mathfrak{b} := d/(a+1)$. Then for any $\varepsilon \in (0, q-1)$ and $n > a+1$, there exists a constant $C > 0$ such that*

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

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

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

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

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

where we twice used Hölder's inequality for operators to obtain the second line from the right side of the first. We notice that $\phi_\theta \boldsymbol{m}_{n_\alpha}^{-1}$ is of the form $g(-i\nabla)f(x)$, so that since $\alpha \geq 2$, by the Kato–Seiler–Simon inequality (see e.g., [Simon 2005, Theorem 4.1]),

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

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 $C_{d,n_\alpha,\alpha} := \|m_{n_\alpha}^{-1}\|_{L^\alpha} < \infty$, this yields

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

Then a direct computation of the integral of ϕ_θ yields

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

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

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

Therefore, (34) leads to

$$\begin{aligned} \|[K(\cdot - z), \boldsymbol{\rho}]\|_p &\leq \int_0^\infty \frac{C_{\boldsymbol{\rho}} h^{1-d(1/\alpha+1/\beta)}}{t^{(1/2)(d/\alpha+d/\beta+1-a)}} \left(\int_0^1 \frac{\mathrm{d}\theta}{\theta^{(d+\alpha)/(2\alpha)}(1-\theta)^{d/(2\beta)}}\right) \mathrm{d}t \\ &\leq \int_0^\infty \frac{C_{\boldsymbol{\rho}} h^{1+d/p'-d/q'}}{t^{(d/2)(1/p-1/q-1/\mathfrak{b})+1}} \left(\int_0^1 \frac{\mathrm{d}\theta}{\theta^{(d+\alpha)/(2\alpha)}(1-\theta)^{d/(2\beta)}}\right) \mathrm{d}t, \end{aligned}$$

where

$$C_{\boldsymbol{\rho}} = \left(\frac{\omega_d}{\omega_{d+\alpha}}\right)^{1/\alpha} \frac{C_{d,n_\alpha,\alpha} C_{d,n_\beta,\beta}}{\beta^{d/(2\beta)} \alpha^{(d+\alpha)/(2\alpha)}} \|\boldsymbol{m}_{n_\alpha} \nabla_\xi \boldsymbol{\rho} \boldsymbol{m}_{n_\beta}\|_q.$$

The integrals in θ and t converge since

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

Then observe that as proved in Appendix B (see (56)),

$$\|\boldsymbol{m}_{n_\alpha} \nabla_\xi \boldsymbol{\rho} \boldsymbol{m}_{n_\beta}\|_q \leq \|\nabla_\xi \boldsymbol{\rho} \boldsymbol{m}_{n_\beta} \boldsymbol{m}_{n_\alpha}\|_q = \|\nabla_\xi \boldsymbol{\rho} \boldsymbol{m}_n\|_q,$$

and we conclude the proof by taking the optimal R as in the proof of Theorem 4.3. □

4B. *Bound for the error term.* In this section, we will prove that the operator B_t defined by (25) is small when h goes to 0.

Proposition 4.7. *Under the hypotheses of Theorem 1.1, if $p \in [1, 2]$ and $n \in 2\mathbb{N}$ with $n > \frac{1}{2}d$, then*

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

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

Proof. Recalling the notation $E = -\nabla K * \rho$ as in [Saffirio 2020a; 2020b], we write a decomposition of B_t as

$$\begin{aligned}\frac{1}{i\hbar}B_t(x,y) &= \int_0^1 E((1-\theta)x+\theta y) - E\big(\tfrac12(x+y)\big)\,\mathrm{d}\theta\cdot\nabla_\xi\boldsymbol{\rho}_f(x,y)\\ &= i\hbar\int_0^1\!\!\int_0^1 \big(\theta-\tfrac12\big)\nabla E\big(((1-\theta)x+\theta y)\theta' + \tfrac12(x+y)(1-\theta')\big)\,\mathrm{d}\theta\,\mathrm{d}\theta' : \nabla_\xi^2\boldsymbol{\rho}_f(x,y)\\ &= i\hbar\int_0^1\!\!\int_0^1 \big(\theta-\tfrac12\big)\nabla E(a_{\theta,\theta'}x + b_{\theta,\theta'}y)\,\mathrm{d}\theta\,\mathrm{d}\theta' : \nabla_\xi^2\boldsymbol{\rho}_f(x,y)\end{aligned}$$

where $a_{\theta,\theta'} = \frac12(\theta'+1) - \theta\theta'$, $b_{\theta,\theta'} = \frac12(1-\theta') + \theta\theta'$ and ":" denotes the double contraction of tensors. In terms of the Fourier transform of ∇E, this yields

$$\frac{1}{i\hbar}B_t(x,y) = i\hbar\int_0^1\!\!\int_0^1\!\!\int_{\mathbb{R}^d}\big(\theta-\tfrac12\big)e^{2i\pi z\cdot(a_{\theta,\theta'}x+b_{\theta,\theta'}y)}\widehat{\nabla E}(z)\,\mathrm{d}\theta\,\mathrm{d}\theta'\,\mathrm{d}z : \nabla_\xi^2\boldsymbol{\rho}_f(x,y).$$

