FROM MANY-BODY QUANTUM DYNAMICS
TO THE HARTREE–FOCK AND VLASOV EQUATIONS
WITH SINGULAR POTENTIALS

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ABSTRACT. We obtain the combined mean-field and semiclassical limit from the N-body Schrödinger equation for fermions interacting via singular potentials. To obtain the result, we first prove the uniformity in Planck's constant h propagation of regularity for solutions to the Hartree–Fock equation with singular pair interaction potentials of the form $\pm|x-y|^{-a}$, including the Coulomb and gravitational interactions.

In the context of mixed states, we use these regularity properties to obtain quantitative estimates on the distance between solutions to the Schrödinger equation and solutions to the Hartree–Fock and Vlasov equations in Schatten norms. For $a \in (0, 1/2)$, we obtain local-in-time results when $N^{-1/2} \ll h \leq N^{-1/3}$. In particular, it leads to the derivation of the Vlasov equation with singular potentials. For $a \in [1/2, 1]$, our results hold only on a small time scale, or with an N-dependent cutoff.

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Part I. **Introduction**

1. Background

1.1. **The Equations.** We consider a system of N identical quantum particles of mass m interacting through a pair potential $K(x - y)$. The state of the system is described by an N-body wave function $\psi_N = \psi_N(t, x_1, x_2, \ldots, x_N)$, belonging to the space of square-integrable complex-valued functions $\mathfrak{h} = L^2(\mathbb{R}^{3N}, \mathbb{C})$, with evolution given by the N-body Schrödinger equation

$$(1) \qquad i\hbar\, \partial_t \psi_N = \sum_{k=1}^{N} -\frac{\hbar^2}{2\,m} \Delta_{x_k} \psi_N + \sum_{1 \leq k < l \leq N} K(x_k - x_l)\, \psi_N,$$

where h is the Planck constant and $\hbar = \frac{h}{2\,\pi}$ is the reduced Planck constant. In applications, one is typically interested in systems where the number of particles N is large, thus making the microscopic description given by the solution to Equation (1) not suitable for studies. In fact, the high dimensionality of the configuration space presents a formidable barrier for understanding the dynamics of the many-body wave function at a microscopic scale. Instead, one can consider the problem at a mesoscopic scale and look at the classical phase space distributions of particles $f = f(t, x, \xi)$, where $(x, \xi) \in \mathbb{R}^3 \times \mathbb{R}^3$ are the spatial and momentum variables. When the collisions are not dominant, the equation governing the dynamics of a large number of interacting particles is given by the Vlasov equation

$$(2) \qquad \partial_t f + \xi \cdot \nabla_x f + E_f \cdot \nabla_\xi f = 0,$$

where $E_f = -\nabla V_f$ is the force field corresponding to the mean-field potential

$$V_f(x) = (K * \rho_f)(x) = \int_{\mathbb{R}^3} K(x-y)\,\rho_f(y)\,\mathrm{d}y$$

and ρ_f is the spatial distribution of particles defined by

$$(3) \qquad \rho_f(x) = \int_{\mathbb{R}^3} f(x,\xi)\,\mathrm{d}\xi.$$

To explore the connection between the microscopic and the mesoscopic scales of the system, we consider the intermediate case of a large number of particles at a microscopic scale where the effective quantum dynamics of the system can be described by its mean-field behavior. Roughly speaking, this means the many-body effects exerted by the system on each particle is well-approximated by an effective interaction potential obtained by averaging the pair potential K with the underlying spatial density of the system. To draw a parallel with the classical theory, one can consider the mean-field equation called the Hartree equation which is the quantum analogue of the Vlasov equation. More precisely, let us take a positive self-adjoint trace class operator $\boldsymbol{\rho}$ acting on $L^2(\mathbb{R}^3, \mathbb{C})$, which can be seen as a positive linear convex combination of projections onto one-particle wave functions. We use the same notation to denote both the operator $\boldsymbol{\rho}$ and its integral kernel $\boldsymbol{\rho}(x,y)$. Here, $\boldsymbol{\rho}$ plays the role of the quantum one-particle phase space distribution of particles. Moreover, the effective one-particle Hamiltonian is given by $H = -\frac{\hbar^2}{2}\Delta + V_{\boldsymbol{\rho}}$, called the Hartree Hamiltonian, where $V_{\boldsymbol{\rho}}$ is the mean-field potential $V_{\boldsymbol{\rho}} = K * \rho(x)$ and $\rho(x)$ is the quantum spatial distribution of particles defined by

$$(4) \qquad \rho(x) = \mathrm{diag}(\boldsymbol{\rho})\,(x) := h^3\,\boldsymbol{\rho}(x,x).$$

With these notations, the Hartree equation reads

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

where $[A, B] := AB - BA$ is the commutator of the operators A and B. If the particles obey the Fermi–Dirac statistics, a more accurate description of their evolution is given by the Hartree–Fock equation

$$(5) \qquad i\hbar\,\partial_t\boldsymbol{\rho} = [H_{\boldsymbol{\rho}}, \boldsymbol{\rho}]\,, \qquad\qquad H_{\boldsymbol{\rho}} = -\frac{\hbar^2}{2}\Delta + V_{\boldsymbol{\rho}} - h^3\,\mathsf{X}_{\boldsymbol{\rho}}\,,$$

where the exchange term $\mathsf{X}_{\boldsymbol{\rho}}$ is the operator with integral kernel

$$(6) \qquad \mathsf{X}_{\boldsymbol{\rho}}(x,y) = K(x-y)\,\boldsymbol{\rho}(x,y).$$

1.2. **The Change of Scaling.** Our goal in this paper is to study simultaneously the mean-field limit, corresponding to the approximations made when the number of particles N is large, and the semiclassical limit, corresponding to a change of scaling where the Planck constant h becomes negligible. More precisely, we consider a solution ψ_N to the Schrödinger equation (1) and define the function $\widetilde{\psi}_N(t, x_1, \ldots, x_N) = \psi_N(T\,t, L\,x_1, \ldots, L\,x_N)$ for some characteristic length L and timescale T. Multiplying equation (1) by $\frac{T}{m\,L^2}$ yields

$$i\,\widetilde{\hbar}\,\partial_t\widetilde{\psi}_N = \sum_{k=1}^{N} -\frac{\widetilde{\hbar}^2}{2}\,\Delta_{x_k}\widetilde{\psi}_N + \frac{1}{N}\sum_{1 \le k < l \le N}\widetilde{K}(x_k - x_l)\,\widetilde{\psi}_N,$$

where $\widetilde{\hbar} = \frac{\hbar T}{m L^2}$ and $\widetilde{K}(x) = \frac{N T^2}{m L^2} K(L x)$. In particular, in the case of a homogeneous interaction $K(x) = \kappa |x|^{-a}$, this gives $\widetilde{K}(x) = \widetilde{\kappa} |x|^{-a}$ where $\widetilde{\kappa} = \frac{\kappa N T^2}{m L^{2+a}}$. In the remainder of the paper, we drop the tilde and study the equation

$$(7) \qquad i\hbar \,\partial_t \psi_N = H_N \,\psi_N, \qquad H_N = \sum_{k=1}^{N} -\frac{\hbar^2}{2}\Delta_{x_k} + \frac{1}{N} \sum_{1 \le k < l \le N} K(x_k - x_l)$$

with scalings such that $\hbar \to 0$, $N \to \infty$ and with

$$(8) \qquad K(x) = \frac{\kappa}{|x|^a},$$

where $\kappa \in \mathbb{R}$ is of order 1 and $a \in (0, 1]$. In fact, we study the time evolution of N-body mixed states, which are self-adjoint, positive trace class operators of rank larger than one. By the spectral theorem, they can be expressed in the following way:

$$(9) \qquad \boldsymbol{\rho}_N = \sum_{j=1}^{\infty} \lambda_j \,|\psi_j\rangle\langle\psi_j| \quad \text{with} \quad \lambda_j \ge 0$$

where $\{\,\psi_j\,\}_{j\in\mathbb{N}} \subset \mathfrak{h}^{\otimes N}$ is an orthonormal set of anti-symmetric wave functions. The operator $\boldsymbol{\rho}_N$ is called a pure state provided it is a rank one projection, that is, $\boldsymbol{\rho}_N = |\psi_N\rangle\langle\psi_N|$. The time evolution equation for density operators is given by the Liouville–von Neumann equation

$$(10) \qquad i\hbar \,\partial_t \boldsymbol{\rho}_N = [H_N, \boldsymbol{\rho}_N]$$

where the Hamiltonian H_N is given in Equation (7), which is the quantum analogue of the classical Liouville equation, equivalent to the N-body Newton laws. The two parameters $\hbar$ and N can a priori be independent, however some restrictions apply in the case of fermions, as shown in Figure 1 and explained in Section 1.4.
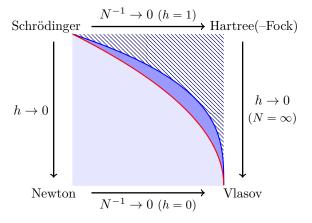

FIGURE 1. The different scalings for the combined mean-field and semiclassical limits. The red line corresponds to the line $h = N^{-1/2}$ and the blue line to $h = N^{-1/3}$.

Notice that the density of particles, i.e. the number of particles per unit of volume, has to be of order $N L^{-3}$, which according to our scaling leads to a quantity proportional to $N h^{3/2} (m/T)^{3/2}$. This explains why the part of Figure (1) that is closer to the Hartree–Fock equation corresponds to relatively higher densities, while the part that is below corresponds to relatively lower densities.

1.3. **State of the Art.** Both the problems of the mean-field limits and the semi-classical limits are well-known questions that are largely addressed in the literature. However, the derivation of the Vlasov–Poisson equation, i.e. the case of the Coulomb and gravitational potentials, remains an open problem, both in the case of quantum mechanics and in the case of classical Newton's laws.

1.3.1. *The Classical Mean-Field Limit.* In the context of classical mechanics, the problem of justifying the Vlasov equation (2) starting from the dynamics of N-particles obeying Newton's laws was first proven for twice differentiable potentials in the pioneering works by Neunzert and Wick [55], Braun and Hepp [18], and then by Dobrushin [25] using the Wasserstein–Monge–Kantorovich distance (see also [71]). The class of potentials was then extended to less regular potentials but still locally Hölder continuous by Hauray and Jabin [40, 41], which was later improved by Jabin and Wang using entropy methods in [43], where the potential is only required to be bounded.

From another point of view, it was also proved in [41] that it is possible to obtain the mean-field limit for potentials with a vanishing cutoff, converging to potentials almost as singular as the Coulomb potential when $N \to \infty$ (see also Boers and Pickl [17]). This is in particular interesting from a numerical point of view. These results were then improved by Lazarovici [48], allowing the cutoff potential to converge to the Coulomb potential, and by Lazarovici and Pickl [49], with a N-dependent cutoff of the order of the inter-particle distance.

1.3.2. *Combined Mean-Field and Semiclassical Limits.* The first rigorous derivation of the Vlasov equation (2) from the N-body Schrödinger equation (1) was proved by Narnhofer and Sewel [54] in the case of smooth potentials, with $\hbar = N^{-1/3}$. Subsequently, the restriction on the potential was substantially relaxed by Spohn [70] to twice differentiable potentials. For the same kind of potentials, a more explicit rate of convergence without assuming $\hbar = N^{-1/3}$ was later obtained by Graffi, Martinez, and Pulvirenti [37] in the case of weak convergence, and more recently by Golse and Paul [34] in the quantum Wasserstein metrics, and by Chen, Lee and Liew for fermions [21] in the scaling $\hbar = N^{-1/3}$.

1.3.3. *Quantum Mean-Field Limit.* It is also possible to first look at the mean-field limit with $\hbar = 1$, i.e. without taking the semiclassical limit, leading to the Hartree and the Hartree–Fock equations. In this case, the situation is better understood, even for the Coulomb and gravitational potentials. For bosons, weak convergence was proved in [10, 28, 8], and explicit rates in stronger norms were obtained in [63, 38, 59, 23, 44, 53, 22, 56]. For fermions, weak convergence was proved in [9] for bounded potentials, and estimates in trace norm and singular potentials such as the Coulomb potential were obtained in [32, 5, 58, 57].

Some of these results have been extended by taking into account the semiclassical parameter $\hbar$. For fermions, taking $\hbar = N^{-1/3}$, convergence of Husimi transform has been proven in [27] for analytic interactions and short times. Schatten norms

estimates have been obtained in [13, 11, 58] for at least twice differentiable potentials. A conditional result was obtained in the case of pure states and singular potentials in [60, 64].

For bosons, results were obtained for at least twice differentiable potentials in [33, 36, 35]

1.3.4. *Semiclassical Limit.* Another possible direction is to look only at the semiclassical limit $\hbar \to 0$, either for the number of particles N fixed or in the mean-field regime. This last case corresponds to going from the Hartree or the Hartree–Fock equation to the Vlasov equation. In the case of the Hartree equation, this was proved in [51] in weak topology, but including singular potentials such as the Coulomb interaction (See also [52, 30]). Explicit rates in stronger norms were then obtained in [4, 1, 12, 34] for at least twice differentiable potentials, and then in [45, 65, 66, 46, 47] for singular interactions.

1.4. **Constraints on the Scalings.** The Fourier transform is defined by

$$
(11) \qquad \widehat{g}(\xi) = \int_{\mathbb{R}^3} e^{-2\pi i\, x \cdot \xi}\, g(x)\, \mathrm{d}x
$$

for $g \in L^2(\mathbb{R}^3)$. We also adopt the following conventions for the time-dependent operator solution $\boldsymbol{\rho} = \boldsymbol{\rho}(t)$ to the Hartree–Fock equation (5)

$$
(12) \qquad \begin{aligned} \|\boldsymbol{\rho}\|_\infty &= \mathcal{C}_\infty, \\ \mathrm{Tr}(\boldsymbol{\rho}) &= h^{-3}. \end{aligned}
$$

for some constant $\mathcal{C}_\infty$. In particular, $\int_{\mathbb{R}^3} \rho(x)\, \mathrm{d}x = h^3\, \mathrm{Tr}(\boldsymbol{\rho}) = 1$. For such an operator, we define its Wigner transform by

$$
f_{\boldsymbol{\rho}}(x,\xi) := \int_{\mathbb{R}^3} e^{-i\, y \cdot \xi / \hbar}\, \boldsymbol{\rho}(x + \tfrac{y}{2}, x - \tfrac{y}{2})\, \mathrm{d}y,
$$

so that it is a function of the phase space with mass $\iint f_{\boldsymbol{\rho}}\, \mathrm{d}x\, \mathrm{d}\xi = h^3\, \mathrm{Tr}(\boldsymbol{\rho}) = 1$. It is well known that, under some regularity assumptions, the Wigner transform of solutions $\boldsymbol{\rho}$ to the Hartree–Fock equation (5) converge to solutions of the Vlasov equation (2) in the semiclassical limit $h \to 0$ (see e.g. [51]). We refer to [51] for a listing of the properties of the Wigner transform. One of them is the fact that

$$
(13) \qquad \|f_{\boldsymbol{\rho}}\|_{L^2(\mathbb{R}^6)} = h^{\frac{3}{2}}\, \|\boldsymbol{\rho}\|_2\,,
$$

where we denote by

$$
(14) \qquad \|\boldsymbol{\rho}\|_p = \left(\mathrm{Tr}(|\boldsymbol{\rho}|^p) \right)^{\frac{1}{p}}
$$

the Schatten norm of order p. Here, the absolute value of an operator A is defined by $|A| = \sqrt{A^* A}$. Since we want to address the case when $f_{\boldsymbol{\rho}}$ converges in $L^2(\mathbb{R}^6)$ to a solution f of the Vlasov equation, this implies that $h^{\frac{3}{2}}\, \|\boldsymbol{\rho}\|_2 \underset{h \to 0}{\to} \|f\|_{L^2(\mathbb{R}^6)}$, so that $\|\boldsymbol{\rho}\|_2$ is of size $h^{-3/2}$.

For an N-particle density operator $\boldsymbol{\rho}_N$, we look at its one-particle reduced density operator $\boldsymbol{\rho}_{N:1}$ defined as the partial trace with of $\boldsymbol{\rho}_N$ respect to the variables 2 to N, that is,

$$
\boldsymbol{\rho}_{N:1} = \mathrm{Tr}_{2,\dots,N}(\boldsymbol{\rho}_N).
$$

Since we also want the corresponding Wigner transform $f_{N:1}$ of the operator $\boldsymbol{\rho}_{N:1}$ of the N-particle density operator to converge to f, we have as well

$$(15) \qquad \|f_{N:1}\|_{L^2(\mathbb{R}^6)} = h^{\frac{3}{2}} \|\boldsymbol{\rho}_{N:1}\|_2 \longrightarrow \|f\|_{L^2(\mathbb{R}^6)} \quad \text{as } N \to \infty \text{ and } h \to 0.$$

However, in the case of fermions, we also know that (as proved for example in [50, 12.5.12], or [69, Theorem 8.4])

$$(16) \qquad 0 \le \boldsymbol{\rho}_{N:1} \le \frac{\operatorname{Tr}(\boldsymbol{\rho}_{N:1})}{N} = \frac{h^{-3}}{N}.$$

Therefore, by bounding the square of the Hilbert–Schmidt norm by the product of the trace norm and the operator norm, we deduce that

$$(17) \qquad \|\boldsymbol{\rho}_{N:1}\|_2^2 \le \|\boldsymbol{\rho}_{N:1}\|_1 \|\boldsymbol{\rho}_{N:1}\|_\infty \le \frac{h^{-6}}{N}.$$

Combining Inequality (17) with Formula (13) with $\boldsymbol{\rho} = \boldsymbol{\rho}_{N:1}$, we obtain

$$(18) \qquad h \le \mathcal{C}_2^{-2/3} N^{-1/3},$$

where $\mathcal{C}_2 = \|f_{N:1}\|_{L^2(\mathbb{R}^6)}$ converges to $\|f\|_{L^2(\mathbb{R}^6)}$, and so remains of order 1. Hence, we are mainly interested in the case when $N h^3$ is bounded above by a constant independent of N and h. This corresponds to the part below the blue line in Figure 1.

Observe our analysis still makes sense if $N h^3 \to \infty$. However, in this situation, even though the solution to the N-body Schrödinger equation and the solution to the Hartree–Fock equation are close, they will not converge in the semiclassical limit to a nontrivial solution of the Vlasov equation, but to zero.

2. Functional Spaces

2.1. **Semiclassical Spaces.** Since we want to look at the convergence in the semiclassical limit $\hbar \to 0$ towards probability distributions of the phase space, we define the semiclassical versions of the Lebesgue norms of the phase space as the following rescaled Schatten norms

$$(19) \qquad \|\boldsymbol{\rho}\|_{\mathcal{L}^p} = h^{\frac{3}{p}} \|\boldsymbol{\rho}\|_p = h^{\frac{3}{p}} \operatorname{Tr}(|\boldsymbol{\rho}|^p)^{\frac{1}{p}}.$$

More generally, given some weight m, we define the weighted spaces by the norm $\|\boldsymbol{\rho}\|_{\mathcal{L}^p(m)} = \|\boldsymbol{\rho}\, m\|_{\mathcal{L}^p}$. To see this definition is compatible with the semiclassical limit, notice that for any operator $\boldsymbol{\rho} \ge 0$ verifying the scaling assumptions (12), one obtains

$$(20) \qquad \|\boldsymbol{\rho}\|_{\mathcal{L}^1} = 1, \qquad\qquad \|\boldsymbol{\rho}\|_{\mathcal{L}^2} = \|f_{\boldsymbol{\rho}}\|_{L^2(\mathbb{R}^6)}, \qquad\qquad \|\boldsymbol{\rho}\|_{\mathcal{L}^\infty} = \mathcal{C}_\infty.$$

One good property of the norm defined by (19) is that it is compatible with taking powers of the operator, in the sense that for any $c > 0$, $\|\boldsymbol{\rho}^c\|_{\mathcal{L}^p} = \|\boldsymbol{\rho}\|_{\mathcal{L}^{pc}}^c$. In particular, in the rest of the paper we will often work with the operator $\sqrt{\boldsymbol{\rho}}$, which verifies, as one would expect, $\left\|\sqrt{\boldsymbol{\rho}}\right\|_{\mathcal{L}^2} = 1$ and $\left\|\sqrt{\boldsymbol{\rho}}\right\|_{\mathcal{L}^\infty} = \sqrt{\mathcal{C}_\infty}$.