Defining e_ω as the operator of multiplication by the function $x\mapsto e^{2i\pi\omega z\cdot x}$, we obtain

$$\frac{1}{i\hbar}B_t = i\hbar\int_0^1\!\!\int_0^1\!\!\int_{\mathbb{R}^d}\big(\theta-\tfrac12\big)\widehat{\nabla E}(z) : e_{a_{\theta,\theta'}}(\nabla_\xi^2\boldsymbol{\rho}_f)e_{b_{\theta,\theta'}}\,\mathrm{d}\theta\,\mathrm{d}\theta'\,\mathrm{d}z,$$

and since e_ω is a bounded (unitary) operator, taking the quantum Lebesgue norms yields

$$\frac{1}{\hbar}\|B_t\|_{\mathcal{L}^p} \le \hbar\int_0^1\!\!\int_0^1\!\!\int_{\mathbb{R}^d}\big|\theta-\tfrac12\big|\,|\widehat{\nabla E}(z)|\,\|e_{a_{\theta,\theta'}}(\nabla_\xi^2\boldsymbol{\rho}_f)e_{b_{\theta,\theta'}}\|_{\mathcal{L}^p}\,\mathrm{d}\theta\,\mathrm{d}\theta'\,\mathrm{d}z \le \tfrac12\hbar\|\widehat{\nabla E}\|_{L^1}\|\nabla_\xi^2\boldsymbol{\rho}_f\|_{\mathcal{L}^p}.$$

- Now to bound $\|\widehat{\nabla E}\|_{L^1}$, we can use the fact that for any $n > \frac12 d$, the Fourier transform maps H^n continuously into L^1 to get

$$\|\widehat{\nabla E}\|_{L^1} \le C_{d,n}\|\nabla^2 K * \rho_f\|_{H^n}.$$

If $a = d-2$, then by the continuity of $\nabla^2 K * \cdot$ in H^n, we get $\|\widehat{\nabla E}\|_{L^1} \le C\|\rho_f\|_{H^n}$. Otherwise, if $a \in \big(\frac12 d - 2, d\big)\setminus\{2\}$, we get

$$\|\widehat{\nabla E}\|_{L^1} \le C_{d,n,a}\|(1+|x|^n)|x|^{a+2-d}\widehat{\rho_f}\|_{L^2} \le C_{d,n,a}\|\rho_f\|_{\dot H^{a+2-d}\cap\dot H^{n+a+2-d}} \le C_{d,n,a}\|\rho_f\|_{L^1\cap H^{(n+a+2-d)_+}},$$

where we used the fact that if $\alpha\in\big(-\frac12 d, 0\big)$, then by Sobolev's inequalities $L^{p^*}\supset\dot H^\alpha$ with $1/p^* = \frac12 - \alpha/d$, and then $L^2\cap L^1\subset L^{p^*}$ since $p^*\in[1,2]$.

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

$$\|\nabla_\xi^2\boldsymbol{\rho}_f\|_{\mathcal{L}^p} \le \|\nabla_\xi^2\boldsymbol{\rho}_f\|_{\mathcal{L}^2}^\theta\|\nabla_\xi^2\boldsymbol{\rho}_f\|_{\mathcal{L}^1}^{1-\theta} = \|\nabla_\xi^2 f\|_{L^2(\mathbb{R}^{2d})}^\theta\|\nabla_\xi^2\boldsymbol{\rho}_f\|_{\mathcal{L}^1}^{1-\theta}, \tag{35}$$

where $\theta = 2/p'$. Then using the fact that $\nabla_\xi^2\boldsymbol{\rho}_f = \boldsymbol{\rho}_\hbar^W(\nabla_\xi^2 f)$, we can use Proposition 3.4 with $g = \nabla_\xi^2 f$, $n_1 = 0$ and $n > \frac12 d$ to get

$$\|\nabla_\xi^2\boldsymbol{\rho}_f\|_{\mathcal{L}^1} \le C\|\nabla_\xi^2 f\|_{H^{2n}_{2n}(\mathbb{R}^{2d})},$$

which using (35) implies that $\|\nabla_\xi^2\boldsymbol{\rho}_f\|_{\mathcal{L}^p} \le C\|\nabla_\xi^2 f\|_{H^{2n}_{2n}(\mathbb{R}^{2d})}$. $\square$

4C. *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.

For $p = 1$, inequality (26) yields

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

Proposition 4.7 gives a bound on the second term on the right-hand side, whereas Theorem 4.3 allows us to bound the last term on the right-hand side uniformly in z. Moreover, because of (11), we have

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

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

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

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

$$\|\operatorname{diag}(|\nabla_\xi \boldsymbol{\rho}_f|)\|_{L^p} \leq \mathcal{C}_{d,n_1}\|\nabla_\xi f\|_{W^{n_0,\infty}(\mathbb{R}^{2d})\cap H^{2n+n_1}_{2n+n_1}(\mathbb{R}^{2d})},$$

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

4D. *Proof of Theorem 1.1.* To prove this theorem, it remains to prove that the assumptions (24a) and (24b) 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 needed in our case in Proposition A.1 in Appendix A. With our assumptions on the initial data, we have $f^{\mathrm{in}} \in W^{\sigma+1,\infty}_m(\mathbb{R}^{2d})$ with $m > d$. Moreover, since $f^{\mathrm{in}} \in H^{\sigma+1}_\sigma(\mathbb{R}^{2d})$ with $\sigma > m + d/(\mathfrak{b}-1)$, by Hölder's inequality we deduce in particular that $f^{\mathrm{in}} \in L^2_\sigma(\mathbb{R}^{2d})$ 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 $n_1 > d/(\mathfrak{b}-1)$. Therefore, Proposition A.1 indeed leads 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 notice that $\sigma > n_0 := 2\lfloor \frac{1}{2}d \rfloor + 2$. Finally, the H^ν bound for ρ also follows from Hölder's inequality since $\sigma > \frac{1}{2}d$, so that

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

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

4E. ***Proof of Theorem 1.4.*** We now prove Theorem 1.4 using the results of Propositions 4.6 and 4.7.

Recall inequality (26). The bound (11) yields

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

The second term on the right-hand side can be estimated thanks to Proposition 4.7 and can then be bounded as in the case $p=1$. The last term on the right-hand side is bounded by Proposition 4.6 by terms of the form $\|\nabla_\xi \boldsymbol{\rho}_f \boldsymbol{m}_n\|_{\mathcal{L}^q}$ with $\boldsymbol{m}_n = 1+|\boldsymbol{p}|^n$, $n > a+1 = d/\mathfrak{b}$ and $1/q$ close to $1/p - 1/\mathfrak{b}$. When $a < \frac{1}{2}(d-2)$, then $q \le 2$ and we can bound them by interpolating between $\mathcal{L}^1$ and $\mathcal{L}^2$ weighted norms, yielding

$$\|\nabla_\xi \boldsymbol{\rho}_f \boldsymbol{m}_n\|_{\mathcal{L}^q} \le \|\nabla_\xi \boldsymbol{\rho}_f \boldsymbol{m}_n\|_{\mathcal{L}^2}^{2/q'} \|\nabla_\xi \boldsymbol{\rho}_f \boldsymbol{m}_n\|_{\mathcal{L}^1}^{1-2/q'},$$

and we can then bound these terms by Propositions 3.3 and 3.4. When $q > 2$, this strategy is no longer possible; however, by the property of the Weyl transform and Calderón–Vaillancourt–Boulkhemair inequality (23) we know that

$$\|\boldsymbol{\rho}_\hbar^W(g)\|_{\mathcal{L}^2} = \|g\|_{L^2(\mathbb{R}^{2d})} \qquad \text{and} \qquad \|\boldsymbol{\rho}_\hbar^W(g)\|_{\mathcal{L}^\infty} \le C_d \|g\|_{W^{n_0,\infty}(\mathbb{R}^{2d})},$$

where $n_0 = 2\lfloor \frac{1}{2}d \rfloor + 2$. Therefore, this time, we interpolate between the $\mathcal{L}^2$- and $\mathcal{L}^\infty$-norm to get

$$\|\boldsymbol{\rho}_\hbar^W(g)\|_{\mathcal{L}^q} \le C_d^\theta \|\boldsymbol{\rho}_\hbar^W(g)\|_{\mathcal{L}^\infty}^\theta \|\boldsymbol{\rho}_\hbar^W(g)\|_{\mathcal{L}^2}^{1-\theta} \le C_d^\theta \|g\|_{W^{n_0,\infty}(\mathbb{R}^{2d})}^\theta \|g\|_{L^2(\mathbb{R}^{2d})}^{1-\theta}, \tag{36}$$

where $\theta = 1 - 2/q$ is close to $2/p' - 1/\mathfrak{b}' \pm \varepsilon$. Using Lemma 3.2, we see that $\nabla_\xi \boldsymbol{\rho}_f \boldsymbol{m}_n$ can be written as a linear combination of terms of the form $\boldsymbol{\rho}_\hbar^W(\xi^\alpha \partial_x^\beta \nabla_\xi f) =: \boldsymbol{\rho}_\hbar^W(g_{\alpha,\beta})$, where α and β are multi-indices satisfying $|\alpha+\beta| \le n$. Therefore, taking $g = g_{\alpha,\beta}$ in (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 1.1. We can therefore conclude by Grönwall's lemma that (12) holds.