The fact that these norms are good analogues of the classical Lebesgue norms can be better understood in light of particular examples. One class of examples is when the density operator has the form $f(x)\, g(\boldsymbol{p})$, where $\boldsymbol{p} = -i\hbar\nabla$ is the momentum operator. Then the Kato-Seiler-Simon inequality [68, Theorem 4.1] reads

$$(21) \qquad \|f(x)\, g(\boldsymbol{p})\|_{\mathcal{L}^p} \le \|f\|_{L^p} \|g\|_{L^p} \quad \text{if } p \in [2, \infty),$$

with equality when $p = 2$, and where $L^p = L^p(\mathbb{R}^3)$. It is the analogue of the function identity $\|f(x)\, g(\xi)\|_{L^p_{x,\xi}} = \|f\|_{L^p}\, \|g\|_{L^p}$. Another class of examples is the class of Töplitz operators, namely when $\boldsymbol{\rho}$ is an averaging of coherent states (see [45, Proposition 7.2] and [51, Exemple III.7]). If $\boldsymbol{\rho}$ is such a state, then its Wigner transform verifies

$$\|f_{\boldsymbol{\rho}}\|_{L^p(\mathbb{R}^6)} \leq \|\boldsymbol{\rho}\|_{\mathcal{L}^p} \quad \text{if } p \in [2, \infty]$$

with equality when $p = 2$. More generally, given such states, for any convex function Φ such that $\Phi(0) = 0$, we have the inequality

$$\iint_{\mathbb{R}^6} \Phi(f_{\boldsymbol{\rho}})\, \mathrm{d}x\, \mathrm{d}\xi \leq h^3 \operatorname{Tr}(\Phi(\boldsymbol{\rho}))\,.$$

We also want to consider the semiclassical version of Sobolev spaces of the phase space. Thus, as in [47], we introduce the following operators

$$(22) \qquad \boldsymbol{\nabla}_x \boldsymbol{\rho} := [\nabla, \boldsymbol{\rho}] \quad \text{and} \quad \boldsymbol{\nabla}_\xi \boldsymbol{\rho} := \left[\frac{x}{i\hbar}, \boldsymbol{\rho}\right],$$

which can be seen as an application of the correspondence principle of quantum mechanics. More precisely, one can observe that these operators correspond to the gradients of the Wigner transform, since

$$(23) \qquad f_{\boldsymbol{\nabla}_x \boldsymbol{\rho}} = \nabla_x f_{\boldsymbol{\rho}} \quad \text{and} \quad f_{\boldsymbol{\nabla}_\xi \boldsymbol{\rho}} = \nabla_\xi f_{\boldsymbol{\rho}}.$$

In the rest of the paper, we will refer to $\boldsymbol{\nabla}_x \boldsymbol{\rho}$ and $\boldsymbol{\nabla}_\xi \boldsymbol{\rho}$ as the quantum gradients or first-order quantum gradients.

We can then define semiclassical analogues of the weighted kinetic homogeneous Sobolev norms by

$$(24\mathrm{a}) \qquad \|\boldsymbol{\rho}\|_{\dot{\mathcal{W}}^{1,p}(m)}^p := \sum_{j=1}^{3} \left\|\boldsymbol{\nabla}_{\xi_j} \boldsymbol{\rho}\right\|_{\mathcal{L}^p(m)}^p + \left\|\boldsymbol{\nabla}_{x_j} \boldsymbol{\rho}\right\|_{\mathcal{L}^p(m)}^p,$$

$$(24\mathrm{b}) \qquad \|\boldsymbol{\rho}\|_{\dot{\mathcal{W}}^{1,\infty}(m)} := \sup_{j \in \{1,2,3\}} \left(\left\|\boldsymbol{\nabla}_{\xi_j} \boldsymbol{\rho}\right\|_{\mathcal{L}^\infty(m)}, \left\|\boldsymbol{\nabla}_{x_j} \boldsymbol{\rho}\right\|_{\mathcal{L}^\infty(m)}\right),$$

and consider the particular case of the weight defined for $n \in \mathbb{N}$ by

$$(25) \qquad m := 1 + |\boldsymbol{p}|^n\,.$$

where $\boldsymbol{p} = -i\hbar\nabla$ so $|\boldsymbol{p}|^2 = -\hbar^2\Delta$. We also define the inhomogeneous version by

$$(26) \qquad \|\boldsymbol{\rho}\|_{\mathcal{W}^{1,p}(m)}^p := \|\boldsymbol{\rho}\|_{\mathcal{L}^p(m)}^p + \|\boldsymbol{\rho}\|_{\dot{\mathcal{W}}^{1,p}(m)}^p,$$

with the usual modification when $p = \infty$. In particular, for $p = 2$, $\|\boldsymbol{\rho}\|_{\mathcal{W}^{1,2}} = \|f_{\boldsymbol{\rho}}\|_{H^1(\mathbb{R}^6)}$.

2.2. Fermionic Fock Space. Let $\mathfrak{h}^{\wedge N} := \mathfrak{h} \wedge \cdots \wedge \mathfrak{h}$ denotes the n-fold anti-symmetric tensor product of $\mathfrak{h}$. We define the fermionic (anti-symmetric) Fock space over $\mathfrak{h}$ to be the closure of

$$(27) \qquad \mathcal{F}(\mathfrak{h}) = \mathcal{F} := \mathbb{C} \oplus \bigoplus_{n=1}^{\infty} \mathfrak{h}^{\wedge n}$$

with respect to the norm induced by the endowed inner product

$$(28) \qquad \langle \psi \mid \varphi \rangle_{\mathcal{F}} = \overline{\psi^{(0)}}\, \varphi^{(0)} + \sum_{n \geq 1} \int_{\mathbb{R}^{3n}} \overline{\psi^{(n)}(\underline{x}_n)}\, \varphi^{(n)}(\underline{x}_n)\, \mathrm{d}x_1 \cdots \mathrm{d}x_n,$$

for any pair of vectors $\psi = (\psi^{(0)}, \psi^{(1)}, \ldots)$ and $\varphi = (\varphi^{(0)}, \varphi^{(1)}, \ldots)$ in $\mathcal{F}$ where $\underline{x}_k = (x_1, \ldots, x_k) \in \mathbb{R}^{3k}$. For simplicity of notation, we will also denote the closure by $\mathcal{F}$. The state with no particles describes the vacuum, defined by the vector $\Omega_{\mathcal{F}} = (1, 0, \ldots) \in \mathcal{F}$. We define the number of particles operator by

$$(29) \qquad \mathcal{N}\psi = \left(n\,\psi^{(n)}\right)_{n \in \mathbb{N}}$$

whose meaning can be interpreted as counting the number of particles in each sector of $\mathcal{F}$. A class of operators on $\mathcal{F}$ that is important to our studies is the class of mixed states on $\mathcal{F}$, which are high rank density matrices on $\mathcal{F}$. More specifically, we are interested in operators of the form

$$(30) \qquad \boldsymbol{\rho}_N := \sum_{j \in \mathbb{N}} \lambda_j \, |\psi_j\rangle \, \langle \psi_j| \,,$$

for some orthonormal set ψ_j of vectors of $\mathcal{F}$ with the normalization

$$(31) \qquad \mathrm{Tr}(\boldsymbol{\rho}_N) = \sum_j \lambda_j = h^{-3} \quad \text{and} \quad h^3 \, \mathrm{Tr}(\mathcal{N}\,\boldsymbol{\rho}_N) = N.$$

Here, N is the mean number of particles. Moreover, for each $(n, m) \in \mathbb{N}^2$, the integral kernel of $\boldsymbol{\rho}_N^{(n,m)}$ has the form

$$(32) \qquad \boldsymbol{\rho}_N^{(n,m)}(\underline{x}_n, \underline{y}_m) = \sum_{j \in \mathbb{N}} \lambda_j \, \psi_j^{(n)}(\underline{x}_n) \, \overline{\psi_j^{(m)}(\underline{y}_m)}.$$

As in the case of the one-particle operator, we define the semiclassical Schatten norms by

$$(33) \qquad \|\boldsymbol{\rho}_N\|_{\mathcal{L}^p(\mathcal{F})} := h^{\frac{3}{p}} \, \mathrm{Tr}(|\boldsymbol{\rho}_N|^p)^{\frac{1}{p}} \,,$$

so that $\|\boldsymbol{\rho}_N\|_{\mathcal{L}^1(\mathcal{F})} = 1$ and $\|\mathcal{N}\boldsymbol{\rho}_N\|_{\mathcal{L}^1(\mathcal{F})} = N$. We also define the one-particle reduced density matrix, i.e. the analogue of the classical first marginal, by

$$\boldsymbol{\rho}_{N:1} := \sum_{n \in \mathbb{N}} \frac{n}{N} \, \mathrm{Tr}_{2..n}\left(\boldsymbol{\rho}_N^{(n,n)}\right),$$

where $\mathrm{Tr}_{2..n}$ indicates the partial trace with respect to all variables except the first.

3. Main Results

3.1. Propagation of Regularity.
Our first result gives the local-in-time and uniform in $\hbar$ propagation of the regularity of the solution to the Hartree–Fock equation (5). Remark that there are no constraints on the scaling here since we are only considering the mean-field equation. Moreover, this result also works in the case of the Coulomb potential.

We define

$$(34) \qquad \mathfrak{b} := \frac{3}{a+1}$$

which corresponds to the integrability of the force field since $\nabla K \in L^{\mathfrak{b},\infty}$.

Theorem 3.1 (Propagation of regularity). *Let $a \in (0,1]$, $m = 1 + |\boldsymbol{p}|^n$ with $n \in \mathbb{N}$ verifying $n \geq 3$ and $\boldsymbol{\rho}$ be a solution to the Hartree–Fock equation (5) with initial condition $\boldsymbol{\rho}^{\mathrm{in}} \in \mathcal{L}^\infty(m)$ satisfying (12) and such that*

$$(35) \qquad \boldsymbol{\rho}^{\mathrm{in}} \in \mathcal{W}^{1,2}(m) \cap \mathcal{W}^{1,4}(m).$$

Then there exists $T > 0$ such that

$$(36) \qquad \boldsymbol{\rho} \in L^\infty([0,T], \mathcal{W}^{1,2}(m) \cap \mathcal{W}^{1,4}(m)),$$

uniformly in $\hbar$.

Remark 3.1 (On the initial data of Hartree equation). *Define $\varphi(y) = e^{-\pi|x|^2/2}$ and $\varphi_{x,\xi}(y) := \frac{1}{h^{9/4}} \varphi\left(\frac{y-x}{\sqrt{h}}\right) e^{i\, y \cdot \xi/\hbar}$. Then one can define an approximation of the Dirac delta on the phase space by $\boldsymbol{\rho}_{x,\xi} := |\varphi_{x,\xi}\rangle \langle\varphi_{x,\xi}|$. Now for any $g : \mathbb{R}^6 \to \mathbb{R}$ such that $g \in W^{1,\infty}(1+|\xi|^n) \cap W^{1,2}(1+|\xi|^n) \cap L^2$, one can define the averaging of coherent states (also called Töplitz operator) as the operator*

$$\mathrm{op}_\varphi(g) := \iint_{\mathbb{R}^6} g(x,\xi)\, \boldsymbol{\rho}_{x,\xi}\, \mathrm{d}x\, \mathrm{d}\xi.$$

This defines a positive compact operator such that (see e.g. [45, Section 7])

$$\left\| \mathrm{op}_\varphi(g) \right\|_{\mathcal{L}^\infty} = \|g\|_{L^\infty(\mathbb{R}^6)}, \qquad \left\| \mathrm{op}_\varphi(g) \right\|_{\mathcal{L}^2} = \|g\|_{L^2(\mathbb{R}^6)}.$$

In particular, in Theorem 3.1, we can take $\boldsymbol{\rho}^{\mathrm{in}} = \mathrm{op}_\varphi(g)$ with $\|g\|_{L^2(\mathbb{R}^6)} = 1$ and $\|g\|_{L^\infty(\mathbb{R}^6)} = \mathcal{C}_\infty^{1/2}$, and then $\boldsymbol{\rho}^{\mathrm{in}}$ verifies (12).

However, we can take more general operators than averaging of coherent states. Taking a function g on the phase space, one can indeed associate to it an operator by doing the inverse of the Wigner transform, called the Weyl transform, and defined as the operator with integral kernel

$$(37) \qquad \boldsymbol{\rho}_g(x,y) = \int_{\mathbb{R}^3} e^{-2i\pi(y-x)\cdot\xi}\, g\left(\tfrac{x+y}{2}, h\xi\right) \mathrm{d}\xi.$$

This operator will verify the hypotheses of the initial condition of Theorem 3.1 if g is sufficiently smooth and decaying at infinity, as proved for example in [47, Section 3].

3.2. **Mean-Field and Semiclassical Limits.** To state our mean-field results, we assume

$$(38) \qquad N^{-\frac{1}{2}} \ll h < \mathcal{C}_\infty N^{-\frac{1}{3}},$$

where $a \ll b$ means that $\frac{a}{b} \to 0$ as $N \to \infty$. Observe that the choice $h = O(N^{-\frac{1}{3}})$ is admissible with a different constant in front. We define the following trace class norm over the Fock space weighted by the number operator

$$(39) \qquad \|\boldsymbol{\rho}_N\|_{\mathcal{L}_k^1(\mathcal{F})} := \left\| (\mathcal{N} + N)^k \boldsymbol{\rho}_N \right\|_{\mathcal{L}^1(\mathcal{F})}.$$

In what follows, for technical reasons related to the well-posedness given in Appendix A, we will assume that the initial quantum spatial distribution of particles (4) verifies

$$\int_{\mathbb{R}^3} \rho^{\mathrm{in}}(x) \langle x \rangle^3\, \mathrm{d}x \le C,$$

where C may depend on h.

Theorem 3.2 (Mean-field limit). *Let $a \in (0, \frac{1}{2})$ and assume Condition (38) is verified. Let $n \in \mathbb{N}$ verifying $n > 3$. Let $\boldsymbol{\rho}$ be a solution to the Hartree–Fock equation (5) with initial condition $\boldsymbol{\rho}^{\mathrm{in}} \in \mathcal{L}^\infty(m)$ verifying (12) and such that*

$$(40a) \qquad \boldsymbol{\rho}^{\mathrm{in}} \in \mathcal{W}^{2,2}(m) \cap \mathcal{W}^{2,4}(m)$$

$$(40b) \qquad \sqrt{\boldsymbol{\rho}^{\mathrm{in}}} \in \mathcal{W}^{1,2}(m) \cap \mathcal{W}^{1,q}(m)$$

with $q \in [\frac{6}{1-2a}, \infty]$. Then there exists $T > 0$, $\boldsymbol{\rho}_{N,\boldsymbol{\rho}}^{\text{in}} \in \mathcal{L}^1(\mathcal{F})$, $\lambda > 0$ and $C > 0$ such that for any $\boldsymbol{\rho}_N$ solution of (10) *with initial condition $\boldsymbol{\rho}_N^{\text{in}} \in \mathcal{L}^1(\mathcal{F})$ commuting with $\mathcal{N}$, for any $t \in [0,T]$*

$$\|\boldsymbol{\rho}_{N:1} - \boldsymbol{\rho}\|_{\mathcal{L}^p} \leq \frac{C \, e^{\lambda t}}{\min(N^{1/2}, N \, h^{3/p'})} \left(1 + \|\boldsymbol{\rho}_N^{\text{in}} - \boldsymbol{\rho}_{N,\boldsymbol{\rho}}^{\text{in}}\|_{\mathcal{L}_k^1(\mathcal{F})}\right)$$

for any $k \geq \frac{1}{2p} + \frac{3}{2}\lceil \frac{\ln N}{p \ln(Nh^2)} \rceil$.

Remark 3.2. *The N-body operator $\boldsymbol{\rho}_{N,\boldsymbol{\rho}}^{\text{in}}$ is explicitly created from $\boldsymbol{\rho}^{\text{in}}$ thanks to the Bogoliubov transformation (see Equation* (85) *in Section 4.3). One should note that $\boldsymbol{\rho}_{N,\boldsymbol{\rho}}^{\text{in}}$ is constructed so that its one-particle reduced density matrix coincides with the solution $\boldsymbol{\rho}$ to the Hartree–Fock equation.*

Remark 3.3. *In the particular case $h = N^{-\frac{1}{3}}$, $\|\boldsymbol{\rho}_N^{\text{in}} - \boldsymbol{\rho}_{N,\boldsymbol{\rho}}^{\text{in}}\|_{\mathcal{L}^1(\mathcal{F})} \leq CN^{-4}$ and $\|\mathcal{N}^4 (\boldsymbol{\rho}_N - \boldsymbol{\rho}_{N,\boldsymbol{\rho}})\|_{\mathcal{L}^1(\mathcal{F})} \leq C$, then for any $t \in [0,T]$, one obtains*

$$\|f_{N:1} - f_{\boldsymbol{\rho}}\|_{L^2} = \|\boldsymbol{\rho}_{N:1} - \boldsymbol{\rho}\|_{\mathcal{L}^2} \leq \frac{C_T}{N^{1/2}}.$$

where we denote by $f_{N:1}$ the Wigner transform of $\boldsymbol{\rho}_{N:1}$.

One can combine the above theorem with the result proved in [47] by two of the authors to obtain an estimate directly between the solution of the N-body Schrödinger equation (1) and the Vlasov equation (2). To simplify, we restrict our attention to the case when $p \leq 2$.

Theorem 3.3 (Combined mean-field and semiclassical limits)**.** *Assume the conditions of Theorem 3.2 and that f is a positive solution of the Vlasov equation* (2) *with initial condition satisfying*

$$\left(1 + |x|^8 + |\xi|^8\right) \nabla_x^{\ell_0} \nabla_\xi^\ell f^{\text{in}} \in L^\infty(\mathbb{R}^6) \cap L^2(\mathbb{R}^6) \quad \text{where} \quad \ell_0 + \ell \leq 9.$$

Moreover, assume $\boldsymbol{\rho}_N^{\text{in}} \in \mathcal{L}^1(\mathcal{F})$ is such that $[\mathcal{N}, \boldsymbol{\rho}_N^{\text{in}}] = 0$. Then, for any $p \in [1,2]$, there exists $T > 0, C_T > 0$ and an operator $\boldsymbol{\rho}_{N,f}^{\text{in}} \in \mathcal{L}^1(\mathcal{F})$ such that for any solution $\boldsymbol{\rho}_N$ to (10) *with initial condition $\boldsymbol{\rho}_N^{\text{in}}$, the estimate*

$$\|\boldsymbol{\rho}_{N:1} - \boldsymbol{\rho}_f\|_{\mathcal{L}^p} \leq C_T \left(\frac{1}{N \, h^{3/p'}} + h\right) \left(1 + \|\boldsymbol{\rho}_N^{\text{in}} - \boldsymbol{\rho}_{N,f}^{\text{in}}\|_{\mathcal{L}_k^1(\mathcal{F})}\right),$$

holds for any $t \in [0,T]$ and any $k \geq \frac{1}{2p} + \frac{3}{2}\lceil \frac{\ln N}{p \ln(Nh^2)} \rceil$.