Now we prove (13). Consider (12) and the bound

$$\|\boldsymbol{\rho}-\boldsymbol{\rho}_f\|_{\mathcal{L}^\infty} \le \|\boldsymbol{\rho}\|_{\mathcal{L}^\infty} + \|\boldsymbol{\rho}_f\|_{\mathcal{L}^\infty}. \tag{37}$$

As for the first term on the right-hand side, we know that all $\mathcal{L}^p$-norms are propagated by the Hartree equation, therefore $\|\boldsymbol{\rho}\|_{\mathcal{L}^\infty} = \|\boldsymbol{\rho}^{\mathrm{in}}\|_{\mathcal{L}^\infty}$ and hence it is bounded by assumption. In the second term on the right-hand side we again use the Calderón–Vaillancourt–Boulkhemair inequality (23). Hence, if $f \in W^{n_0,\infty}(\mathbb{R}^{2d})$ and $\boldsymbol{\rho}^{\mathrm{in}} \in \mathcal{L}^\infty$, the $\mathcal{L}^\infty$-norm of the difference $\boldsymbol{\rho}-\boldsymbol{\rho}_f$ is bounded uniformly in $\hbar$. To conclude, we bound the $\mathcal{L}^q$-norm using the $\mathcal{L}^\infty$-norm and the $\mathcal{L}^p$-norm with $p = \mathfrak{b} - \varepsilon$, for $\varepsilon > 0$ small enough, and get

$$\|\boldsymbol{\rho}-\boldsymbol{\rho}_f\|_{\mathcal{L}^q} \le \|\boldsymbol{\rho}-\boldsymbol{\rho}_f\|_{\mathcal{L}^p}^{p/q} \|\boldsymbol{\rho}-\boldsymbol{\rho}_f\|_{\mathcal{L}^\infty}^{1-p/q},$$

since $q \in (p,\infty)$. Then (12) yields

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

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

5. Proof of Theorem 1.6

We recall that $\mathsf{X} = \mathsf{X}_{\boldsymbol{\rho}}$ is the operator of the time-dependent integral kernel $\mathsf{X}_{\boldsymbol{\rho}}(x, y) = K(x - y)\boldsymbol{\rho}(x, y)$, where $\boldsymbol{\rho}$ is the integral kernel of the operator $\boldsymbol{\rho}$. Under the conditions of Theorem 1.6, the associated energy is bounded and we have the following inequalities.

Proposition 5.1. *Let $a \in [0, d)$, $s := d - a$ and $\boldsymbol{\rho}$ be a positive trace class operator. Then if $K \in \dot{H}^{s,1}_w$, we have that*

$$\operatorname{Tr}(\mathsf{X}\boldsymbol{\rho}) \le C h^s \|K\|_{\dot{H}^{s,1}_w} \||\boldsymbol{p}|^{a/2}\boldsymbol{\rho}\|^2_{\mathcal{L}^2}. \tag{38}$$

Moreover, if $a \in \left[0, \frac{1}{2}d\right)$ and $K^2 \in \dot{H}^{2s-d,1}_w$, then for any $p \in [1, 2]$ and $q = (2p)/(2 - p) \in [2, \infty]$ there exists a constant such that for any operator $\boldsymbol{\rho}_2$,

$$\|\mathsf{X}_{\boldsymbol{\rho}}\boldsymbol{\rho}_2\|_{\mathcal{L}^p} \le C h^s \|K^2\|^{1/2}_{\dot{H}^{2s-d,1}_w} \||\boldsymbol{p}|^{a/2}\boldsymbol{\rho}\|_{\mathcal{L}^2} \|\boldsymbol{\rho}_2\|_{\mathcal{L}^q}. \tag{39a}$$

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

$$\|\mathsf{X}_{\boldsymbol{\rho}}\boldsymbol{\rho}_2\|_{\mathcal{L}^p} \le C h^{s+d(1/p-1/2)} \|K^2\|^{1/2}_{\dot{H}^{2s-d,1}_w} \||\boldsymbol{p}|^{a/2}\boldsymbol{\rho}\|_{\mathcal{L}^2} \|\boldsymbol{\rho}_2\|_{\mathcal{L}^\infty}, \tag{39b}$$