Remark 3.4. *In particular, when $\|\boldsymbol{\rho}_N^{\text{in}} - \boldsymbol{\rho}_{N,f}\|_{\mathcal{L}_k^1(\mathcal{F})} \leq C$ and $p = 2$, then, by Identity* (13)*, we obtain again a L^2 convergence result with the quantitative bound*

$$\|f_{N:1} - f\|_{L^2(\mathbb{R}^6)} \leq C_T \left(\frac{1}{N \, h^{3/2}} + h\right),$$

where $f_{N:1}$ is the Wigner transform of $\boldsymbol{\rho}_{N:1}$.

It is interesting to notice that the semiclassical error h is larger than the mean-field error when $N \gg h^{-5/2}$, and smaller when $N \ll h^{-5/2}$. When the two are of the same order, one obtains an error of order $h = N^{-2/5}$, which is the best of the rates in term of the number of particles, while the rate is of order $h = N^{-1/3}$ in the critical scaling.

Remark 3.5. *In the particular case of the Coulomb potential, we can still obtain an estimate for small times or with a N dependent cutoff (see Theorem 4.1 and Remark 4.2). Our results are summarized in the following table.*

Potential	$a \in (0, 1/2)$	$a \in [1/2, 1]$
Regularity	$t < T$	$t < T$
Mean-field	$t < T$	$t \ll h^{a-1/2}$ or cutoff
Mean-field + semiclassical	$t < T$	$t \ll h^{a-1/2}$ or cutoff

4. The Strategy and the General Result

4.1. **Second Quantization.** The method of second quantization provides a mathematical framework for studying the notion of quantum fluctuations. The goal of this section is to recast the original Cauchy problem (10) with a mixed state initial data on $\mathfrak{h}^{\wedge N}$ to a problem on the Fock space $\mathcal{F}$. We briefly present the method of second quantization and state the corresponding Hamiltonian evolution problem on $\mathcal{F}$. We refer the interested reader to [15, 62, 31, 24, 6] for a more complete presentation.

For every $f \in \mathfrak{h}$, we define the associated creation operator $a^*(f)$ and its adjoint the annihilation operator $a(f)$ on $\mathcal{F}$ by their actions on the n-sector of $\mathcal{F}$ as follows

$$(a^*(f)\psi)^{(n)}(\underline{x}_n) := \frac{1}{\sqrt{n}} \sum_{j=1}^{n} (-1)^{j-1} f(x_j)\, \psi^{(n-1)}(\underline{x}_{n\setminus j})$$

$$(a(f)\psi)^{(n)}(\underline{x}_n) := \sqrt{n+1} \int_{\mathbb{R}^3} \overline{f(x)}\, \psi^{(n+1)}(x, \underline{x}_n)\, \mathrm{d}x,$$

where $\underline{x}_{n\setminus j} := (x_1, \ldots, \cancel{x}_j, \ldots, x_n)$. Moreover, the action of the annihilation operator on the vacuum of $\mathcal{F}$ is $a(f)\Omega_{\mathcal{F}} = 0$. Then, we extend the operators linearly to the whole $\mathcal{F}$. It can easily be checked that the collection of creation and annihilation operators on $\mathcal{F}$ satisfies the canonical anti-commutation relations (CAR) making it a CAR algebra:

$$(41) \qquad [a(f), a^*(g)]_+ = \langle f, g\rangle_{\mathfrak{h}}, \quad [a(f), a(g)]_+ = [a^*(f), a^*(g)]_+ = 0$$

for all $f, g \in \mathfrak{h}$ where $[A, B]_+ = AB + BA$ is the anti-commutator of the operators A, B. Moreover, from relation (41), we have the identity

$$(42) \qquad \|a(f)\psi\|_{\mathcal{F}}^2 + \|a^*(f)\psi\|_{\mathcal{F}}^2 = \|f\|_{\mathfrak{h}}^2 \|\psi\|_{\mathcal{F}}^2 \implies \left\|a^{\sharp}(f)\right\|_{\infty} = \|f\|_{\mathfrak{h}}$$

for all $f \in \mathfrak{h}$ where $a^{\sharp}$ is either a^* or a. Thus, both the creation and annihilation operators are bounded operators on $\mathcal{F}$.

At times, it is more convenient to deal with localized object as opposed to $a^*(f)$ and $a(f)$. Thus, it is useful to introduce, at least formally, the fermionic creation and annihilation operator-valued distributions at the position x, denoted respectively by a_x^* and a_x, as follows

$$(43a) \qquad (a_x^*\psi)^{(n)}(\underline{x}_n) = \frac{1}{\sqrt{n}} \sum_{j=1}^{n} (-1)^{j-1}\, \delta(x - x_j)\, \psi^{(n-1)}(\underline{x}_{n\setminus j}),$$

$$(43b) \qquad (a_x\psi)^{(n)}(\underline{x}_n) = \sqrt{n+1}\, \psi^{(n+1)}(x, \underline{x}_n).$$

It is also straightforward to check that a_x^* and a_x satisfy the anticommutation relations:

$$(44) \qquad \left[a_x, a_y^*\right]_+ = \delta(x - y), \qquad \left[a_x, a_y\right]_+ = \left[a_x^*, a_y^*\right]_+ = 0,$$

and that the creation and annihilation operators can be rewritten as follows

$$(45) \qquad a^*(f) = \int_{\mathbb{R}^3} f(x)\, a_x^*\, \mathrm{d}x, \qquad a(f) = \int_{\mathbb{R}^3} \overline{f(x)}\, a_x\, \mathrm{d}x.$$

To every observable O on $\mathfrak{h}$ corresponds an induced linear operator $\mathrm{d}\Gamma(O) : \mathcal{F} \to \mathcal{F}$ called the *second quantization* of O on $\mathcal{F}$, defined as

$$(46) \qquad \mathrm{d}\Gamma(O) = 0 \oplus \bigoplus_{n=1}^{\infty} \mathrm{d}\Gamma_n(O)$$

where $\mathrm{d}\Gamma_n(O)$ is the N-particle operator

$$(47) \qquad \mathrm{d}\Gamma_n(O) = \sum_{j=1}^{n} 1_{\mathfrak{h}^{j-1}} \otimes O \otimes 1_{\mathfrak{h}^{n-j}}.$$

An important example of second quantized operator is the number operator which is simply the second quantization of the identity operator. Another relevant class of operators are the trace class operators. It is straightforward to check that the second quantization of trace class operators on $\mathfrak{h}$ are also trace class operators on $\mathcal{F}$, that is, the second quantization of mixed states on $\mathfrak{h}$ are mixed states on $\mathcal{F}$.

If the observable O has a distributional kernel $O(x, y)$, then we could rewrite $\mathrm{d}\Gamma(O)$ in terms of the operator-valued distributions a_x^* and a_x as follows

$$(48) \qquad \mathrm{d}\Gamma(O) = \int_{\mathbb{R}^6} O(x, y)\, a_x^*\, a_y\, \mathrm{d}x\, \mathrm{d}y.$$

In particular, the number operator can be rewritten as

$$(49) \qquad \mathcal{N} = \int_{\mathbb{R}^3} a_x^*\, a_x\, \mathrm{d}x.$$

4.2. **State Purification and Time Evolution.** We define the Fock space Hamiltonian by

$$(50) \qquad \mathsf{H}_N = \int_{\mathbb{R}^3} a_x^* \left(-\hbar^2 \Delta_x\right) a_x\, \mathrm{d}x + \frac{1}{2N} \int_{\mathbb{R}^6} K(x - y)\, a_x^*\, a_y^*\, a_y\, a_x\, \mathrm{d}x\, \mathrm{d}y.$$

By direct computation, we see that H_N commutes with the number operator, which implies that the expectation of the number of particles is conserved under the Hamiltonian dynamics. Moreover, its action on the n-sector is given by

$$(51) \qquad (\mathsf{H}_N \psi)^{(n)} = \mathsf{H}_N^{(n)} = \sum_{k=1}^{n} -\frac{\hbar^2}{2} \Delta_{x_k} \psi^{(n)} + \frac{1}{N} \sum_{k<l}^{n} K(x_l - x_k)\, \psi^{(n)},$$

which, on the N-sector of $\mathcal{F}$, coincides with the mean-field Hamiltonian defined in Equation (7). We consider the Cauchy problem

$$(52) \qquad i\hbar\, \partial_t \boldsymbol{\rho}_N = [\mathsf{H}_N, \boldsymbol{\rho}_N], \quad \text{with} \quad \boldsymbol{\rho}_N(t = 0) = \boldsymbol{\rho}_N^{\mathrm{in}} = \sum_{\mathsf{j}} \lambda_{\mathsf{j}}\, |\psi_{\mathsf{j}}\rangle\langle\psi_j|$$

where the data are defined as in (30). Following the idea of [11], we reformulate problem (52) as an evolution problem of a pure state[1] in the fermionic Fock space

$$\mathcal{G} := \mathcal{F}(\mathfrak{h} \oplus \mathfrak{h}) \tag{53}$$

which hereinafter will be referred to as the double Fock space. This procedure is commonly known as purification of mixed states. For completeness, we devote the remainder of this section to review the state purification process.

For any operator $\boldsymbol{\rho}_N$ as defined in (30) and any orthonormal basis ϕ_j of $\mathcal{F}$, we construct the following Hilbert–Schmidt operator on $\mathcal{F}$

$$\boldsymbol{v}_N := \sum_{j \in \mathbb{N}} \varepsilon_j \, |\psi_j\rangle \, \langle \phi_j| \,, \tag{54}$$

where $|\varepsilon_j|^2 = \lambda_j$ (cf. Equation (30)). Then, we see that $\boldsymbol{\rho}_N = |\boldsymbol{v}_N|^2$, which is called the Schmidt decomposition of $\boldsymbol{\rho}_N$. In particular, its scaled Hilbert–Schmidt norm, defined by $\|\boldsymbol{v}\|_{\mathcal{L}^2(\mathcal{F})}^2 = h^3 \operatorname{Tr}\!\left(|\boldsymbol{v}|^2\right)$, is

$$\|\boldsymbol{v}_N\|_{\mathcal{L}^2(\mathcal{F})}^2 = \|\boldsymbol{\rho}_N\|_{\mathcal{L}^1(\mathcal{F})} = 1. \tag{55}$$

It is important to notice the decomposition is not unique. In fact, we will need to make a definite choice later.

Recall that the space of Hilbert–Schmidt operators $\mathcal{L}^2(\mathcal{F})$ is isomorphic to the tensor product $\mathcal{F}(\mathfrak{h}) \otimes \mathcal{F}(\mathfrak{h})$, as Hilbert spaces, via the linear mapping $\mathsf{J}_h = \mathsf{J}$ that maps $|\phi\rangle\langle\psi| \mapsto h^{-\frac{3}{2}} \phi \otimes \overline{\psi}$. One can then associate to $\boldsymbol{v}_N$ an element of $\mathcal{F}(\mathfrak{h}) \otimes \mathcal{F}(\mathfrak{h})$ as follows

$$\mathsf{J}\boldsymbol{v}_N = h^{-\frac{3}{2}} \sum_{j \in \mathbb{N}} \varepsilon_j \, \phi_j \otimes \overline{\psi_j}. \tag{56}$$

Furthermore, we can associate to every element (56) a vector in the double Fock space $\mathcal{G}$ via the isomorphism $\mathsf{U} : \mathcal{F} \otimes \mathcal{F} \to \mathcal{G}$ defined by the following: for $f \in \mathfrak{h}^{\wedge n}$ and $g \in \mathfrak{h}^{\wedge m}$

$$\mathsf{U}\left(f \otimes g\right) = \sqrt{\frac{(n+m)!}{n! \, m!}} \left(J_l^{\otimes n} f\right) \otimes_a \left(J_r^{\otimes m} g\right), \tag{57}$$

where $J_l, J_r : \mathfrak{h} \to \mathfrak{h} \oplus \mathfrak{h}$ are respectively the canonical embedding of $\mathfrak{h}$ into the *left* and the *right* coordinate of $\mathfrak{h} \oplus \mathfrak{h}$, and $\otimes_a$ is the antisymmetric tensor product. Then extend the mapping linearly to to the whole $\mathcal{F} \otimes \mathcal{F}$. The unitary map U is known as the exponential law for Fock spaces and it verifies the following properties (see [24, Theorem 3.43] or [6, Chapter 3])

$$\Omega_{\mathcal{G}} = \mathsf{U}(\Omega_{\mathcal{F}} \otimes \Omega_{\mathcal{F}}) \tag{58a}$$

$$a_l^\sharp(f) := a^\sharp(f \oplus 0) = \mathsf{U}\left(a^\sharp(f) \otimes 1\right) \mathsf{U}^* \tag{58b}$$

$$a_r^\sharp(f) := a^\sharp(0 \oplus f) = \mathsf{U}\left((-1)^{\mathcal{N}} \otimes a^\sharp(f)\right) \mathsf{U}^*, \tag{58c}$$

with $a^\sharp = a$ or a^*. The presence of the operator $(-1)^{\mathcal{N}}$ ensures that the operators satisfy the CAR. It can also be readily checked that $a_l^\sharp(f)$ anti-commutes with $a_r^\sharp(g)$ for all $f, g \in \mathfrak{h}$.

---

[1]Here, we make the identification of $|\Psi\rangle\langle\Psi|$ with $\Psi \in \mathcal{G}$. In other words, pure state density matrices are simply vectors.

Just like in the case of $\mathcal{F}$, it is useful to define the left and right creation and annilihation operator-valued distributions at the position x by

$$(59a) \quad (a_{x,l}^* \Psi)^{(n,m)}(\underline{x}_n, \underline{y}_m) := \frac{1}{\sqrt{n}} \sum_{j=1}^{n} (-1)^{j-1} \, \delta(x - x_j) \, \Psi^{(n-1,m)}(\underline{x}_{n \backslash j}, \underline{y}_m),$$

$$(59b) \quad (a_{x,l} \Psi)^{(n,m)}(\underline{x}_n, \underline{y}_m) := \sqrt{n+1} \, \Psi^{(n+1,m)}(x, \underline{x}_n, \underline{y}_m),$$

$$(59c) \quad (a_{x,r}^* \Psi)^{(n,m)}(\underline{x}_n, \underline{y}_m) := \frac{1}{\sqrt{m}} \sum_{j=1}^{m} (-1)^{n+j-1} \, \delta(x - y_j) \, \Psi^{(n,m-1)}(\underline{x}_n, \underline{y}_{m \backslash j}),$$

$$(59d) \quad (a_{x,r} \Psi)^{(n,m)}(\underline{x}_n, \underline{y}_m) := (-1)^{n} \sqrt{m+1} \, \Psi^{(n,m+1)}(\underline{x}_n, x, \underline{y}_m).$$

This allows us to write

$$(60) \qquad a_\sigma(f) = \int_{\mathbb{R}^3} \overline{f(x)} \, a_{x,\sigma} \, \mathrm{d}x \quad \text{and} \quad a_\sigma^*(f) = \int_{\mathbb{R}^3} f(x) a_{x,\sigma}^* \, \mathrm{d}x$$

where $\sigma \in \{l, r\}$. It is again straightforward to check the CAR relations: $\left[a_{x,\sigma}, a_{y,\sigma}^*\right]_+ = \delta(x - y)$ and $\left[a_{x,\sigma}^\sharp, a_{y,\sigma'}^\sharp\right]_+ = 0$ where $\sigma, \sigma' \in \{l, r\}$.

For every observable O on $\mathfrak{h}$, we can define the left or right induced linear operator $\mathrm{d}\Gamma_l(O), \mathrm{d}\Gamma_r(O) : \mathcal{G} \to \mathcal{G}$

$$(61) \qquad \mathrm{d}\Gamma_l(O) := \mathrm{d}\Gamma(O \oplus 0) = \mathsf{U} \left(\mathrm{d}\Gamma(O) \otimes 1\right) \mathsf{U}^* = \int_{\mathbb{R}^6} O(x,y) \, a_{x,l}^* \, a_{y,l} \, \mathrm{d}x \, \mathrm{d}y,$$

$$(62) \qquad \mathrm{d}\Gamma_r(O) := \mathrm{d}\Gamma(0 \oplus O) = \mathsf{U} \left(1 \otimes \mathrm{d}\Gamma(O)\right) \mathsf{U}^* = \int_{\mathbb{R}^6} O(x,y) \, a_{x,r}^* \, a_{y,r} \, \mathrm{d}x \, \mathrm{d}y.$$

The number operator on $\mathcal{G}$ is defined by

$$(63) \qquad \mathcal{N} = \mathcal{N}_l + \mathcal{N}_r = \mathsf{U} \left(\mathcal{N} \otimes 1 + 1 \otimes \mathcal{N}\right) \mathsf{U}^*.$$

We will denote by

$$(64) \qquad \mathsf{I}_\mathcal{G} := \mathsf{U}\mathsf{J}$$

the transformation from $\mathcal{L}^2(\mathcal{F})$ to $\mathcal{G}$ mapping density operators to vectors of the double Fock space. Then for an operator $\boldsymbol{v}_N \in \mathcal{L}^2(\mathcal{F})$, the action of the operator $\mathcal{N}$ in $\mathcal{G}$ becomes $\mathcal{N} \mathsf{I}_\mathcal{G}(\boldsymbol{v}_N) = \mathsf{I}_\mathcal{G}(\mathcal{N}\boldsymbol{v}_N + \boldsymbol{v}_N \mathcal{N})$.

With the above purification process, we can recast our Cauchy problem for mixed states to a Cauchy problem for states exhibiting in the double Fock space $\mathcal{G}$ the structure of pure states. Recall the solution to the Cauchy problem (52) in the Schrödinger picture is given by

$$(65) \qquad \boldsymbol{\rho}_N = e^{-i(t/\hbar) \, \mathsf{H}_N} \, \boldsymbol{\rho}_N^{\text{in}} \, e^{i(t/\hbar) \, \mathsf{H}_N}.$$

We define the time evolution of $\boldsymbol{v}_N$ with initial state $\boldsymbol{v}_N^{\text{in}}$ by

$$(66) \qquad \boldsymbol{v}_N = e^{-i(t/\hbar) \, \mathsf{H}_N} \, \boldsymbol{v}_N^{\text{in}} \, e^{i(t/\hbar) \, \mathsf{H}_N}.$$

Then $\boldsymbol{\rho}_N = |\boldsymbol{v}_N|^2$ solves Equation (10) with initial data $\boldsymbol{\rho}_N^{\text{in}} = |\boldsymbol{v}_N^{\text{in}}|^2$. In the double Fock space $\mathcal{G}$, this corresponds to say that the evolution is given by $\Phi = \Phi(t)$ with

$$(67) \qquad \Phi := \mathsf{I}_\mathcal{G}(\boldsymbol{v}_N) = e^{-i(t/\hbar) \, \mathsf{L}_N} \mathsf{I}_\mathcal{G}(\boldsymbol{v}_N^{\text{in}}) = e^{-i(t/\hbar) \, \mathsf{L}_N} \Phi^{\text{in}}$$

where the Liouvillian L_N is defined by $\mathsf{L}_N = \mathsf{U} \left(\mathsf{H}_N \otimes 1 - 1 \otimes \mathsf{H}_N\right) \mathsf{U}^*$. In particular, for any observable O of $\mathcal{F}$, we have the relation

$$(68) \qquad \mathrm{Tr}_\mathcal{F}\left(\mathsf{O}\boldsymbol{\rho}_N\right) = \langle \Phi \, | \, (\mathsf{O} \otimes 1) \, \Phi \rangle_\mathcal{G} = \mathrm{Tr}_\mathcal{G}\left((\mathsf{O} \otimes 1) \, |\Phi\rangle\langle\Phi|\right).$$

which allows us to compute the mean value of the observable O with respect to the mixed state $\boldsymbol{\rho}_N$ in terms of the purified state Φ. In particular, we could express the one-particle reduced density matrix of $\boldsymbol{\rho}_N$ in terms of Φ, that is, the integral kernel of $\boldsymbol{\rho}_{N:1}$ is given by

$$(69) \qquad \boldsymbol{\rho}_{N:1}(x,y) = \frac{1}{N\,h^3} \left\langle \Phi \,\middle|\, a^*_{x,l}\, a_{y,l}\, \Phi \right\rangle.$$

Notice that we are using the normalization $\mathrm{Tr}(\boldsymbol{\rho}_{N:1}) = h^{-3}$.

4.3. **Bogoliubov Transformation and Quasi-Free States.** In general, we do not expect the evolution of the Cauchy problem (52) to be well-approximated by its mean-field dynamics. In fact, for initial data that are far from equilibrium, the effects of quantum fluctuation about its mean-field dynamics are not expected to be small. Thus, it is natural to restrict our studies to a subclass of initial data that are in close proximity to equilibrium states. As explained in [11], equilibrium states at finite positive temperature are believed to be well-approximated by mixed quasi-free states. Furthermore, mixed quasi-free states has the important property that it can be represented by a Bogoliubov transformation acting on the vacuum of the double Fock space $\mathcal{G}$ which is a key object in our study of the mean-field limit.

In this section, we give a brief overview of rudimentary facts about Bogoliubov transformation in the framework of the double Fock space $\mathcal{G}$ and construct a class quasi-free states exhibiting the structure of pure states in $\mathcal{G}$, with average number of particles N and pairing density equal to zero. We follow closely to the presentation given in [69].

4.3.1. *Bogoliubov Transformation.* For the pairs $f = f_1 \oplus f_2, g = g_1 \oplus g_2 \in \mathfrak{h} \oplus \mathfrak{h}$, we define the corresponding field operators by

$$(70a) \qquad A(f,g) := a(f) + a^*(\overline{g}) = a_l(f_1) + a_r(f_2) + a^*_l(\overline{g_1}) + a^*_r(\overline{g_2})$$

$$(70b) \qquad A^*(f,g) := (A(f,g))^* = a_l(\overline{g_1}) + a_r(\overline{g_2}) + a^*_l(f_1) + a^*_r(f_2).$$

Notice the field operator $A(f,g)$ and its adjoint satisfy the relation

$$(71) \qquad\qquad\qquad A^*(f,g) = A(C(f,g))$$

for all $f, g \in \mathfrak{h} \oplus \mathfrak{h}$ where $C : (\mathfrak{h} \oplus \mathfrak{h}) \oplus (\mathfrak{h} \oplus \mathfrak{h}) \to (\mathfrak{h} \oplus \mathfrak{h}) \oplus (\mathfrak{h} \oplus \mathfrak{h})$ is the anti-linear map (antiunitary involution) defined by $C(f_1 \oplus f_2, g_1 \oplus g_2) = (\overline{g_1} \oplus \overline{g_2}, \overline{f_1} \oplus \overline{f_2})$. We can also readily check the collection of field operators satisfy the anticommutation relations:

$$(72) \quad [A(f,g), A^*(h,k)]_+ = \langle (f,g) \,|\, (h,k) \rangle_{(\mathfrak{h} \oplus \mathfrak{h}) \oplus (\mathfrak{h} \oplus \mathfrak{h})}, \quad \left[A^\sharp(f,g), A^\sharp(h,k) \right]_+ = 0$$

where $A^\sharp = A$ or A^* and $f, g, h, k \in \mathfrak{h} \oplus \mathfrak{h}$.

A linear isomorphism $\nu : (\mathfrak{h} \oplus \mathfrak{h}) \oplus (\mathfrak{h} \oplus \mathfrak{h}) \to (\mathfrak{h} \oplus \mathfrak{h}) \oplus (\mathfrak{h} \oplus \mathfrak{h})$ is called a Bogoliubov (canonical) transformation of $(\mathfrak{h} \oplus \mathfrak{h}) \oplus (\mathfrak{h} \oplus \mathfrak{h})$ provided it preserves the anticommutation relations (72), that is, we have that

$$(73) \qquad\qquad [A(\nu(f,g)), A^*(\nu(h,k))]_+ = \langle (f,g) \,|\, (h,k) \rangle_{(\mathfrak{h} \oplus \mathfrak{h}) \oplus (\mathfrak{h} \oplus \mathfrak{h})}$$

for all $f, g, h, k \in \mathfrak{h} \oplus \mathfrak{h}$ and, likewise, for the other relations. Hence, it follows from (71) and (73) that ν is a Bogoliubov transformation provided it satisfies the conditions

$$(74) \qquad\qquad \nu\, C = C\, \nu, \qquad \text{and} \qquad \nu^* \nu = \nu \nu^* = I,$$

where I is the corresponding identity map.

It is more convenient to express conditions (74) as follows: ν is a Bogoliubov transformation on $(\mathfrak{h} \oplus \mathfrak{h}) \oplus (\mathfrak{h} \oplus \mathfrak{h})$ if there exist operators U, $V : \mathfrak{h} \oplus \mathfrak{h} \to \mathfrak{h} \oplus \mathfrak{h}$ satisfying the properties

$$(75) \qquad U^*U + V^*V = I \qquad \text{and} \qquad U^*\overline{V} + V^*\overline{U} = 0$$

such that ν has the form

$$(76) \qquad \nu = \begin{pmatrix} U & \overline{V} \\ V & \overline{U} \end{pmatrix}.$$

Moreover, we say that the Bogoliubov transformation ν is (unitarily) implementable on $\mathcal{G}$ if there exists a unitary map $\mathsf{R}_\nu : \mathcal{G} \mapsto \mathcal{G}$ such that

$$(77) \qquad \mathsf{R}_\nu^* A(f,g) \mathsf{R}_\nu = A(\nu(f,g))$$

for all $f, g \in \mathfrak{h} \oplus \mathfrak{h}$. A necessary and sufficient condition for the transformation ν to be implementable is given by Shale and Stinespring in [67]: ν is implementable if and only if V is a Hilbert–Schmidt operator. In particular, if $\mathrm{Tr}(V^*V)$ is finite, then ν is an implementable Bogoliubov transformation. It is common to refer to R_ν as the Bogoliubov transformation on $\mathcal{G}$.

4.3.2. *Quasi-Free States.* A state $\boldsymbol{\rho}_N$ on $\mathcal{F}$ is said to be quasi-free if

$$(78\text{a}) \qquad \mathrm{Tr}_{\mathcal{F}}\left(a^{\sharp_1}(f_1) \cdots a^{\sharp_{2n+1}}(f_{2n+1})\boldsymbol{\rho}_N\right) = 0,$$

$$(78\text{b}) \qquad \mathrm{Tr}_{\mathcal{F}}\left(a^{\sharp_1}(f_1) \cdots a^{\sharp_{2n+1}}(f_{2n})\boldsymbol{\rho}_N\right)$$

$$= \sum_\pi (-1)^\pi \prod_{j=1}^n \mathrm{Tr}_{\mathcal{F}}\left(a^{\sharp_{\pi(j)}}(f_{\pi(j)}) a^{\sharp_{\pi(j+n)}}(f_{\pi(j+n)})\boldsymbol{\rho}_N\right),$$

where $f_i \in \mathfrak{h}$ and the sum is over all permutations π satisfying

$$(79) \qquad \pi(1) < \pi(2) < \ldots < \pi(n) \quad \text{and} \quad \pi(j) < \pi(j+n), \; j = 1, \ldots, n.$$

In short, a state is said to be quasi-free if the higher-order reduced density matrices of $\boldsymbol{\rho}_N$ are completely determined by the generalized one-particle reduced density matrix. We could also express Conditions (78) in terms of the purified state Φ. This means that any quasi-free mixed state can be viewed as the partial trace of a quasi-free pure state. Moreover, using the fact that pure quasi-free states are completely characterized by its generalized one-particle reduced density matrix, it can be shown that a pure quasi-free state Φ on $\mathcal{G}$ can be written as $\Phi = \mathsf{R}_\nu\Omega$ for some Bogoliubov transformation R_ν.

Let us now construct the Bogoliubov transformation and its corresponding class of quasi-free states that we will study in Part III of the paper. Let ω be a one-particle density operator on $\mathfrak{h}$ satisfying the properties: $0 \le \omega \le 1$ and $\mathrm{Tr}(\omega) = N$. Define the map $\nu : (\mathfrak{h} \oplus \mathfrak{h}) \oplus (\mathfrak{h} \oplus \mathfrak{h}) \mapsto (\mathfrak{h} \oplus \mathfrak{h}) \oplus (\mathfrak{h} \oplus \mathfrak{h})$ given by Equation (76) with U and V having the explicit forms

$$(80) \qquad U = \begin{pmatrix} u & 0 \\ 0 & \overline{u} \end{pmatrix} \qquad \text{and} \qquad V = \begin{pmatrix} 0 & \overline{v} \\ -v & 0 \end{pmatrix}$$

with

$$(81) \qquad u := \sqrt{1-\omega} \qquad \text{and} \qquad v := \sqrt{\omega}.$$

Notice U and V verify Equation (75) which means ν is a Bogoliubov transformation. Furthermore, V is a Hilbert–Schmidt operator. Indeed, since $\mathrm{Tr}(V^*V) = 2\,\mathrm{Tr}(\omega) = 2\,N$ is clearly finite, then, by the Shale–Stinespring condition [67], ν is

implementable. Hence, there exists a unitary map $\mathsf{R}_\nu : \mathcal{G} \mapsto \mathcal{G}$ implementing ν. Consequentially, Equation (77) yields the relations

$$(82) \qquad\qquad \mathsf{R}_\nu^* a_{x,l} \mathsf{R}_\nu = a_l(u_x) - a_r^*(\overline{v_x}),$$

$$(83) \qquad\qquad \mathsf{R}_\nu^* a_{x,r} \mathsf{R}_\nu = a_r(\overline{u_x}) + a_l^*(v_x).$$

where we used the notation $u_x(y) = u(y, x), v_x(y) = v(y, x)$.

Let us now use the Bogoliubov transformation to represent quasi-free mixed states. The construction we present here is an example of the well-known Araki–Wyss representation, see [3, 2, 24]. More precisely, we are interested in constructing a quasi-free mixed state with one-particle reduced density $\boldsymbol{\rho}$ on the double Fock space $\mathcal{G}$. To this end, we define $\mathsf{R}_{\boldsymbol{\rho}}$ as the Bogoliubov transform with $\omega = N h^3 \boldsymbol{\rho}$, and we let the unitary map $\mathsf{R}_{\boldsymbol{\rho}}$ act on the vacuum $\Omega_\mathcal{G}$, i.e.

$$(84) \qquad\qquad \Phi_{\boldsymbol{\rho}} := \mathsf{R}_{\boldsymbol{\rho}} \Omega_\mathcal{G} \in \mathcal{G}.$$

We can now compute the integral kernel of one-particle reduced density matrix associated with the state $\Phi_{\boldsymbol{\rho}}$:

$$\boldsymbol{\rho}_{N:1}(x, y) = \frac{1}{N h^3} \left\langle \Phi_{\boldsymbol{\rho}} \,\middle|\, a_{l,y}^* \, a_{l,x} \Phi_{\boldsymbol{\rho}} \right\rangle = \frac{1}{N h^3} \left\langle \Omega_\mathcal{G} \,\middle|\, \mathsf{R}_{\boldsymbol{\rho}}^* a_{l,y}^* \mathsf{R}_{\boldsymbol{\rho}} \mathsf{R}_{\boldsymbol{\rho}}^* a_{l,x} \mathsf{R}_{\boldsymbol{\rho}} \Omega_\mathcal{G} \right\rangle$$

$$= \frac{1}{N h^3} \left\langle \Omega_\mathcal{G} \,\middle|\, a_l(\overline{v_y}) \, a_r^*(\overline{v_x}) \, \Omega_\mathcal{G} \right\rangle = \frac{1}{N h^3} (v^* v)(x, y) = \boldsymbol{\rho}(x, y).$$

Therefore, the one-particle reduced density matrix associated with $\Phi_{\boldsymbol{\rho}}$ corresponds to the operator $\boldsymbol{\rho}$. Furthermore, the off-diagonal term associated with the state $\Phi_{\boldsymbol{\rho}}$, referred to as pairing density, is zero. Indeed,

$$\alpha_{\Phi_{\boldsymbol{\rho}}}(x, y) := \left\langle R_{\boldsymbol{\rho}} \Omega_\mathcal{G} \,\middle|\, a_{l,y} \, a_{l,x} \, R_{\boldsymbol{\rho}} \Omega_\mathcal{G} \right\rangle = \left\langle \Omega_\mathcal{G} \,\middle|\, a_l(u_y) \, a_l(\overline{v_x}) \, \Omega_\mathcal{G} \right\rangle = 0$$

where we used that $[a_l(u_y), a_r^*(\overline{v_x})]_+ = 0$. Undoing the purification process, we can now define the reference state (mean-field approximation) $\boldsymbol{\rho}_{N,\boldsymbol{\rho}}$, associated to the solution $\boldsymbol{\rho}$ of the Hartree–Fock equation (5), as stated in Theorem 3.2 by

$$(85) \qquad\qquad \boldsymbol{\rho}_{N,\boldsymbol{\rho}} = \left| \mathsf{I}_\mathcal{G}^{-1}(\Phi_{\boldsymbol{\rho}}) \right|^2.$$

4.4. **The General Result.** In this section, we state our more general result from which our main results follow. Our result is obtained by controlling the growth of the weighted norm

$$\|\Psi\|_{\mathcal{G}_k} := \left\| (\mathcal{N} + 1)^k \, \Psi \right\|_\mathcal{G}.$$

Theorem 4.1. *Let $a \in [0, 1]$ and assume Condition (38) is verified. Let $(k, n) \in \mathbb{N}^2$ and $\alpha \in [0, 1]$ verifying $n > 3$ and $\alpha > a - \frac{1}{2}$. Let $\boldsymbol{\rho}$ be a solution of the Hartree–Fock equation (5) with initial condition $\boldsymbol{\rho}^{\mathrm{in}} \in \mathcal{L}^\infty(m)$ satisfying (12) and such that*

$$(86) \qquad\qquad \boldsymbol{\rho}^{\mathrm{in}} \in \mathcal{W}^{2,2}(m) \cap \mathcal{W}^{2,4}(m)$$

$$(87) \qquad\qquad \sqrt{\boldsymbol{\rho}^{\mathrm{in}}} \in \mathcal{W}^{1,2}(m) \cap \mathcal{W}^{1,q}(m)$$

with $q \in [2, \infty]$ verifying

$$(88) \qquad\qquad \frac{3}{q} \in \left[2 \left(\alpha - a - \frac{1}{4} \right), \alpha - a + \frac{1}{2} \right].$$

Let $\Psi^{in} \in \mathcal{G}$. Then, there exists $T > 0$ and $C > 0$ such that for any $t \in [0, T]$ and any $p \in [1, \infty)$

$$\|\boldsymbol{\rho}_{N:1} - \boldsymbol{\rho}\|_{\mathcal{L}^p} \le \frac{C \, e^{\lambda \, h^{-\alpha} t}}{\min(N^{\frac{1}{2}}, N \, h^{\frac{3}{p'}})} \left(\left\|\Psi^{in}\right\|_{\mathcal{G}_{\frac{3}{2}k + \frac{1}{2p}}}^2 + \frac{h^{2k(\alpha-1)}}{N^{k - \frac{1}{p}}} t^2 \left\|\Psi^{in}\right\|_{\mathcal{G}_{\frac{3}{2}k}}^2 \right).$$

where $\lambda = C_{a,\alpha} |\kappa| C_{\boldsymbol{\rho}}$ for some constant $C_{\boldsymbol{\rho}}$ depending only on T and the initial condition of the Hartree–Fock equation.

In the above theorem, we assumed we know the perturbation of the vacuum, Ψ^{in}. As done in (85) for the reference state $\boldsymbol{\rho}_{N,\boldsymbol{\rho}}$, we can associate to Ψ^{in} an operator $\boldsymbol{\rho}_N = \left|I_{\mathcal{G}}^{-1}(R_{\boldsymbol{\rho}}\Psi)\right|^2$ which solves the Schrödinger equation (52).

Remark 4.1. *In particular, notice that*

$$\frac{h^{2k(\alpha-1)}}{N^{k-\frac{1}{p}}} \le 1 \iff k \ge \frac{\ln N}{p \ln \left(N h^{2(1-\alpha)}\right)}.$$

More specifically, if $N = h^{-c}$, then this is equivalent to $k \ge \frac{c}{p(c+2(\alpha-1))}$. For instance, take $c = 3$. Then for any $a < 1/2$, we can take $\alpha = 0$ and $k = 3$, leading to

$$\|\boldsymbol{\rho}_{N:1} - \boldsymbol{\rho}\|_{\mathcal{L}^p} \le \frac{C \, e^{\lambda t}}{N^{\min(\frac{1}{2}, \frac{1}{p})}} \|\Psi\|_{\mathcal{G}_5}^2.$$

In the case of the Coulomb potential $a = 1$, we can take $k = 2$ and any $\alpha > 1/2$, leading to

$$\|\boldsymbol{\rho}_{N:1} - \boldsymbol{\rho}\|_{\mathcal{L}^p} \le \frac{C}{N^{\min(\frac{1}{2}, \frac{1}{p})}} \|\Psi\|_{\mathcal{G}_4}^2 e^{\lambda t / h^{\alpha}},$$

which is small only for small times $t \ll N^{-1/6} = h^{1/2}$. This is an improvement in comparison to non semiclassical estimates which are valid only for $t \ll h$.

Remark 4.2. *When $a \ge 1/2$, one can also consider the potential with a h-dependent cut-off. For example, a way to get a potential bounded at distance $|x| \le R$ is to take*

$$(89) \qquad K_R(x) = \frac{\omega_a \, \kappa}{2} \int_0^{R^{-2}} s^{\frac{a}{2}-1} e^{-\pi |x|^2 s} \, ds \xrightarrow[R \to 0]{} \kappa \frac{1}{|x|^a},$$

which is a radial decreasing potential verifying $K_R(x) \le |\kappa| \max\left(\frac{1}{|x|^a}, \frac{\omega_a}{aR^a}\right)$. For the Coulomb interaction potential for example, assuming $R \le 1$ and $N = h^{-c}$ and taking $c = 3$ and $p \le 2$, this leads to

$$\|\boldsymbol{\rho}_{N:1} - \boldsymbol{\rho}\|_{\mathcal{L}^p} \le \frac{C \, e^{\lambda t / \sqrt{R}}}{N^{1/2}} \|\Psi\|_{\mathcal{G}_5}^2.$$

Thus, one obtains a quantitative convergence result as soon as $R > \frac{4\lambda^2 t^2}{(\ln N)^2}$.

Remark 4.3. *Let $\boldsymbol{\rho}_{N,\boldsymbol{\rho}}$ be defined by (85). Then the standard deviation of the number of particles $\sigma_{\mathcal{N}}^2 := h^3 \operatorname{Tr}\left(\mathcal{N}_l^2 \boldsymbol{\rho}_{N,\boldsymbol{\rho}}\right) - \left(h^3 \operatorname{Tr}\left(\mathcal{N}_l \boldsymbol{\rho}_{N,\boldsymbol{\rho}}\right)\right)^2$ is given by*

$$\sigma_{\mathcal{N}}^2 = \operatorname{Tr}\left(\omega - \omega^2\right) = N \left(1 - \mathcal{C}_2^2 N h^3\right).$$

In particular, $\sigma_{\mathcal{N}} \le \sqrt{N}$.

Notice also that $\sigma_{\mathcal{N}} = 0 \iff \omega = \omega^2 \iff \mathcal{C}_2^2 N h^3 = 1$. This implies that in order for the reference state $\boldsymbol{\rho}_{N,\boldsymbol{\rho}}$ to have a fixed number of particles, it has to

be a pure state and the scaling has to be the critical scaling $Nh^3 = \mathcal{C}_2^{-2}$. In this case, the regularity conditions (35) are not expected to hold. However, it is a good question to know whether it is possible to find a state $\boldsymbol{\rho}_N = \left| I_{\mathcal{G}}^{-1}(R_{\boldsymbol{\rho}}\Psi) \right|^2$ with a fixed number of particles but still closed to $\boldsymbol{\rho}_{N,\boldsymbol{\rho}}$, in the sense that the associated Ψ verifies $\|\Psi\|_{\mathcal{G}_5} \ll N^{\frac{1}{2}}$.