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

Remark 5.2. We can control the weighted $\mathcal{L}^2$-norms by the inequality

$$\||\boldsymbol{p}|^{a/2}\boldsymbol{\rho}\|^2_{\mathcal{L}^2} \le \|\boldsymbol{\rho}\|_{\mathcal{L}^\infty} \operatorname{Tr}(|\boldsymbol{p}|^a\boldsymbol{\rho}). \tag{40}$$

Notice 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 $\operatorname{Tr}(|\boldsymbol{p}|^a\boldsymbol{\rho})$ on the right-hand side. However, by definition of the absolute value for operators and by cyclicity of the trace, we get

$$\||\boldsymbol{p}|^{a/2}\boldsymbol{\rho}\|^2_2 = \operatorname{Tr}(\boldsymbol{\rho}|\boldsymbol{p}|^a\boldsymbol{\rho}) = \operatorname{Tr}(\boldsymbol{\rho}\boldsymbol{\rho}^{1/2}|\boldsymbol{p}|^a\boldsymbol{\rho}^{1/2}) = \operatorname{Tr}(\boldsymbol{\rho}||\boldsymbol{p}|^{a/2}\boldsymbol{\rho}^{1/2}|^2).$$

Now, Hölder's inequality gives

$$\operatorname{Tr}(\boldsymbol{\rho}||\boldsymbol{p}|^{a/2}\boldsymbol{\rho}^{1/2}|^2) \le \|\boldsymbol{\rho}\|_\infty \operatorname{Tr}(||\boldsymbol{p}|^{a/2}\boldsymbol{\rho}^{1/2}|^2) = \|\boldsymbol{\rho}\|_\infty \operatorname{Tr}(|\boldsymbol{p}|^a\boldsymbol{\rho}),$$

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

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

- *Proof of inequality (38).* Use (14) to get

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

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

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

Now we concentrate on bounding the double integral. First we observe that by the change of variable $z = x - y - w$ we have

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

Then, by the Hardy–Rellich inequality (see e.g., [Yafaev 1999]), since $a \in [0, d)$, for any $\varphi \in H^{a/2}$, we have that

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

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

$$\mathcal{E}_a \le \mathcal{C}_{d,a} \iint_{\mathbb{R}^{2d}} |\Delta_z^{a/4} \boldsymbol{\rho}(z + y + w, y)|^2 \,\mathrm{d}z\,\mathrm{d}y = \mathcal{C}_{d,a} \iint_{\mathbb{R}^{2d}} |\Delta_x^{a/4} \boldsymbol{\rho}(x, y)|^2 \,\mathrm{d}x\,\mathrm{d}y.$$

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

$$\mathcal{E}_a \le C_{d,a} h^{d-a} \| |\boldsymbol{p}|^{a/2} \boldsymbol{\rho} \|_{\mathcal{L}^2}^2,$$

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

- *Proof of inequality* (39a). Since $\mathsf{X}_{\boldsymbol{\rho}}$ is a positive operator, $\mathsf{X}_{\boldsymbol{\rho}}^2 = |\mathsf{X}_{\boldsymbol{\rho}}|^2$. Moreover, denoting by $\tilde{\mathsf{X}}_{\boldsymbol{\rho}}$ the exchange operator associated to the kernel K^2, the following interesting property holds:

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

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

$$\|\mathsf{X}_{\boldsymbol{\rho}} \boldsymbol{\rho}_2\|_p \le \|\boldsymbol{\rho}_2\|_q \|\mathsf{X}_{\boldsymbol{\rho}}\|_2 \le h^{d/q'} \|\boldsymbol{\rho}_2\|_{\mathcal{L}^q} \operatorname{Tr}(\tilde{\mathsf{X}}_{\boldsymbol{\rho}} \boldsymbol{\rho})^{1/2},$$

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

- *Proof of inequality* (39b). We use the fact that $\|\mathsf{X}_{\boldsymbol{\rho}} \boldsymbol{\rho}_2\|_p \le \|\mathsf{X}_{\boldsymbol{\rho}} \boldsymbol{\rho}_2\|_2$ for any $p \ge 2$ and then we use (39a) for $p = 2$ to get

$$\|\mathsf{X}_{\boldsymbol{\rho}} \boldsymbol{\rho}_2\|_{\mathcal{L}^p} \le h^{(d/2 - d/p')} \|\mathsf{X}_{\boldsymbol{\rho}} \boldsymbol{\rho}_2\|_{\mathcal{L}^2} \le C h^{s + d(1/p - 1/2)} \|K^2\|_{\dot{H}_w^{2s-d,1}}^{1/2} \| |\boldsymbol{p}|^{a/2} \boldsymbol{\rho}\|_{\mathcal{L}^2} \|\boldsymbol{\rho}\|_{\mathcal{L}^\infty}.$$

The use of the nonsemiclassical inequality $\|\mathsf{X}_{\boldsymbol{\rho}} \boldsymbol{\rho}_2\|_p \le \|\mathsf{X}_{\boldsymbol{\rho}} \boldsymbol{\rho}_2\|_2$ explains the deterioration of the rate, which might not be optimal. □

When $a < 0$, we have similar bounds using moments in x instead of moments in $\boldsymbol{p}$.