Part II. **Propagation of Regularity**

This part is devoted to the proof of Theorem 3.1 about the propagation of the semiclassical regularity of the solutions of the Hartree–Fock equation (5), and also of higher regularity properties needed to obtain Theorem 3.2.

5. The Classical Case: Regularity for the Vlasov Equation

As a warm-up and an explanation of our strategy, we start by the analogue of our method in the classical case of the kinetic Vlasov equation. We define

$$N_{p,x} := \iint_{\mathbb{R}^6} |\nabla_x f|^p\, m \text{ and } N_{p,\xi} := \iint_{\mathbb{R}^6} |\nabla_\xi f|^p\, m.$$

Denoting $\mathsf{T} := \xi \cdot \nabla_x + E \cdot \nabla_\xi$, then we have

$$\partial_t(\nabla_x f) = -\mathsf{T}\nabla_x f - \nabla E \cdot \nabla_\xi f \tag{90}$$

$$\partial_t(\nabla_\xi f) = -\mathsf{T}\nabla_\xi f - \nabla_x f. \tag{91}$$

Proposition 5.1. *Let $n > 3$ and f be a solution of Equation (2) with initial condition verifying*

$$\nabla_{x,\xi} f^{\mathrm{in}} \in L^p(1 + |\xi|^n)$$

for any $p \in [1, \infty)$. Then there exists a time $T > 0$ such that

$$\nabla_{x,\xi} f \in L^\infty((0,T), L^p(1 + |\xi|^n)).$$

Proof. Let $m := 1 + |\xi|^{np}$. To simplify the computations, we remark that $\mathsf{T}^* = -\mathsf{T}$ and $\mathsf{T}(uv) = u\,\mathsf{T}(v) + \mathsf{T}(u)\,v$, so that by writing $u^p := |u|^{p-1}u$, it holds

$$\iint_{\mathbb{R}^6} \mathsf{T}(u) \cdot u^{p-1} m = -\iint_{\mathbb{R}^6} u \cdot \mathsf{T}(u^{p-1})\, m + |u|^p\, \mathsf{T}(m).$$

But

$$u \cdot (\mathsf{T}(u^{p-1})) = u^{p-1} \cdot \mathsf{T}(u) + (p-2)\,(\mathsf{T}(u) \cdot u)\, |u|^{p-2}$$
$$= (p-1)\, u^{p-1} \cdot \mathsf{T}(u).$$

We deduce

$$-p \iint_{\mathbb{R}^6} \mathsf{T}(u) \cdot u^{p-1} m = \iint_{\mathbb{R}^6} |u|^p\, \mathsf{T}(m).$$

Therefore, differentiating the weighted L^p norms, we obtain

$$\frac{\mathrm{d}N_{p,x}}{\mathrm{d}t} = \iint_{\mathbb{R}^6} |\nabla_x f|^p\, \mathsf{T}(m) - p\,(\nabla_x f)^{p-1} \cdot \nabla E \cdot \nabla_\xi f\, m\, \mathrm{d}x\, \mathrm{d}\xi$$

$$\frac{\mathrm{d}N_{p,\xi}}{\mathrm{d}t} = \iint_{\mathbb{R}^6} |\nabla_\xi f|^p\, \mathsf{T}(m) - p\,(\nabla_\xi f)^{p-1} \cdot \nabla_x f\, m\, \mathrm{d}x\, \mathrm{d}\xi.$$

Then by Young's inequality for the product

$$\mathsf{T}(m) = n\, p\, E \cdot \xi^{np-1} \le np\, \|E\|_{L^\infty}\, m.$$

We cut $\nabla K = F_1 + F_2 \in L^{\mathfrak{b}_1} + L^{\mathfrak{b}_2}$. The difficult term is

$$\iint_{\mathbb{R}^6} (\nabla_x f)^{p-1} \cdot \nabla E \cdot \nabla_\xi f \, m \, \mathrm{d}x \, \mathrm{d}\xi \leq \|\nabla K * \nabla \rho\|_{L^\infty} \iint_{\mathbb{R}^6} |\nabla_x f|^{p-1} \, |\nabla_\xi f| \, m \, \mathrm{d}x \, \mathrm{d}\xi$$

$$\leq \left(\|F_1\|_{L^{\mathfrak{b}_1}} \|\nabla \rho\|_{L^{\mathfrak{b}_1'}} + \|F_2\|_{L^{\mathfrak{b}_2}} \|\nabla \rho\|_{L^{\mathfrak{b}_2'}} \right) N_{p,x}^{1-1/p} N_{p,\xi}^{1/p}$$

$$\leq B_K \left(\|\nabla \rho\|_{L^{\mathfrak{b}_1'}} + \|\nabla \rho\|_{L^{\mathfrak{b}_2'}} \right) N_{p,x}^{1-1/p} N_{p,\xi}^{1/p},$$

with $B_K = \|\nabla K\|_{L^{\mathfrak{b}_1}+L^{\mathfrak{b}_2}}$ and where we used three times Hölder's inequality. Then, when $n \geq 3/\mathfrak{b}$, we get

$$\|\nabla \rho\|_{L^{\mathfrak{b}'}} = \left\| \int_{\mathbb{R}^3} \nabla_x f \, \mathrm{d}\xi \right\|_{L^{\mathfrak{b}'}} \leq \|\nabla_x f \, \langle \xi \rangle^n\|_{L_{x,\xi}^{\mathfrak{b}'}} \leq C \, N_{\mathfrak{b}',x}^{1/\mathfrak{b}'}.$$

Therefore, taking respectively $p = \mathfrak{b}_1'$ and $p = \mathfrak{b}_2'$ and using the notation $u_k = u_k(t) := N_{\mathfrak{b}_k',x}^{\frac{1}{\mathfrak{b}_k'}}$ and $v_k = v_k(t) := N_{\mathfrak{b}_k',\xi}^{\frac{1}{\mathfrak{b}_k'}}$, for $k = 1$ and $k = 2$, it holds

$$\frac{\mathrm{d}}{\mathrm{d}t} u_k \leq n \|E\|_{L^\infty} u_k + B_K \left(u_1 + u_2 \right) v_k$$

$$\frac{\mathrm{d}}{\mathrm{d}t} v_k \leq n \|E\|_{L^\infty} v_k + u_k v_k,$$

so that defining $U := u_1 + u_2 + v_1 + v_2$ we get

$$(92) \qquad \frac{\mathrm{d}}{\mathrm{d}t} U \leq n \|E\|_{L^\infty} U + \left(B_K + \frac{1}{2} \right) U^2,$$

where we used the fact $2uv \leq u^2 + v^2$, and we obtain by Grönwall's inequality that U remains finite as long as $t < T$ where T depends on the growth of $\|E(t, \cdot)\|_{L^\infty}$, which we can control by

$$\|E\|_{L^\infty} \leq C_K \left(\|\nabla \rho\|_{L^{c_1'}} + \|\nabla \rho\|_{L^{c_2'}} \right) \leq C_K \left(N_{c_1',x}^{1/c_1'} + N_{c_2',x}^{1/c_2'} \right),$$

with $C_K = \|K\|_{L^{c_1}+L^{c_2}}$. In particular, for the Coulomb interaction, one can choose $c_1 = \mathfrak{b}_1 < 3/2$ and $c_2 = \mathfrak{b}_2 > 3$. $\qquad \square$

6. The Quantum Case: Propagation of Regularity for the Hartree–Fock Equation

In this section, we prove the semiclassical analogue of the propagation of regularity for the Vlasov equation shown in Section 5. The main difficulty is to close the Grönwall's inequality, which we managed to do by propagating at the same time the $\mathcal{L}^\infty(m)$, the $\mathcal{W}^{1,2}(m)$, and the $\mathcal{W}^{1,q}(m)$ norms with $q \geq 2$ and

$$m = 1 + |\boldsymbol{p}|^n,$$

where $n > 0$. This first step allows us to prove that the $\mathcal{W}^{1,q}(m)$ norm remains bounded on some time interval for $q \in [2, q_a)$ with $q_a := \infty$ if $\mathfrak{b} := \frac{3}{a+1} \geq 2$ and

$$\frac{1}{q_a} := \frac{1}{\mathfrak{b}} - \frac{1}{2}$$

when $\mathfrak{b} < 2$. It is the content of the following proposition, where we only consider $q \in [2, 4]$ for simplicity.

Proposition 6.1. *Fix $a \in (0,1]$. If $\boldsymbol{\rho}^{\mathrm{in}} \in \mathcal{W}^{1,2}(m) \cap \mathcal{W}^{1,4}(m) \cap \mathcal{L}^{\infty}(m)$, then there exists $T > 0$ such that*

$$\boldsymbol{\rho} \in L^{\infty}((0,T), \mathcal{W}^{1,2}(m) \cap \mathcal{W}^{1,4}(m) \cap \mathcal{L}^{\infty}(m)),$$
$$\rho \in L^{\infty}((0,T), H^1 \cap W^{1,4} \cap L^1 \cap L^{\infty}).$$

Now that we know that the first-order semiclassical Sobolev norms remain bounded for some finite time $T > 0$ for $q \in [2, q_a)$, we can use this first result and a similar strategy to prove the propagation of higher Sobolev norms on the same time scale. This is done in the following proposition.

Proposition 6.2. *Under the hypotheses of Proposition 6.1, if $\boldsymbol{\rho}^{\mathrm{in}} \in \mathcal{W}^{2,2}(m) \cap \mathcal{W}^{2,4}(m)$, then*

$$\boldsymbol{\rho} \in L^{\infty}((0,T), \mathcal{W}^{2,2}(m) \cap \mathcal{W}^{2,4}(m) \cap \mathcal{W}^{1,\infty}(m)),$$
$$\rho \in L^{\infty}((0,T), H^2 \cap W^{2,4}).$$

Remark 6.1. *The propagation of the second-order Sobolev norms will allow us to remove the constraint $q \in [2, q_a)$ and to get the boundedness of first-order Sobolev norms also for $q \geq q_a$. This is relevant when $a \geq \frac{1}{2}$.*

In order to perform the mean-field limit, we actually need to prove the propagation of these norms for $\sqrt{\boldsymbol{\rho}}$ instead of $\boldsymbol{\rho}$ (Cf. Equations (177a)-(177b)), which works in a similar way.

Proposition 6.3. *Under the hypotheses of Proposition 6.2, if $\sqrt{\boldsymbol{\rho}^{\mathrm{in}}} \in \mathcal{W}^{1,q}(m)$ for some $q \in [2,\infty]$, then*

$$\sqrt{\boldsymbol{\rho}} \in L^{\infty}((0,T), \mathcal{W}^{1,q}(m)).$$

This proposition then implies also the regularity of $\boldsymbol{\rho}$ as indicated in next lemma.

Lemma 6.1. *Let $\boldsymbol{\rho} \geq 0$ be a compact operator. Then for any $q \in [1,\infty]$,*

$$(93) \qquad \|\boldsymbol{\rho}\|_{\dot{\mathcal{W}}^{1,q}(m)} \leq 2 \left\|\sqrt{\boldsymbol{\rho}}\right\|_{\mathcal{L}^{\infty}(m)} \left\|\sqrt{\boldsymbol{\rho}}\right\|_{\dot{\mathcal{W}}^{1,q}(m)}.$$

Proof of Lemma 6.1. By the product rule for commutators and Hölder's inequality for Schatten norms, for any $\eta \in \{x, \xi\}$,

$$\|\boldsymbol{\nabla}_{\eta}\boldsymbol{\rho}\|_{\mathcal{L}^q} = \|(\boldsymbol{\nabla}_{\eta}(\sqrt{\boldsymbol{\rho}})\sqrt{\boldsymbol{\rho}} + \sqrt{\boldsymbol{\rho}}\,\boldsymbol{\nabla}_{\eta}(\sqrt{\boldsymbol{\rho}}))\,m\|_{\mathcal{L}^q}$$
$$\leq \|\boldsymbol{\nabla}_{\eta}(\sqrt{\boldsymbol{\rho}})\|_{\mathcal{L}^q} \|\sqrt{\boldsymbol{\rho}}\,m\|_{\mathcal{L}^{\infty}} + \|\sqrt{\boldsymbol{\rho}}\|_{\mathcal{L}^{\infty}} \|\boldsymbol{\nabla}_{\eta}\sqrt{\boldsymbol{\rho}}\,m\|_{\mathcal{L}^q},$$

which implies Inequality (93). $\qquad\qquad\square$

6.1. **The Strategy.** Both the Hartree and the Hartree–Fock equations can be written in the form

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

with $H = \frac{|\boldsymbol{p}|^2}{2} + V_{\boldsymbol{\rho}} - h^3 \mathsf{X}_{\boldsymbol{\rho}}$ (with $\mathsf{X}_{\boldsymbol{\rho}} = 0$ in the case of the Hartree equation). If we look at the time derivatives of quantum gradients, since $\boldsymbol{\nabla}_x H = \nabla V_{\boldsymbol{\rho}} = -E_{\boldsymbol{\rho}}$ and $\frac{1}{i\hbar}[\boldsymbol{\nabla}_{\xi}H, \boldsymbol{\rho}] = \frac{1}{i\hbar}[\boldsymbol{p}, \boldsymbol{\rho}] = -\boldsymbol{\nabla}_x\boldsymbol{\rho}$ and since $[x, \mathsf{X}_{\boldsymbol{\rho}}] = \mathsf{X}_{[x,\boldsymbol{\rho}]}$ and $[\nabla, \mathsf{X}_{\boldsymbol{\rho}}] = \mathsf{X}_{[\nabla,\boldsymbol{\rho}]}$ (see Lemma 6.6), we obtain

$$(94) \qquad \partial_t \boldsymbol{\nabla}_x \boldsymbol{\rho} = \frac{1}{i\hbar}[H, \boldsymbol{\nabla}_x\boldsymbol{\rho}] - \frac{1}{i\hbar}[h^3\mathsf{X}_{\boldsymbol{\nabla}_x\boldsymbol{\rho}}, \boldsymbol{\rho}] - \frac{1}{i\hbar}[E_{\boldsymbol{\rho}}, \boldsymbol{\rho}]$$

$$\partial_t \boldsymbol{\nabla}_{\xi} \boldsymbol{\rho} = \frac{1}{i\hbar}[H, \boldsymbol{\nabla}_{\xi}\boldsymbol{\rho}] - \frac{1}{i\hbar}[h^3\mathsf{X}_{\boldsymbol{\nabla}_{\xi}\boldsymbol{\rho}}, \boldsymbol{\rho}] - \boldsymbol{\nabla}_x\boldsymbol{\rho}.$$

These equations are of the form

$$i\hbar\,\partial_t\boldsymbol{\mu} = [\mathsf{A},\boldsymbol{\mu}] + [\mathsf{B},\boldsymbol{\rho}]\,, \tag{95}$$

with A and B self-adjoint. Our goal is to propagate the weighted Schatten norms for solutions of these equations. Computing the time derivative of such quantities, we get the following result.

Lemma 6.2. *Let $\boldsymbol{\rho}$, A and B be self-adjoint operators and $\boldsymbol{\mu} = \boldsymbol{\mu}(t)$ be a family of self-adjoint operators verifying Equation* (95). *Then, formally, for any even integer $q \geq 2$ we have*

$$\frac{\mathrm{d}}{\mathrm{d}t}\,\|\boldsymbol{\mu}\,m\|_q \leq \frac{1}{\hbar}\,\|[\mathsf{A},m]\,\boldsymbol{\mu}\|_q + \frac{1}{\hbar}\,\|[\mathsf{B},\boldsymbol{\rho}]\,m\|_q\,.$$

Applying this lemma for $\boldsymbol{\mu} = \boldsymbol{\rho}$ solution of the Hartree–Fock equation or for $\boldsymbol{\mu} = \boldsymbol{\nabla}_x\boldsymbol{\rho}$ or $\boldsymbol{\mu} = \boldsymbol{\nabla}_\xi\boldsymbol{\rho}$, and with $m = 1$ or $m = \boldsymbol{p}_{\mathsf{j}}^n$ for some $\mathsf{j} \in \{1,2,3\}$, we obtain

$$\frac{\mathrm{d}}{\mathrm{d}t}\,\|\boldsymbol{\rho}\,m\|_q \leq \frac{1}{\hbar}\,\|[V_{\boldsymbol{\rho}},m]\,\boldsymbol{\rho}\|_q + \frac{1}{\hbar}\,\big\|\big[h^3\mathsf{X}_{\boldsymbol{\rho}},m\big]\,\boldsymbol{\rho}\big\|_q\,, \tag{96}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\,\|\boldsymbol{\nabla}_x\boldsymbol{\rho}\,m\|_q \leq \frac{1}{\hbar}\,\|[V_{\boldsymbol{\rho}},m]\,\boldsymbol{\nabla}_x\boldsymbol{\rho}\|_q + \frac{1}{\hbar}\,\|[E_{\boldsymbol{\rho}},\boldsymbol{\rho}]\,m\|_q$$

$$+ \frac{1}{\hbar}\,\big\|\big[h^3\mathsf{X}_{\boldsymbol{\rho}},m\big]\,\boldsymbol{\nabla}_x\boldsymbol{\rho}\big\|_q + \frac{1}{\hbar}\,\big\|\big[h^3\mathsf{X}_{\boldsymbol{\nabla}_x\boldsymbol{\rho}},\boldsymbol{\rho}\big]\,m\big\|_q\,, \tag{97}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\,\|\boldsymbol{\nabla}_\xi\boldsymbol{\rho}\,m\|_q \leq \frac{1}{\hbar}\,\|[V_{\boldsymbol{\rho}},m]\,\boldsymbol{\nabla}_\xi\boldsymbol{\rho}\|_q + \|\boldsymbol{\nabla}_x\boldsymbol{\rho}\,m\|_q$$

$$+ \frac{1}{\hbar}\,\big\|\big[h^3\mathsf{X}_{\boldsymbol{\rho}},m\big]\,\boldsymbol{\nabla}_\xi\boldsymbol{\rho}\big\|_q + \frac{1}{\hbar}\,\big\|\big[h^3\mathsf{X}_{\boldsymbol{\nabla}_\xi\boldsymbol{\rho}},\boldsymbol{\rho}\big]\,m\big\|_q\,, \tag{98}$$

where we used the fact that $[H,m] = \big[V_{\boldsymbol{\rho}} - h^3\mathsf{X}_{\boldsymbol{\rho}},m\big]$ since $\big[|\boldsymbol{p}|^2,m\big] = 0$. In the next sections, we will bound all the weighted Schatten norms of the commutators appearing on the right-hand side of inequalities (96), (97) and (98) in order to get a Grönwall-type inequality.