Proposition 5.3. *Let $a < 0$ and $K(x) = |x|^{|a|}$. Then for any positive operator $\boldsymbol{\rho}$,*

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

Moreover, for any $p \in [1, \infty]$, *there exists a constant* $C > 0$ *such that for any operator* $\boldsymbol{\rho}_2$,

$$\|\mathsf{X}_{\boldsymbol{\rho}}\boldsymbol{\rho}_2\|_{\mathcal{L}^p} \leq C h^d \||x|^{|a|/2}\boldsymbol{\rho}\|_{\mathcal{L}^2}\|\boldsymbol{\rho}_2\|_{\mathcal{L}^q} \quad \text{when } p \in [1, 2), \tag{42a}$$

$$\|\mathsf{X}_{\boldsymbol{\rho}}\boldsymbol{\rho}_2\|_{\mathcal{L}^p} \leq C h^{d(1/p+1/2)} \||x|^{|a|/2}\boldsymbol{\rho}\|_{\mathcal{L}^2}\|\boldsymbol{\rho}_2\|_{\mathcal{L}^\infty} \quad \text{when } p \in [2, \infty], \tag{42b}$$

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

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

$$\iint_{\mathbb{R}^{2d}} K(x-y)|\boldsymbol{\rho}(x,y)|^2 \,\mathrm{d}x\,\mathrm{d}y \leq C \iint_{\mathbb{R}^{2d}} (|x|^{|a|} + |y|^{|a|})|\boldsymbol{\rho}(x,y)|^2 \,\mathrm{d}x\,\mathrm{d}y$$

and observing that the right-hand side is exactly the right-hand side of (41). The two other inequalities follow by taking K^2 instead of K and using Hölder's inequality as in the proof of Proposition 5.3. □

Proof of Theorem 1.6. We proceed as in the proof of Theorem 1.1 and consider the one-parameter group of unitary transformations $\mathcal{U}_t$ generated by the Hartree–Fock Hamiltonian, i.e.,

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

and compute

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

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

$$\begin{aligned}\|\boldsymbol{\rho} - \boldsymbol{\rho}_\hbar^W(f)\|_{\mathcal{L}^p} \leq \|\boldsymbol{\rho}^{\mathrm{in}} - \boldsymbol{\rho}_f^{\mathrm{in}}\|_{\mathcal{L}^p} + \frac{1}{\hbar}\int_0^t \|[K*(\rho-\rho_f), \boldsymbol{\rho}_\hbar^W(f)]\|_{\mathcal{L}^p}\,\mathrm{d}s \\ + \frac{1}{\hbar}\int_0^t \|B_s\|_{\mathcal{L}^p}\,\mathrm{d}s + \frac{1}{\hbar}\int_0^t \|[\mathsf{X}_{\boldsymbol{\rho}}, (\boldsymbol{\rho} - \boldsymbol{\rho}_\hbar^W(f))]\|_{\mathcal{L}^p}\,\mathrm{d}s.\end{aligned} \tag{43}$$

The second and third terms on the right-hand side in (43) can be bounded as in Theorem 1.1. As for the fourth term, we use Proposition 5.1.

More precisely, when $K(x) = \pm|x|^{-a}$ with $a \in \left[0, \frac{1}{2}d\right)$, using (39a) or (39b) yields

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

with $\tilde{s} = d - a - d(1/2 - 1/p)_+$. When $\tilde{s} \geq 2$, this does not change the order of the rate of convergence $O(h)$. When $\tilde{s} < 2$ (i.e., for high values of a and p), the contribution of the exchange term becomes bigger than that of the second term on the right-hand side of (43), thus leading to a rate of convergence of the order $O(h^{\tilde{s}-1})$.

When $K(x) = \pm|x|^{-a}$ with $a \in (-1, 0)$, we use (42a) or (39b) to get bounds in terms of $\||x|^{|a|/2}\boldsymbol{\rho}\|_{\mathcal{L}^2}$ instead of $\||\boldsymbol{p}|^{|a|/2}\boldsymbol{\rho}\|_{\mathcal{L}^2}$.

When $K(x) = \pm\ln(|x|)$, we write $K(x) \leq C_\varepsilon(|x|^\varepsilon + |x|^{-\varepsilon})$ and use both types of inequalities to get bounds with $\|(|x|^{\varepsilon/2} + |\boldsymbol{p}|^{\varepsilon/2})\boldsymbol{\rho}\|_{\mathcal{L}^2}$ instead.

For all the choices of K, when $p = 1$, we can therefore conclude that

$$\|\boldsymbol{\rho} - \boldsymbol{\rho}^W_\hbar(f)\|_{\mathcal{L}^1} \leq (\|\boldsymbol{\rho}^{\text{in}} - \boldsymbol{\rho}^{\text{in}}_f\|_{\mathcal{L}^1} + C_0(t)\hbar + C_1(t)\hbar^{s-1})e^{\lambda(t)}. \tag{44}$$

When $p \in (1, \mathfrak{b})$, we proceed as in the proof of (12) (the Hartree case) and use (44) to get

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

Moreover, when $p \in [\mathfrak{b}, \infty)$, again as in the Hartree case, we proceed as in the proof of (13). Following the exact same argument, $\|\boldsymbol{\rho} - \boldsymbol{\rho}^W_\hbar(f)\|_{\mathcal{L}^\infty}$ is bounded uniformly in $\hbar$ as soon as $\boldsymbol{\rho}^{\text{in}} \in \mathcal{L}^\infty$ and $f \in W^{2\lfloor d/2\rfloor+2,\infty}$. Hence,

$$\|\boldsymbol{\rho} - \boldsymbol{\rho}^W_\hbar(f)\|_{\mathcal{L}^p} \leq C(t)(\|\boldsymbol{\rho}^{\text{in}} - \boldsymbol{\rho}^{\text{in}}_f\|_1^{1-\theta} + C_0\hbar^{p/q} + C_1\hbar^{(\tilde{s}-1)p/q})e^{\lambda(t)}.$$

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

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 [1992] or Lions and Perthame [1991], 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 by Han-Kwan [2019] or in Appendix A in the work by the second author [Saffirio 2020b]. 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 $W^{\sigma,\infty}_n(\mathbb{R}^{2d})$. We prefer to work in the framework of [Lions and Perthame 1991], which allows us to have noncompactly 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 $K = 1/|x|^a$ with $a \in (-1, d-2]$ and let $(n, \sigma, n_1) \in \mathbb{N}^3$ be such that $n > d$ and $n_1 > d/(\mathfrak{b}-1)$ with $\mathfrak{b} = d/(a+1)$. Let $f \geq 0$ be a solution of the Vlasov equation (1) with initial data $f^{\text{in}} \in W^{\sigma,\infty}_n(\mathbb{R}^{2d})$ satisfying*

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

Then the following regularity estimates hold:

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

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

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

$$f \in L^\infty_{\text{loc}}(\mathbb{R}_+, H^\sigma_k(\mathbb{R}^{2d})).$$

The proof works in two steps. We first explain in the next lemma how to get 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.2. *Let f be a solution of the Vlasov equation (1) as in Proposition A.1 with $\sigma \geq 1$ and assume moreover that*

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

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

Proof. For clarity, we first start with the case $\sigma = 1$ for which we present 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 [Golse 2013].

Case 1: $\sigma = 1$. Define the transport operator $\mathsf{T} := \xi \cdot \nabla_x + E \cdot \nabla_\xi$. Then we have

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

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

To simplify the computations, recall that $\mathsf{T}^* = -\mathsf{T}$ and $\mathsf{T}(uv) = u\mathsf{T}(v) + \mathsf{T}(u)v$. Hence, by writing $m_n := 1 + |\xi|^{np} + |x|^{np}$ and using the notation $u^p := |u|^{p-1}u$, we have

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

However, noticing that

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

we can simplify (49) as

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

Now define

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

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

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

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

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

Then again by Young's inequality for products,

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

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

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

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

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

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 that in [Beale et al. 1984] which can be found in the course notes [Golse 2013] and can be written as

$$\|\nabla E\|_{L^\infty} \leq C(1 + M_0 + \|\rho_f\|_{L^\infty} \ln(1 + \|\nabla \rho_f\|_{L^\infty})) \leq C_t(1 + \ln(1 + \|\nabla \rho_f\|_{L^\infty})) =: J(t).$$

Combining these bounds we arrive at $\frac{\mathrm{d}}{\mathrm{d}t} M_{x,\xi} \leq p(1+n) J(t) M_{x,\xi}$, which by Grönwall's lemma implies

$$M_{x,\xi}^{1/p}(t) \leq M_{x,\xi}^{1/p}(0) e^{(1+n)\int_0^t J}.$$

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

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

However, since $n > d$, we have

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

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

$$\begin{aligned} J(t) &\leq C_t + C_t \ln((1 + C_{d,n}\|f^{\mathrm{in}}\|_{W_n^{1,\infty}(\mathbb{R}^{2d})}) e^{(1+n)\int_0^t J}) \\ &\leq C_t + C_t \ln(1 + C_{d,n}\|f^{\mathrm{in}}\|_{W_n^{1,\infty}(\mathbb{R}^{2d})}) + C_t(1+n)\int_0^t J. \end{aligned}$$

Hence, by Grönwall's lemma,

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

We then deduce the bounds on $\|f\|_{W_n^{1,\infty}(\mathbb{R}^{2d})}$ and $\nabla \rho_f$ by (51) and (52).