Proof of Lemma 6.2. First notice that

$$\partial_t\boldsymbol{\mu}^2 = \frac{1}{i\hbar}\,\big[\mathsf{A},\boldsymbol{\mu}^2\big] + \frac{1}{i\hbar}\,([\mathsf{B},\boldsymbol{\rho}]\,\boldsymbol{\mu} + \boldsymbol{\mu}\,[\mathsf{B},\boldsymbol{\rho}])\,.$$

Therefore, using that $2p := q$ is even and the cyclicity of the trace, we get

$$\frac{\mathrm{d}}{\mathrm{d}t}\,\|\boldsymbol{\mu}\,m\|_{2p}^{2p} = \frac{\mathrm{d}}{\mathrm{d}t}\,\mathrm{Tr}\Big(\big(m\boldsymbol{\mu}^2 m\big)^p\Big) = p\,\mathrm{Tr}\bigg(m\left(\frac{\mathrm{d}}{\mathrm{d}t}(\boldsymbol{\mu}^2)\right)m\,\big(m\boldsymbol{\mu}^2 m\big)^{p-1}\bigg)$$

$$= \frac{p}{i\hbar}\,\mathrm{Tr}\Big(m\,\big([\mathsf{A},\boldsymbol{\mu}^2] + [\mathsf{B},\boldsymbol{\rho}]\,\boldsymbol{\mu} + \boldsymbol{\mu}\,[\mathsf{B},\boldsymbol{\rho}]\big)\,m\,\big(m\boldsymbol{\mu}^2 m\big)^{p-1}\Big) =: I_{\mathsf{A}} + I_{\mathsf{B}}. \tag{99}$$

For I_{A}, we use again the cyclicity of the trace to write

$$I_{\mathsf{A}} = \frac{p}{i\hbar}\,\mathrm{Tr}\big(\mathsf{A}\boldsymbol{\mu}^2 m^2(\boldsymbol{\mu}^2 m^2)^{p-2}\boldsymbol{\mu}^2 m^2 - \boldsymbol{\mu}^2\mathsf{A}m^2(\boldsymbol{\mu}^2 m^2)^{p-2}\boldsymbol{\mu}^2 m^2\big)$$

$$= \frac{p}{i\hbar}\,\mathrm{Tr}\big(m^2\mathsf{A}\boldsymbol{\mu}^2 m^2(\boldsymbol{\mu}^2 m^2)^{p-2}\boldsymbol{\mu}^2 - \mathsf{A}m^2(\boldsymbol{\mu}^2 m^2)^{p-2}\boldsymbol{\mu}^2 m^2\boldsymbol{\mu}^2\big)$$

$$= \frac{p}{i\hbar}\,\mathrm{Tr}\Big(\big[m^2,\mathsf{A}\big]\,\big(\boldsymbol{\mu}^2 m^2\big)^{p-1}\boldsymbol{\mu}^2\Big)\,.$$

This can also be written as

$$I_{\mathsf{A}} = \frac{p}{i\hbar} \operatorname{Tr}\Big(\boldsymbol{\mu} \left([m, \mathsf{A}] \, m + m \, [m, \mathsf{A}] \right) \boldsymbol{\mu} \, |m\boldsymbol{\mu}|^{2(p-1)} \Big)$$
$$= \frac{2p}{i\hbar} \operatorname{Im}\Big(\operatorname{Tr}\Big(\boldsymbol{\mu} \, m \, [m, \mathsf{A}] \, \boldsymbol{\mu} \, |m\boldsymbol{\mu}|^{2(p-1)} \Big) \Big).$$

Therefore, by Hölder's inequality for the trace, we obtain

$$|I_{\mathsf{A}}| \leq \frac{2p}{\hbar} \, \|\boldsymbol{\mu} \, m\|_{2p} \, \|[m, \mathsf{A}] \, \boldsymbol{\mu}\|_{2p} \, \|m \, \boldsymbol{\mu}\|_{2p}^{2(p-1)}$$

$$(100) \qquad\qquad \leq \frac{q}{\hbar} \, \|\boldsymbol{\mu} \, m\|_q^{q-1} \, \|[\mathsf{A}, m] \, \boldsymbol{\mu}\|_q \,,$$

where we used the fact that since $\boldsymbol{\mu}$ and m are self-adjoint, and since the Schatten norm is invariant by taking the adjoint, we have $\|m \, \boldsymbol{\mu}\|_{2p} = \|\boldsymbol{\mu} \, m\|_{2p}$. For the B term, we get more easily

$$I_{\mathsf{B}} = \frac{2p}{i\hbar} \operatorname{Im}\Big(\operatorname{Tr}\Big(m \, [\mathsf{B}, \boldsymbol{\rho}] \, \boldsymbol{\mu} \, m \, |m\boldsymbol{\mu}|^{2(p-1)} \Big) \Big) .$$

By using again Hölder's inequality and the commutation in the Schatten norm, we obtain

$$(101) \qquad\qquad |I_{\mathsf{B}}| \leq \frac{q}{\hbar} \, \|m \, [\mathsf{B}, \boldsymbol{\rho}]\|_q \, \|\boldsymbol{\mu} \, m\|_q^{q-1} \,.$$

We conclude the proof by combining inequalities (100) and (101) on Formula (99) and using the fact that $\frac{\mathrm{d}}{\mathrm{d}t} \|\boldsymbol{\mu} \, m\|_q = \frac{1}{q} \|\boldsymbol{\mu} \, m\|_q^{1-q} \frac{\mathrm{d}}{\mathrm{d}t} \|\boldsymbol{\mu} \, m\|_q^q$. $\qquad\square$

6.2. **Preliminary Inequalities.** In order to simplify the computations, we will sometimes use weights of the form

$$m = 1 + |\boldsymbol{p}|^n$$

and

$$\tilde{m} = 1 + \sum_{\mathrm{j}=1}^{3} \boldsymbol{p}_{\mathrm{j}}^n.$$

Thanks to the following lemma, these weights define equivalent weighted Schatten norms.

Lemma 6.3. *Let $n \in \mathbb{R}$. Then there exists $C > 0$ such that for any $p \in [1, \infty]$ and any operator $\boldsymbol{\rho}$*

$$(102) \qquad\qquad C^{-1} \, \|\boldsymbol{\rho} \, \tilde{m}\|_p \leq \|\boldsymbol{\rho} \, m\|_p \leq C \, \|\boldsymbol{\rho} \, \tilde{m}\|_p$$

$$(103) \qquad\qquad C^{-1} \, \big\|\boldsymbol{\rho} \, \boldsymbol{p}_{\mathrm{j}}^n\big\|_p \leq \|\boldsymbol{\rho} \, m\|_p \leq C \left(\|\boldsymbol{\rho}\|_p + \sum_{\mathrm{j}=1}^{3} \big\|\boldsymbol{\rho} \, \boldsymbol{p}_{\mathrm{j}}^n\big\|_p \right).$$

Proof. We remark that $\tilde{m}$ and m commute, m is invertible, and $m^{-1}\tilde{m} = g(\boldsymbol{p})$ with $\|g\|_{L^\infty} < C$ uniformly in $\hbar$. Therefore, we obtain

$$\|\boldsymbol{\rho} \, \tilde{m}\|_p = \|\boldsymbol{\rho} \, m \, g(\boldsymbol{p})\|_p \leq C \, \|\boldsymbol{\rho} \, m\|_p \,,$$

which proves the first inequality of Equation (102). The second one follows by reversing the role of $\tilde{m}$ and m, and the first inequality of Equation (103) by replacing $\tilde{m}$ by $\boldsymbol{p}_{\mathrm{j}}^n$. The second inequality of Equation (103) follows from the second inequality of Equation (102) and the triangle inequality for Schatten norms. $\qquad\square$

We will need the following *unmixing inequality* similar to [47, Equation (56)].

Lemma 6.4. *Let $p \geq 1$ and $(n, m) \in \mathbb{N}^2$. Then for any self-adjoint operators A and B, the following inequality holds*

$$(104) \qquad \left\| B^n A B^m \right\|_p \leq 2 \left\| A B^{n+m} \right\|_p.$$

Proof of Lemma (6.4). Assume that $A \geq 0$. Then by Hölder's inequality, we have

$$(105) \qquad \| B^n A B^m \|_p \leq \left\| B^n A^{\frac{n}{n+m}} \right\|_{\frac{n+m}{n} p} \left\| A^{\frac{m}{n+m}} B^m \right\|_{\frac{n+m}{m} p}.$$

Now observe that since by definition of the absolute value $|BA| = ||B|A|$, we get $\left\| B^n A^{\frac{n}{n+m}} \right\|_{\frac{n+m}{n} p} = \left\| |B|^n A^{\frac{n}{n+m}} \right\|_{\frac{n+m}{n} p}$, and since the Schatten norm is invariant by taking the adjoint

$$\left\| A^{\frac{m}{n+m}} B^m \right\|_{\frac{n+m}{m} p} = \left\| B^m A^{\frac{m}{n+m}} \right\|_{\frac{n+m}{m} p} = \left\| |B|^m A^{\frac{m}{n+m}} \right\|_{\frac{n+m}{m} p}.$$

Now, by the Araki-Lieb-Thirring inequality

$$\left\| |B|^n A^{\frac{n}{n+m}} \right\|_{\frac{n+m}{n} p} \leq \left\| |B|^{n+m} A \right\|_p^{\frac{n}{n+m}} = \left\| A B^{n+m} \right\|_p^{\frac{n}{n+m}},$$

$$\left\| |B|^m A^{\frac{m}{n+m}} \right\|_{\frac{n+m}{m} p} \leq \left\| |B|^{n+m} A \right\|_p^{\frac{m}{n+m}} = \left\| A B^{n+m} \right\|_p^{\frac{m}{n+m}}.$$

Combining these inequalities with Inequality (105) leads to

$$(106) \qquad \| B^n A B^m \|_p \leq \left\| A B^{n+m} \right\|_p.$$

In the more general case of a self-adjoint operator A possibly not nonnegative, we write $A = A_+ - A_-$ with $A_+ = \frac{|A|+A}{2}$ and $\frac{|A|-A}{2}$. Then by Inequality (106) and the triangle inequality for Schatten norms, we get

$$\| B^n A B^m \|_p \leq \left\| A_+ B^{n+m} \right\|_p + \left\| A_- B^{n+m} \right\|_p$$
$$\leq \frac{1}{2} \left(\left\| |A| B^{n+m} + A B^{n+m} \right\|_p + \left\| |A| B^{n+m} - A B^{n+m} \right\|_p \right)$$
$$\leq \left\| |A| B^{n+m} \right\|_p + \left\| A B^{n+m} \right\|_p$$

and we conclude by using again the fact that $||A|B| = |AB|$. $\qquad \square$

Let us define the adjoint representation of A as

$$\mathrm{ad}_A(B) := [A, B].$$

Then, using the above Lemma, we can prove the following inequality.

Lemma 6.5. *Let $n \in \mathbb{N}$. Then for any self-adjoint operators A and B, we have*

$$\left\| \mathrm{ad}_B^n(A) \right\|_p \leq 2^{n+1} \left\| A B^n \right\|_p.$$

Proof. This follows from the expansion

$$\mathrm{ad}_B^n(A) = \sum_{k=0}^{n} \binom{n}{k} (-1)^k B^{n-k} A B^k,$$

together with the triangle inequality for the Schatten norms and the unmixing inequality (104). $\qquad \square$

The next proposition allows us to control $\| \nabla \rho \|_{L^p}$ by $\| \boldsymbol{\nabla}_x \boldsymbol{\rho} \, m \|_{\mathcal{L}^p}$ for some weight m. Notice that it can be viewed as a trace-type inequality.

Proposition 6.4. *Let $p \in [1, \infty]$ and $n > \frac{3}{p'}$. Then there exists a constant $C > 0$ such that for any compact self-adjoint operator $\boldsymbol{\mu}$*

$$\|\mathrm{diag}(\boldsymbol{\mu})\|_{L^p} \le C \, \|\boldsymbol{\mu} \, m\|_{\mathcal{L}^p} \,,$$

with $m = 1 + |\boldsymbol{p}|^n$.

Remark 6.2. *In particular, since for $k \in \mathbb{N}$, $\nabla^k \rho = \mathrm{diag}\left(\boldsymbol{\nabla}_x^k \boldsymbol{\rho}\right)$, the above estimate implies*

$$\left\|\nabla^k \rho\right\|_{L^p} \le C \left\|\boldsymbol{\nabla}_x^k \boldsymbol{\rho} \, m\right\|_{\mathcal{L}^p} \,.$$

Proof. Let $\rho_{\boldsymbol{\mu}}(x) := \mathrm{diag}(\boldsymbol{\mu})(x) = h^3 \boldsymbol{\mu}(x, x)$. Then, using the dual formulation of the L^p norm and separating φ into the sum of its positive and negative parts $\varphi := \varphi_+ + \varphi_-$, we have

$$\|\rho_{\boldsymbol{\mu}}\|_{L^p} \le \sup_{\|\varphi\|_{L^{p'}} \le 1} \left(\left| \int_{\mathbb{R}^3} \rho_{\boldsymbol{\mu}} \, \varphi_- \right| + \left| \int_{\mathbb{R}^3} \rho_{\boldsymbol{\mu}} \, \varphi_+ \right| \right),$$

from which we deduce that we can actually restrict ourselves to nonnegative functions φ and identifying the function φ with the multiplication operator by the function φ, we get

$$(107) \qquad \|\rho_{\boldsymbol{\mu}}\|_{L^p} \le 2 \sup_{\substack{\varphi \ge 0 \\ \|\varphi\|_{L^{p'}} \le 1}} \left| \int_{\mathbb{R}^3} \rho_{\boldsymbol{\mu}} \, \varphi \right| = 2 \sup_{\substack{\varphi \ge 0 \\ \|\varphi\|_{L^{p'}} \le 1}} \left| h^3 \, \mathrm{Tr}(\boldsymbol{\mu} \, \varphi) \right|.$$

Taking $m(y) := \sqrt{1 + |y|^n}$ and $w(y) = m(y)^{-1}$, we see that $\boldsymbol{m} := m(\boldsymbol{p})$ is a positive invertible operator and its inverse $\boldsymbol{w} := w(\boldsymbol{p})$ is a compact operator. By Hölder's inequality for the trace, we have

$$(108) \qquad h^3 \, \mathrm{Tr}(\boldsymbol{\mu} \, \varphi) = h^3 \, \mathrm{Tr}(\boldsymbol{m} \, \boldsymbol{\mu} \, \boldsymbol{m} \, \boldsymbol{w} \, \varphi \, \boldsymbol{w}) \le \|\boldsymbol{m} \, \boldsymbol{\mu} \, \boldsymbol{m}\|_{\mathcal{L}^p} \, \|\boldsymbol{w} \, \varphi \, \boldsymbol{w}\|_{\mathcal{L}^{p'}} \,.$$

However, since φ is a nonnegative function, we get that it is also a positive operator. Hence

$$\|\boldsymbol{w} \, \varphi \, \boldsymbol{w}\|_{\mathcal{L}^{p'}} = \left\| \left| \sqrt{\varphi} \, \boldsymbol{w} \right|^2 \right\|_{\mathcal{L}^{p'}} = \|\sqrt{\varphi} \, \boldsymbol{w}\|_{\mathcal{L}^{2p'}}^2 \le \|\varphi\|_{L^{p'}} \, \|w\|_{L^{2p'}}^2$$

where to get the last inequality we used the Kato-Seiler-Simon Inequality (21) since $2p' \ge 2$. Combining the above inequality with inequalities (107) and (108) yields

$$\|\rho_{\boldsymbol{\mu}}\|_{L^p} \le C_{p,n} \, \|\boldsymbol{m} \, \boldsymbol{\mu} \, \boldsymbol{m}\|_{\mathcal{L}^p} \le C_{p,n} \, \|\boldsymbol{\mu} \, m^2\|_{\mathcal{L}^p}$$

where the second inequality is a consequence of Lemma 6.4, and $C_{p,n} = 2 \, \|w\|_{L^{2p'}}^2$ is finite because $n > \frac{3}{p'}$ by assumption. $\qquad \square$

6.3. **Commutators Involving the Direct Term.** In the semiclassical case, instead of $\nabla E_{\boldsymbol{\rho}} \cdot \nabla_\xi f$ (see Equation (90)), the time derivative of the gradient let appear the term $\frac{1}{i\hbar} [E_{\boldsymbol{\rho}}, \boldsymbol{\rho}]$ (see Equation (94)). Hence we will need to get semiclassical estimates on this quantity, which is the purpose of the following proposition.

Proposition 6.5 (Commutator estimates). *Let $a \in (0, 1]$, $\mathfrak{b} = \frac{3}{a+1}$ and $(q, r) \in [2, \infty]^2$ be such that $\frac{1}{r} + \frac{1}{q} = \frac{1}{2}$. Then for any compact operator $\boldsymbol{\rho}_2$ it holds*

$$(109) \qquad \frac{1}{\hbar} \, \|[E_{\boldsymbol{\rho}}, \boldsymbol{\rho}_2]\|_{\mathcal{L}^q} \le C \, \|\rho\|_{B_{r,1}^{1-3\left(\frac{1}{r'} - \frac{1}{\mathfrak{b}}\right)}} \, \|\boldsymbol{\nabla}_\xi \boldsymbol{\rho}_2\|_{\mathcal{L}^q} \,.$$

When $q = 2$ and $r = \infty$, we also have

$$(110) \qquad \frac{1}{\hbar} \left\| [E_{\boldsymbol{\rho}}, \boldsymbol{\rho}_2] \right\|_{\mathcal{L}^2} \le C \left\| \nabla \rho \right\|_{L^{\mathfrak{b}',1}} \left\| \boldsymbol{\nabla}_\xi \boldsymbol{\rho}_2 \right\|_{\mathcal{L}^2}$$

for $a \in \left[\frac{1}{2}, 1 \right]$, and

$$(111) \qquad \frac{1}{\hbar} \left\| [E_{\boldsymbol{\rho}}, \boldsymbol{\rho}_2] \right\|_{\mathcal{L}^2} \le C \left\| \rho \right\|_{L^{\frac{3}{1-a},1}} \left\| \boldsymbol{\nabla}_\xi \boldsymbol{\rho}_2 \right\|_{\mathcal{L}^2}$$

for $a \in \left(0, \frac{1}{2} \right)$.

From the fact that $(L^r, W^{1,r})_{s,1} = B^s_{r,1}$ for any $r \in [1, \infty)$ and $s \in (0, 1)$, we deduce the following inequality in terms of more classical Sobolev spaces.

Corollary 6.1. *Let $(q, r) \in (2, \infty] \times (\mathfrak{b}', \infty)$ be such that $\frac{1}{r} + \frac{1}{q} = \frac{1}{2}$. Then it holds*

$$\frac{1}{\hbar} \left\| [E_{\boldsymbol{\rho}}, \boldsymbol{\rho}_2] \right\|_{\mathcal{L}^q} \le C \left\| \rho \right\|_{L^r}^{1-s} \left\| \rho \right\|_{W^{1,r}}^s \left\| \boldsymbol{\nabla}_\xi \boldsymbol{\rho}_2 \right\|_{\mathcal{L}^q}$$

with $s = 1 - 3 \left(\frac{1}{r'} - \frac{1}{\mathfrak{b}} \right)$.

From the fact that $\frac{1}{r} + \frac{1}{q} = \frac{1}{2}$ and the fact that $r > \mathfrak{b}'$, when $a \ge 1/2$, the above results only work when $q < q_a$ with $\frac{1}{q_a} = \frac{1}{\mathfrak{b}} - \frac{1}{2}$.

Proof of Proposition 6.5. First observe that the integral kernel of the operator $[E_{\boldsymbol{\rho}}, \boldsymbol{\rho}_2]$ can be written as

$$[E_{\boldsymbol{\rho}}, \boldsymbol{\rho}_2](x, y) = (E_{\boldsymbol{\rho}}(x) - E_{\boldsymbol{\rho}}(y)) \, \boldsymbol{\rho}_2(x, y)$$
$$= \frac{(E_{\boldsymbol{\rho}}(x) - E_{\boldsymbol{\rho}}(y)) \otimes (x - y)}{|x - y|^2} \cdot (x - y) \, \boldsymbol{\rho}_2(x, y).$$

Thus, we can explicitly compute its Hilbert–Schmidt norm by computing the L^2 norm of the kernel, and since the kernel of the operator $\boldsymbol{\nabla}_\xi \boldsymbol{\rho}_2$ is $\frac{x-y}{i\hbar} \boldsymbol{\rho}_2(x, y)$, we get the following estimate

$$(112) \quad \frac{1}{\hbar} \left\| [E_{\boldsymbol{\rho}}, \boldsymbol{\rho}_2] \right\|_2 = \left(\iint_{\mathbb{R}^6} \left| \frac{(E_{\boldsymbol{\rho}}(x) - E_{\boldsymbol{\rho}}(y)) \otimes (x - y)}{|x - y|^2} \cdot \boldsymbol{\nabla}_\xi \boldsymbol{\rho}_2(x, y) \right|^2 \mathrm{d}x \, \mathrm{d}y \right)^{\frac{1}{2}}$$
$$\le \left\| \nabla E_{\boldsymbol{\rho}} \right\|_{L^\infty} \left\| \boldsymbol{\nabla}_\xi \boldsymbol{\rho}_2 \right\|_2.$$

In particular, for $a \in \left[\frac{1}{2}, 1 \right]$, since $\nabla E_{\boldsymbol{\rho}} = \nabla K * \nabla \rho$ with $\nabla K \in L^{\mathfrak{b},\infty}$, we deduce Inequality (110) using the fact that the dual of $L^{\mathfrak{b}',1}$ is $L^{\mathfrak{b},\infty}$ (see e.g. [42])

If $a \in \left(0, \frac{1}{2} \right)$, we use that $\nabla E_{\boldsymbol{\rho}} = \nabla^2 K * \rho$ with $\nabla^2 K \in L^{\frac{3}{a+2},\infty}$. Thus Inequality (111) follows from Hölder's inequality for Lorentz norms.

A second possibility is to use the fundamental theorem of calculus for $E_{\boldsymbol{\rho}}$ and then the Fourier inversion theorem to rewrite the integral kernel of the commutator as

$$\frac{1}{i\hbar} [E_{\boldsymbol{\rho}}, \boldsymbol{\rho}_2](x, y) = \int_0^1 \nabla E_{\boldsymbol{\rho}}((1 - \theta)x + \theta y) \, \mathrm{d}\theta \cdot (\boldsymbol{\nabla}_\xi \boldsymbol{\rho}_2)(x, y)$$
$$= \int_{[0,1] \times \mathbb{R}^3} \widehat{\nabla E_{\boldsymbol{\rho}}}(z) \, e^{2i\pi z \cdot (1-\theta)x} \cdot (\boldsymbol{\nabla}_\xi \boldsymbol{\rho}_2)(x, y) \, e^{2i\pi z \cdot \theta y} \, \mathrm{d}\theta \, \mathrm{d}z,$$

which implies that by writing e_ω the operator of multiplication by $e^{2i\pi\omega\cdot x}$, it holds

$$\frac{1}{i\hbar}[E_{\boldsymbol{\rho}},\boldsymbol{\rho}_2] = \int_{[0,1]\times\mathbb{R}^3} \widehat{\boldsymbol{\nabla}E_{\boldsymbol{\rho}}}(z)\, e_{(1-\theta)z}\, (\boldsymbol{\nabla}_\xi\boldsymbol{\rho}_2)\, e_{\theta z}\, \mathrm{d}\theta\, \mathrm{d}z.$$

Since the operators e_ω are bounded operators of norm $\|e_\omega\|_\infty = 1$, we deduce the following estimate on the operator norm of the commutator

$$(113)\quad \frac{1}{\hbar}\left\|[E_{\boldsymbol{\rho}},\boldsymbol{\rho}_2]\right\|_\infty \le \int_{[0,1]\times\mathbb{R}^3} \left|\widehat{\boldsymbol{\nabla}E_{\boldsymbol{\rho}}}(z)\right| \|\boldsymbol{\nabla}_\xi\boldsymbol{\rho}_2\|_\infty\, \mathrm{d}\theta\, \mathrm{d}z = \left\|\widehat{\boldsymbol{\nabla}E_{\boldsymbol{\rho}}}\right\|_{L^1} \|\boldsymbol{\nabla}_\xi\boldsymbol{\rho}_2\|_\infty\,.$$

In order to get a result for a general $q \in [2,\infty]$, we proceed by complex interpolation. Defining the vector-valued Hilbert–Schmidt operator $\boldsymbol{\mu} := \boldsymbol{\nabla}_\xi\boldsymbol{\rho}_2$, we remark that $\boldsymbol{\rho}_2(x,y) = i\hbar\frac{x-y}{|x-y|^2}\cdot\boldsymbol{\mu}(x,y)$ and the commutator can be rewritten as the bilinear operator

$$\Lambda(E,\boldsymbol{\mu}) := \left[E, \frac{x-y}{|x-y|^2}\cdot\boldsymbol{\mu}\right] = \frac{1}{i\hbar}[E,\boldsymbol{\rho}_2].$$

Thus, using the fact that $B^0_{\infty,1} \subset L^\infty$ and $B^{\frac{3}{2}}_{2,1} \subset \mathcal{F}(L^1)$, inequalities (112) and (113) imply

$$\|\Lambda(E,\boldsymbol{\mu})\|_2 \le C\, \|E\|_{B^1_{\infty,1}} \|\boldsymbol{\mu}\|_2\,,$$

$$\|\Lambda(E,\boldsymbol{\mu})\|_\infty \le C\, \|E\|_{B^{1+\frac{3}{2}}_{2,1}} \|\boldsymbol{\mu}\|_\infty\,.$$

By the same proof, one obtains the inequality for any vector-valued Hilbert–Schmidt operator $\boldsymbol{\mu}$. Finally, we use the fact that the complex interpolation space between the involved Besov spaces is given by $[B^1_{\infty,1}, B^{1+\frac{3}{2}}_{2,1}]_{\frac{2}{r}} = B^{1+\frac{3}{r}}_{r,1}$ (see for example [16, Theorem 6.4.5]), while the complex interpolation of Schatten spaces $\mathfrak{S}^q$ gives $[\mathfrak{S}^2,\mathfrak{S}^\infty]_{1-\frac{2}{q}} = \mathfrak{S}^q$ (see for example [73, Section 1.19.7]), so that by bilinear interpolation (see [72, Chapter 28]), we obtain

$$\|\Lambda(E,\boldsymbol{\mu})\|_q \le C\, \|E\|_{B^{1+\frac{3}{r}}_{r,1}} \|\boldsymbol{\mu}\|_q \qquad\qquad \text{with } \frac{1}{r} = \frac{1}{2} - \frac{1}{q}.$$

If we take $E_{\boldsymbol{\rho}} = \nabla K * \rho$ with $\rho \in L^1 \cap L^p$ for some $p \in (1,\infty)$ and $\nabla K \in L^{\flat,\infty}$, we know that $E_{\boldsymbol{\rho}} \in L^{\tilde{r}}$ for some $\tilde{r} \in (1,\infty)$. Moreover, $E_{\boldsymbol{\rho}}$ is proportional to $(-\Delta)^{\frac{a-3}{2}}\nabla\rho$, therefore we can apply [7, Proposition 2.30] and deduce that

$$\|E_{\boldsymbol{\rho}}\|_{B^{1+\frac{3}{r}}_{r,1}} \le C\, \|\rho\|_{B^{\frac{3}{r}+a-1}_{r,1}} = \|\rho\|_{B^{1-3\left(\frac{1}{r'}-\frac{1}{\flat}\right)}_{r,1}}\,.$$

Taking $\boldsymbol{\mu} = \boldsymbol{\nabla}_\xi\boldsymbol{\rho}_2$ yields the results. $\qquad\qquad\square$

To get estimates with weights, remark that we can write $[E_{\boldsymbol{\rho}},\rho]\,\boldsymbol{p}_\mathrm{j}^{2n}$ in the following form

$$\frac{1}{i\hbar}[E_{\boldsymbol{\rho}},\rho]\,\boldsymbol{p}_\mathrm{j}^{2n} = \frac{1}{i\hbar}\left[E_{\boldsymbol{\rho}},\rho\,\boldsymbol{p}_\mathrm{j}^{2n}\right] - \frac{1}{i\hbar}\left[E_{\boldsymbol{\rho}},\boldsymbol{p}_\mathrm{j}^{2n}\right]\rho.$$

To control the $\mathcal{L}^q$ norm of the first term of the right-hand side we use Proposition 6.5, which gives

$$\frac{1}{\hbar}\left\|\left[E_{\boldsymbol{\rho}},\rho\,\boldsymbol{p}_\mathrm{j}^{2n}\right]\right\|_{\mathcal{L}^q} \le C\, \|\rho\|_{B^{1-3\left(\frac{1}{r'}-\frac{1}{\flat}\right)}_{r,1}} \left\|\boldsymbol{\nabla}_\xi(\rho\,\boldsymbol{p}_\mathrm{j}^{2n})\right\|_{\mathcal{L}^q}\,,$$

and we can also replace $\|\rho\|_{B_{r,1}^{1-3\left(\frac{1}{r'}-\frac{1}{\mathfrak{b}}\right)}}$ by $\|\nabla\rho\|_{L^{\mathfrak{b}',1}}$ when $q = 2$. To bound the second term, we will use the following proposition.

Proposition 6.6 (Weighted commutator estimate)**.** *Let* $a \in (0, 1]$ *and* $\mathfrak{b} = \frac{3}{a+1}$. *For* $a \in \left[\frac{1}{2}, 1\right]$ *take* $(q, r, r_1) \in \left[\frac{3}{2}, \infty\right] \times \left(\frac{3}{3-a}, \mathfrak{b}'\right) \times [1, \infty]$, *for* $a \in \left(0, \frac{1}{2}\right)$ *take* $(q, r, r_1) \in \left[\frac{3}{2}, \infty\right] \times \left(\frac{3}{3-a}, \frac{3}{1-a}\right) \times [1, \infty]$, *such that*

$$(114) \qquad \frac{1}{r} + \frac{1}{r_1} = \frac{1}{q} + \frac{1}{\mathfrak{b}'}.$$

Let $n \in \mathbb{N}$ *and* $m := 1 + |\boldsymbol{p}|^{2n}$. *Then there exists a constant* $C > 0$ *such that*

$$\frac{1}{\hbar} \left\| \left[E_{\boldsymbol{\rho}}, \boldsymbol{p}_{\mathrm{j}}^{2n}\right] \boldsymbol{\mu} \right\|_{\mathcal{L}^q} \leq C \left\| \boldsymbol{\nabla}_{x_{\mathrm{j}}} \boldsymbol{\rho}\, m \right\|_{\mathcal{L}^r} \|\boldsymbol{\mu}\, m\|_{\mathcal{L}^{r_1}}.$$

If $r = \mathfrak{b}'$, *we need to replace* $\mathcal{L}^r$ *by* $\mathcal{L}^{r-\varepsilon} \cap \mathcal{L}^{r+\varepsilon}$ *for some* $\varepsilon \in (0, \mathfrak{b}' - 1)$.

With a similar proof, one obtains a similar result replacing $E_{\boldsymbol{\rho}}$ by $V_{\boldsymbol{\rho}} = K * \rho$. This yields the following inequalities.

Proposition 6.7. *With the same hypotheses as in Proposition 6.6, it holds*

$$\frac{1}{\hbar} \left\| \left[V_{\boldsymbol{\rho}}, \boldsymbol{p}_{\mathrm{j}}^{2n}\right] \boldsymbol{\mu} \right\|_{\mathcal{L}^q} \leq C \|\boldsymbol{\rho}\, m\|_{\mathcal{L}^r} \|\boldsymbol{\mu}\, m\|_{\mathcal{L}^{r_1}},$$

with the same additional constraints in the endpoint cases.

Proof of Proposition 6.6. Let $E := E_{\boldsymbol{\rho}}$. We remark that $\left[E, \boldsymbol{p}_{\mathrm{j}}\right] = E\,\boldsymbol{p}_{\mathrm{j}} - \boldsymbol{p}_{\mathrm{j}}\, E = i\hbar\, \partial_{\mathrm{j}} E$ is the operator of multiplication by $x \mapsto i\hbar\, \partial_{\mathrm{j}} E(x)$, and since $\boldsymbol{p}_{\mathrm{j}}^2 = \boldsymbol{p}_{\mathrm{j}} \boldsymbol{p}_{\mathrm{j}}$, we get

$$\frac{1}{i\hbar} \left[E, \boldsymbol{p}_{\mathrm{j}}^2\right] = \frac{1}{i\hbar} \left(\left[E, \boldsymbol{p}_{\mathrm{j}}\right] \boldsymbol{p}_{\mathrm{j}} + \boldsymbol{p}_{\mathrm{j}} \left[E, \boldsymbol{p}_{\mathrm{j}}\right]\right) = (\partial_{\mathrm{j}} E)\, \boldsymbol{p}_{\mathrm{j}} + \boldsymbol{p}_{\mathrm{j}}\, (\partial_{\mathrm{j}} E),$$

and more generally, for any $n \in \mathbb{N}$

$$\frac{1}{i\hbar} \left[E, \boldsymbol{p}_{\mathrm{j}}^{2n}\right] = \sum_{k=0}^{n-1} \boldsymbol{p}_{\mathrm{j}}^{2k} \left(\partial_{\mathrm{j}} E\, \boldsymbol{p}_{\mathrm{j}} + \boldsymbol{p}_{\mathrm{j}}\, \partial_{\mathrm{j}} E\right) \boldsymbol{p}_{\mathrm{j}}^{2(n-k-1)} = \sum_{k=0}^{2n-1} \boldsymbol{p}_{\mathrm{j}}^k\, \partial_{\mathrm{j}} E\, \boldsymbol{p}_{\mathrm{j}}^{2n-1-k}.$$

From this formula and the triangle inequality for Schatten norms, we deduce

$$\frac{1}{\hbar} \left\| \left[E, \boldsymbol{p}_{\mathrm{j}}^{2n}\right] \boldsymbol{\mu} \right\|_{\mathcal{L}^q} \leq \sum_{k=0}^{2n-1} \left\| \boldsymbol{p}_{\mathrm{j}}^k\, \partial_{\mathrm{j}} E\, \boldsymbol{p}_{\mathrm{j}}^{2n-1-k} \boldsymbol{\mu} \right\|_{\mathcal{L}^q}.$$

We cannot directly apply Hölder's inequality here since $\boldsymbol{p}_{\mathrm{j}}^k E$ is an unbounded operator, therefore we have to make some commutations between $\boldsymbol{p}_{\mathrm{j}}^k$ and $\partial_{\mathrm{j}} E$. By Leibniz formula

$$\boldsymbol{p}_{\mathrm{j}}^k\, \partial_{\mathrm{j}} E = \sum_{\ell=0}^k \binom{k}{\ell} g_\ell\, \boldsymbol{p}_{\mathrm{j}}^{k-\ell},$$

where g_ℓ is the function defined by $g_\ell(x) = (\boldsymbol{p}_{\mathrm{j}}^\ell(\partial_{\mathrm{j}} E))(x)$. Multiplying and dividing by $m_{\ell+1} := 1 + |\boldsymbol{p}|^{\ell+1}$, we deduce that

$$\frac{1}{\hbar} \left\| \left[E, \boldsymbol{p}_{\mathrm{j}}^{2n} \right] \boldsymbol{\mu} \right\|_{\mathcal{L}^q} \le \sum_{k=0}^{2n-1} \sum_{\ell=0}^{k} \binom{k}{\ell} \left\| g_\ell \, m_{\ell+1}^{-1} m_{\ell+1} \, \boldsymbol{p}_{\mathrm{j}}^{2n-1-\ell} \boldsymbol{\mu} \right\|_{\mathcal{L}^q}$$
$$\le \sum_{\ell=0}^{2n-1} C_\ell \left\| g_\ell \, m_{\ell+1}^{-1} m_{\ell+1} \, \boldsymbol{p}_{\mathrm{j}}^{2n-1-\ell} \boldsymbol{\mu} \right\|_{\mathcal{L}^q},$$

where $C_\ell = \sum_{k=\ell}^{2n-1} \binom{k}{\ell}$.

1. Case ℓ small. In this case we define $\frac{1}{\sigma} = \frac{1}{q} - \frac{1}{r_1}$. By the relation (114) and the fact that $r \in (\frac{3}{3-a}, \mathfrak{b}']$, we deduce that

$$\frac{1}{\sigma} = \frac{1}{r} - \frac{1}{\mathfrak{b}'} \in \left[0, \frac{1}{3} \right),$$

or equivalently $\sigma \in (3, \infty]$. Thus, we can use Hölder's inequality for Schatten norms and the Kato-Seiler-Simon Inequality (21) to deduce that

$$\left\| g_\ell \, m_{\ell+1}^{-1} m_{\ell+1} \, \boldsymbol{p}_{\mathrm{j}}^{2n-1-\ell} \boldsymbol{\mu} \right\|_{\mathcal{L}^q} \le \left\| g_\ell \, m_{\ell+1}^{-1} \right\|_{\mathcal{L}^\sigma} \left\| m_{\ell+1} \, \boldsymbol{p}_{\mathrm{j}}^{2n-1-\ell} \boldsymbol{\mu} \right\|_{\mathcal{L}^{r_1}}$$
$$\le C_m^{1/\sigma} \left\| g_\ell \right\|_{L^\sigma} \left\| \boldsymbol{\mu} \, m_{2n} \right\|_{\mathcal{L}^{r_1}},$$

where $C_m = \int_{\mathbb{R}^3} \frac{\mathrm{d}x}{(1+|x|^{\ell+1})^\sigma}$ is finite because $\sigma > 3$ implies that $\sigma > \frac{3}{\ell+1}$. Then observe that

$$g_\ell = -\nabla K * (\boldsymbol{p}_{\mathrm{j}}^\ell \partial_{\mathrm{j}} \rho) = -\nabla K * \mathrm{diag}\left(\mathrm{ad}_{\boldsymbol{p}_{\mathrm{j}}}^\ell (\boldsymbol{\nabla}_{x_{\mathrm{j}}} \boldsymbol{\rho}) \right).$$

We first consider $a \in \left[\frac{1}{2}, 1 \right]$. If $r < \mathfrak{b}'$, then $\sigma < \infty$. Therefore, since $\nabla K \in L^{\mathfrak{b},\infty}$, $(\sigma, \mathfrak{b}) \in (1, \infty)^2$ and from Formula (114), $\frac{1}{r} = \frac{1}{\mathfrak{b}'} + \frac{1}{\sigma}$, by the Hardy–Littlewood–Sobolev inequality,

$$\left\| g_\ell \right\|_{L^\sigma} \le C_K \left\| \mathrm{diag}\left(\mathrm{ad}_{\boldsymbol{p}_{\mathrm{j}}}^\ell (\boldsymbol{\nabla}_{x_{\mathrm{j}}} \boldsymbol{\rho}) \right) \right\|_{L^r},$$

where $C_K = \left\| \nabla K \right\|_{L^{\mathfrak{b},\infty}}$. By Proposition 6.4 and Lemma 6.5, we get that for $\ell < 2n - 3/r'$ we have

$$\left\| g_\ell \right\|_{L^\sigma} \le C_K \left\| \mathrm{ad}_{\boldsymbol{p}_{\mathrm{j}}}^\ell \left(\boldsymbol{\nabla}_{x_{\mathrm{j}}} \boldsymbol{\rho} \right) m_{2n-\ell} \right\|_{\mathcal{L}^r} \le 2^{\ell+1} C_K \left\| \boldsymbol{\nabla}_{x_{\mathrm{j}}} \boldsymbol{\rho} \, m_{2n} \right\|_{\mathcal{L}^r}.$$

Since $\frac{1}{r} > 1 - \frac{2n}{3}$, this includes at least the case $\ell = 0$.

If $r = \mathfrak{b}'$, then $\sigma = \infty$ and we use Young's inequality instead of the Hardy–Littlewood–Sobolev inequality, and the fact that $\nabla K \in L^{\mathfrak{b}+\epsilon} + L^{\mathfrak{b}-\epsilon}$ for any $\epsilon \in (0, \mathfrak{b} - 1]$ to get

$$\left\| g_\ell \right\|_{L^\sigma} \le C_K \left\| \mathrm{diag}\left(\mathrm{ad}_{\boldsymbol{p}_{\mathrm{j}}}^\ell (\boldsymbol{\nabla}_{x_{\mathrm{j}}} \boldsymbol{\rho}) \right) \right\|_{L^{r+\varepsilon} \cap L^{r-\varepsilon}},$$

for any $\varepsilon \in (0, \mathfrak{b}' - 1]$, and the proof follows similarly.