Case 2: $\sigma > 1$. We give details for $\sigma = 2$. The generalization to $\sigma \geq 2$ follows in the same way. In the case $\sigma = 2$, (48b) and (48a) become

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

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

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

and compute their time derivatives, using Young's inequality for products, the bound on $\mathsf{T}(m_n)$ as in Case 1 and the fact that $p>1$:

$$\begin{aligned}
\frac{\mathrm{d}M_{\xi\xi}}{\mathrm{d}t}&\le p(n\|E\|_{L^\infty}+n+2)M_{\xi\xi}+2pM_{x\xi},\\
\frac{\mathrm{d}M_{x\xi}}{\mathrm{d}t}&\le p(n\|E\|_{L^\infty}+n+1+\|\nabla E\|_{L^\infty})M_{x\xi}+pM_{xx}+p\|\nabla E\|_{L^\infty}M_{\xi\xi},\\
\frac{\mathrm{d}M_{xx}}{\mathrm{d}t}&\le p(n\|E\|_{L^\infty}+n+2\|\nabla E\|_{L^\infty}+\|\nabla^2 E\|_{L^\infty})M_{xx}+2p\|\nabla E\|_{L^\infty}M_{x\xi}+p\|\nabla^2 E\|_{L^\infty}M_{\xi},
\end{aligned}$$

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

$$\frac{\mathrm{d}}{\mathrm{d}t}M_2\le Cp(n\|E\|_{L^\infty}+n+2+2\|\nabla E\|_{L^\infty}+\|\nabla^2 E\|_{L^\infty})M_2.$$

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

$$M_2^{1/p}(t)\le M_2^{1/p}(0)e^{C_t},\tag{53}$$

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

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

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 $\sigma=|\boldsymbol{\sigma}|$ stands for the sum of the components of the multi-index $\boldsymbol{\sigma}=(\sigma_1,\sigma_2,\dots)$. □

Proof of Proposition A.1. It just remains to prove that assumption (47) holds. First notice that the method used in [Lions and Perthame 1991, 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 $p=1+n_1/d$ by the kinetic interpolation inequality. Then, by Young's inequality, since $n_1>d/(\mathfrak{b}-1)$, we deduce that

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

Finally, as proved in [Lafleche 2019, 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

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

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 $H_k^\sigma(\mathbb{R}^{2d})$-norm is also initially bounded, we can again use (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. Again we conclude the proof using Grönwall's lemma. □

Appendix B: Operator identities

Here we list some formulas for operators which are used in this paper. First, if A and B are self-adjoint, then we have

$$\|AB\|_p = \|BA\|_p, \tag{54}$$

which follows from the fact that the singular values are the same for an operator and its adjoint [Simon 2005, (1.3)]. Then we shall remember Hölder's inequality for operators [Simon 2005, Theorem 2.8], which says that for any bounded operators A and B and any $(p,q,r)\in[1,\infty]^3$ such that $1/p=1/q+1/r$,

$$\|AB\|_p \leq \|A\|_q\|B\|_r. \tag{Hölder}$$

The second important inequality is the Araki–Lieb–Thirring inequality [Araki 1990, Theorem 1] which states that for any operators $A, B\geq 0$ and any $(q,r)\in[1,\infty)\times\mathbb{R}_+$, the following inequality is true:

$$\mathrm{Tr}((BAB)^{qr}) \leq \mathrm{Tr}((B^qA^qB^q)^r).$$

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

$$\|AB\|_{qr}^q \leq \|A^qB^q\|_r. \tag{55}$$

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 $A, B\geq 0$, $p\geq 1$ and $r\geq 0$, the following mixing inequality holds:

$$\|B^rAB\|_p \leq \|AB^{r+1}\|_p. \tag{56}$$

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

$$\|B^rAB\|_p \leq \|B^rA^{r/(r+1)}\|_{((r+1)/r)p}\|A^{1/(r+1)}B\|_{(r+1)p}.$$

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

$$\|B^rA^{r/(r+1)}\|_{((r+1)/r)p} \leq \|AB^{r+1}\|_p^{r/(r+1)} \quad \text{and} \quad \|A^{1/(r+1)}B\|_{(r+1)p} \leq \|AB^{r+1}\|_p^{1/(r+1)},$$

which yield the result. □

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