Now we consider $a \in \left(0, \frac{1}{2} \right)$ and rewrite g_ℓ as

$$g_\ell = -\nabla^2 K * (\boldsymbol{p}_{\mathrm{j}}^\ell \rho) = -\nabla^2 K * \mathrm{diag}\left(\mathrm{ad}_{\boldsymbol{p}_{\mathrm{j}}}^\ell (\boldsymbol{\rho}) \right).$$

If $r < \mathfrak{b}'$, then $\sigma < \infty$. Therefore, since $\nabla^2 K \in L^{\frac{3}{a+2},\infty}$, $(\sigma, \mathfrak{b}) \in (1,\infty)^2$ and from Formula (114), $\frac{1}{r} = \frac{1}{\mathfrak{b}'} + \frac{1}{\sigma}$, by the Hardy–Littlewood–Sobolev inequality,

$$\|g_\ell\|_{L^\sigma} \leq C_K \left\| \mathrm{diag}\left(\mathrm{ad}_{\boldsymbol{p}_{\mathrm{j}}}^\ell(\boldsymbol{\rho}) \right) \right\|_{L^r},$$

where $C_K = \left\| \nabla^2 K \right\|_{L^{\frac{3}{a+2},\infty}}$. By Proposition 6.4 and Lemma 6.5, we get that for $\ell < 2n - 3/r'$ we have

$$\|g_\ell\|_{L^\sigma} \leq C_K \left\| \mathrm{ad}_{\boldsymbol{p}_{\mathrm{j}}}^\ell(\boldsymbol{\rho})\, m_{2n-\ell} \right\|_{\mathcal{L}^r} \leq 2^{\ell+1} C_K \left\| \boldsymbol{\rho}\, m_{2n} \right\|_{\mathcal{L}^r}.$$

Since $\frac{1}{r} > 1 - \frac{2n}{3}$, this includes at least the case $\ell = 0$.

If $r = \mathfrak{b}'$, then $\sigma = \infty$ and we use Young's inequality instead of the Hardy–Littlewood–Sobolev inequality, and the fact that $\nabla^2 K \in L^{\frac{3}{a+2}+\epsilon} + L^{\frac{3}{a+2}-\epsilon}$ for any $\epsilon \in (0, \frac{3}{a+2} - 1]$ to get

$$\|g_\ell\|_{L^\sigma} \leq C_K \left\| \mathrm{diag}\left(\mathrm{ad}_{\boldsymbol{p}_{\mathrm{j}}}^\ell(\boldsymbol{\rho}) \right) \right\|_{L^{r+\varepsilon} \cap L^{r-\varepsilon}},$$

for any $\varepsilon \in (0, \frac{3}{a+2} - 1]$, and the proof follows similarly.

2. Case $\ell > 0$. Let $\frac{1}{\tilde{q}} = \frac{1}{q} + \frac{1}{3}$. Then since $\tilde{q} \leq q$,

$$\|\cdot\|_{\mathcal{L}^q} = h^{3/q} \|\cdot\|_q \leq h^{3/q} \|\cdot\|_{\tilde{q}} = h^{-1} \|\cdot\|_{\mathcal{L}^{\tilde{q}}}.$$

Similarly as in the step 1, we define $\frac{1}{\tilde{\sigma}} = \frac{1}{\tilde{q}} - \frac{1}{\tilde{r}_1}$ and by Formula (114) we get

$$\frac{1}{\tilde{\sigma}} = \frac{1}{3} + \frac{1}{\tilde{r}} - \frac{1}{\mathfrak{b}'} \in \left(\frac{a}{3}, \frac{1}{2} \right)$$

or equivalently $\tilde{\sigma} \in \left(2, \frac{3}{a} \right)$, and we deduce

$$\left\| g_\ell\, m_{\ell+1}^{-1}\, m_{\ell+1}\, \boldsymbol{p}_{\mathrm{j}}^{2n-1-\ell} \boldsymbol{\mu} \right\|_{\mathcal{L}^q} \leq h^{-1} \left\| g_\ell\, m_{\ell+1}^{-1} m_{\ell+1}\, \boldsymbol{p}_{\mathrm{j}}^{2n-1-\ell} \boldsymbol{\mu} \right\|_{\mathcal{L}^{\tilde{q}}}$$
$$\leq C_m^{1/\tilde{\sigma}}\, h^{-1} \|g_\ell\|_{L^{\tilde{\sigma}}} \left\| \boldsymbol{\mu}\, m_{2n} \right\|_{\mathcal{L}^{\tilde{r}_1}},$$

where $C_m = \int_{\mathbb{R}^3} \frac{\mathrm{d}x}{(1+|x|^{\ell+1})^\sigma}$. Since $\tilde{\sigma} > \frac{3}{2}$ and $\ell \geq 1$, we have $\tilde{\sigma} > \frac{3}{\ell+1}$ and so $C_m < \infty$. Note that since $\ell \geq 1$

$$g_\ell = -\partial_{\mathrm{j}} \nabla K * \boldsymbol{p}_{\mathrm{j}}^\ell \rho = i\hbar\, (\partial_{\mathrm{j}} \nabla K) * \mathrm{diag}\left(\mathrm{ad}_{\boldsymbol{p}_{\mathrm{j}}}^{\ell-1}(\boldsymbol{\nabla}_{x_{\mathrm{j}}} \boldsymbol{\rho}) \right).$$

To control g_ℓ, when $a = 1$, we use the fact that $\partial_{\mathrm{j}} \nabla K$ is continuous from $L^{\tilde{\sigma}}$ to $L^{\tilde{\sigma}}$ by the Calderón-Zygmund Theorem (see e.g. [26, Theorem 5.1]). When $a \in \left[\frac{1}{2}, 1 \right)$, $|\partial_{\mathrm{j}} \nabla K| \leq \frac{1}{|x|^{a+2}}$ and we use the Hardy–Littlewood–Sobolev inequality. In both cases, we obtain

$$\|g_\ell\|_{L^{\tilde{\sigma}}} \leq C_K\, h \left\| \mathrm{diag}\left(\mathrm{ad}_{\boldsymbol{p}_{\mathrm{j}}}^{\ell-1}(\boldsymbol{\nabla}_{x_{\mathrm{j}}} \boldsymbol{\rho}) \right) \right\|_{L^{\tilde{r}}}$$

since $1 + \frac{1}{\tilde{\sigma}} = \frac{1}{3} + \frac{1}{\tilde{r}} + \frac{1}{\mathfrak{b}} = \frac{1}{\tilde{r}} + \frac{a+2}{3}$. By Proposition 6.4 and Lemma 6.5, we get that for $\ell < 2n + 1 - \frac{3}{\tilde{r}'}$ we have

$$h^{-1} \|g_\ell\|_{L^{\tilde{r}}} \leq C_K \left\| \mathrm{ad}_{\boldsymbol{p}_{\mathrm{j}}}^{\ell-1}(\boldsymbol{\nabla}_{x_{\mathrm{j}}} \boldsymbol{\rho})\, m_{2n-\ell+1} \right\|_{\mathcal{L}^{\tilde{r}}} \leq 2^\ell C_K \left\| \boldsymbol{\nabla}_{x_{\mathrm{j}}} \boldsymbol{\rho}\, m_{2n} \right\|_{\mathcal{L}^{\tilde{r}}}.$$

Since $\tilde{r} < 3$, we have $\frac{3}{\tilde{r}'} < 2$, so $2n + 1 - \frac{3}{\tilde{r}'} > 2n - 1$, therefore this works for any $1 \leq \ell \leq 2n - 1$. By choosing $\tilde{r} = r$ we conclude the proof.

When $a \in \left(0, \frac{1}{2} \right)$, we obtain

$$\|g_\ell\|_{L^{\tilde{\sigma}}} \leq C_K\, h \left\| \mathrm{diag}\left(\mathrm{ad}_{\boldsymbol{p}_{\mathrm{j}}}^{\ell-1}(\boldsymbol{\rho}) \right) \right\|_{L^{\tilde{r}}}$$

where $C_K = \left\|\nabla^2 K\right\|_{L^{\frac{3}{a+2},\infty}}$, and $1 + \frac{1}{\bar{\sigma}} = \frac{1}{3} + \frac{1}{\bar{r}} + \frac{1}{6} = \frac{1}{\bar{r}} + \frac{a+2}{3}$. By Proposition 6.4 and Lemma 6.5, we get that for $\ell < 2n + 1 - \frac{3}{\bar{r}'}$ we have

$$h^{-1} \left\|g_\ell\right\|_{L^{\bar{r}}} \le C_K \left\|\mathrm{ad}_{\boldsymbol{p}_{\mathrm{j}}}^{\ell-1}(\boldsymbol{\rho})\, m_{2n-\ell+1}\right\|_{\mathcal{L}^{\bar{r}}} \le 2^\ell C_K \left\|\boldsymbol{\rho}\, m_{2n}\right\|_{\mathcal{L}^{\bar{r}}}.$$

Since $\tilde{r} < 3$, we have $\frac{3}{\bar{r}'} < 2$, so $2n + 1 - \frac{3}{\bar{r}'} > 2n - 1$, therefore this works for any $1 \le \ell \le 2n - 1$. By choosing $\tilde{r} = r$ we conclude the proof. $\qquad\square$

6.4. Preliminary Properties of the Exchange Operator.

6.4.1. *Preliminary Identities.* Let $\mathsf{X} = \mathsf{X}_{\boldsymbol{\rho}}$ be the operator of integral kernel $\mathsf{X}(x, y) = K(x - y)\,\boldsymbol{\rho}(x, y)$ with $K(x) = |x|^{-a}$ and recall the notation of the adjoint representation of A, $\mathrm{ad}_A(B) = [A, B]$.

Lemma 6.6. *Let $a \in (0, 1]$. Then the following identities holds true*

$$[x, \mathsf{X}_{\boldsymbol{\rho}}] = \mathsf{X}_{[x,\boldsymbol{\rho}]}, \qquad\qquad [\nabla, \mathsf{X}_{\boldsymbol{\rho}}] = \mathsf{X}_{[\nabla,\boldsymbol{\rho}]},$$

and more generally, with the adjoint notation, $\mathrm{ad}_x^n(\mathsf{X}_{\boldsymbol{\rho}}) = \mathsf{X}_{\mathrm{ad}_x^n(\boldsymbol{\rho})}$ and $\mathrm{ad}_\nabla^n(\mathsf{X}_{\boldsymbol{\rho}}) = \mathsf{X}_{\mathrm{ad}_\nabla^n(\boldsymbol{\rho})}$. In particular, since $\boldsymbol{\nabla}_x\boldsymbol{\rho} = \mathrm{ad}_\nabla(\boldsymbol{\rho})$ and $\boldsymbol{\nabla}_\xi\boldsymbol{\rho} = \frac{1}{i\hbar}\,\mathrm{ad}_x(\boldsymbol{\rho})$, it can be written $\boldsymbol{\nabla}_\xi^n(\mathsf{X}_{\boldsymbol{\rho}}) = \mathsf{X}_{\boldsymbol{\nabla}_\xi^n\boldsymbol{\rho}}$, and $\boldsymbol{\nabla}_x^n(\mathsf{X}_{\boldsymbol{\rho}}) = \mathsf{X}_{\boldsymbol{\nabla}_x^n\boldsymbol{\rho}}$.

Proof. The first identity follows immediately by looking at the integral kernel of the operator

$$[x, \mathsf{X}_{\boldsymbol{\rho}}]\,(x, y) = \frac{(x - y)\,\boldsymbol{\rho}(x, y)}{|x - y|^a} = \mathsf{X}_{[x,\boldsymbol{\rho}]}(x, y).$$

To get the second we take $\varphi \in C_c^\infty$, integrate by parts and use the fact that $\nabla_x K(x - y) = -\nabla_y K(x - y)$ to get

$$[\nabla, \mathsf{X}_{\boldsymbol{\rho}}]\varphi(x) = \nabla \int_{\mathbb{R}^3} \frac{\boldsymbol{\rho}(x, y)}{|x - y|^a}\,\varphi(y)\,\mathrm{d}y - \int_{\mathbb{R}^3} \frac{\boldsymbol{\rho}(x, y)}{|x - y|^a}\,\nabla\varphi(y)\,\mathrm{d}y$$

$$= \int_{\mathbb{R}^3} (\nabla_x + \nabla_y)\left(\frac{\boldsymbol{\rho}(x, y)}{|x - y|^a}\right)\varphi(y)\,\mathrm{d}y = \int_{\mathbb{R}^3} \frac{(\nabla_x + \nabla_y)(\boldsymbol{\rho}(x, y))}{|x - y|^a}\,\varphi(y)\,\mathrm{d}y,$$

and we conclude by remarking that $(\nabla_x + \nabla_y)(\boldsymbol{\rho}(x, y))$ is nothing but the integral kernel of the operator $[\nabla, \boldsymbol{\rho}]$. $\qquad\square$

Lemma 6.7. *Let $\eta = 1$, $\eta = \boldsymbol{p}_{\mathrm{j}}$ or $\eta = x_{\mathrm{j}}$, then we have*

$$(115) \qquad\qquad \eta^n\,\mathsf{X}_{\boldsymbol{\rho}} = \sum_{k=0}^n \binom{n}{k}\mathsf{X}_{\mathrm{ad}_\eta^k(\boldsymbol{\rho})}\,\eta^{n-k}$$

$$(116) \qquad\qquad [\eta^n, \mathsf{X}_{\boldsymbol{\rho}}] = \sum_{k=1}^n \binom{n}{k}\mathsf{X}_{\mathrm{ad}_\eta^k(\boldsymbol{\rho})}\,\eta^{n-k}.$$

Proof. Since $A^k B = (A^{k-1}B)A + A^{k-1}\,\mathrm{ad}_A(B)$, we easily deduce the following commutator expansion

$$A^n B = \sum_{k=0}^n \binom{n}{k}\mathrm{ad}_A^k(B)\,A^{n-k}.$$

Therefore, we deduce the result by taking $B = \mathsf{X}_{\boldsymbol{\rho}}$ and by Lemma 6.6. $\qquad\square$

6.4.2. *Preliminary Inequalities.* We know from [47, Equation (39a)] that if $a \in [0, 3/2)$ and $q = 2$, then

$$(117) \qquad \|\mathsf{X}_{\boldsymbol{\rho}}\|_q \leq C \, h^{-a} \, \|\boldsymbol{\rho} \, |\boldsymbol{p}|^a\|_2 \, .$$

By the fact that the Schatten norms of smaller order controls the Schatten norms of higher order, we deduce that this inequality actually holds for any $q \in [2, \infty]$. The next proposition will allow us to put the weight $|\boldsymbol{p}|^a$ on an other operator $\boldsymbol{\mu}$ instead of $\boldsymbol{\rho}$.

Lemma 6.8. *Let $\boldsymbol{\mu}$ and $\tilde{\boldsymbol{\mu}}$ be compact operators. Then for any $q \in [2, \infty]$ and any $\theta \in \{0, 1\}$,*

$$(118) \qquad \|\mathsf{X}_{\tilde{\boldsymbol{\mu}}} \, \boldsymbol{\mu}\|_q \leq C_a \, h^{-a} \, \left\| \tilde{\boldsymbol{\mu}} \, |\boldsymbol{p}|^{a(1-\theta)} \right\|_2 \left\| \boldsymbol{\mu}^* \, |\boldsymbol{p}|^{\theta a} \right\|_\infty,$$

where $\boldsymbol{\mu}^*$ is the adjoint operator of $\boldsymbol{\mu}$.

Proof. Take $\boldsymbol{\mu}_2$ a compact but possibly not self-adjoint operator. Then

$$\|\mathsf{X}_{\boldsymbol{\mu}_2}\|_2^2 = \operatorname{Tr}\!\left(\mathsf{X}_{\boldsymbol{\mu}_2}^* \, \mathsf{X}_{\boldsymbol{\mu}_2}\right) = \iint_{\mathbb{R}^6} \frac{\boldsymbol{\mu}_2^*(x,y) \, \boldsymbol{\mu}_2(y,x)}{|x-y|^{2a}} \, \mathrm{d}x \, \mathrm{d}y$$

$$= \iint_{\mathbb{R}^6} \frac{|\boldsymbol{\mu}_2(x,y)|^2}{|x-y|^{2a}} \, \mathrm{d}x \, \mathrm{d}y = \iint_{\mathbb{R}^6} \frac{|\boldsymbol{\mu}_2(x,y+x)|^2}{|y|^{2a}} \, \mathrm{d}x \, \mathrm{d}y,$$

so that by the Hardy-Rellich inequality,

$$\|\mathsf{X}_{\boldsymbol{\mu}_2}\|_2^2 \leq \mathcal{C}_a \iint_{\mathbb{R}^6} \left| \Delta_y^{a/2} \boldsymbol{\mu}_2(x, y+x) \right|^2 \mathrm{d}x \, \mathrm{d}y = \mathcal{C}_a \iint_{\mathbb{R}^6} \left| \Delta_y^{a/2} \boldsymbol{\mu}_2(x, y) \right|^2 \mathrm{d}x \, \mathrm{d}y$$

$$\leq C_a \, h^{-2a} \iint_{\mathbb{R}^6} |(\boldsymbol{\mu}_2 \, |\boldsymbol{p}|^a)(x,y)|^2 \, \mathrm{d}x \, \mathrm{d}y,$$

where $\mathcal{C}_a$ is the constant appearing in the Hardy–Rellich inequality and $C_a = (2\pi)^a \mathcal{C}_a$. From this we deduce the generalization of (117) for possibly not self-adjoint operators

$$(119) \qquad \left\|\mathsf{X}_{\boldsymbol{\mu}_2}\right\|_2 \leq C_a \, h^{-a} \, \|\boldsymbol{\mu}_2 \, |\boldsymbol{p}|^a\|_2 \, .$$

By Hölder's inequality, taking $\boldsymbol{\mu}_2 = \tilde{\boldsymbol{\mu}}$, it implies (118) when $\theta = 0$. Now, remarking that we have the following integration by parts like formula

$$\operatorname{Tr}(\mathsf{X}_{\tilde{\boldsymbol{\mu}}} \, \boldsymbol{\mu}) = \iint_{\mathbb{R}^6} \frac{\tilde{\boldsymbol{\mu}}(x,y) \, \boldsymbol{\mu}(y,x)}{|x-y|^a} \, \mathrm{d}x \, \mathrm{d}y = \operatorname{Tr}(\tilde{\boldsymbol{\mu}} \, \mathsf{X}_{\boldsymbol{\mu}}) \, ,$$

and using the cyclicity of the trace, Hölder's inequality and Inequality (119) with $\boldsymbol{\mu}_2 = \mathsf{X}_{\tilde{\boldsymbol{\mu}}} \, \boldsymbol{\mu} \boldsymbol{\mu}^*$, we get

$$\|\mathsf{X}_{\tilde{\boldsymbol{\mu}}} \, \boldsymbol{\mu}\|_2^2 = \operatorname{Tr}(\mathsf{X}_{\tilde{\boldsymbol{\mu}}^*} \, \mathsf{X}_{\tilde{\boldsymbol{\mu}}} \, \boldsymbol{\mu} \boldsymbol{\mu}^*) = \operatorname{Tr}\!\left(\tilde{\boldsymbol{\mu}}^* \, \mathsf{X}_{(\mathsf{X}_{\tilde{\boldsymbol{\mu}}} \, \boldsymbol{\mu} \boldsymbol{\mu}^*)}\right)$$

$$\leq \|\tilde{\boldsymbol{\mu}}\|_2 \left\|\mathsf{X}_{(\mathsf{X}_{\tilde{\boldsymbol{\mu}}} \, \boldsymbol{\mu} \boldsymbol{\mu}^*)}\right\|_2 \leq C_a \, h^{-a} \, \|\tilde{\boldsymbol{\mu}}\|_2 \, \|\mathsf{X}_{\tilde{\boldsymbol{\mu}}} \, \boldsymbol{\mu} \boldsymbol{\mu}^* \, |\boldsymbol{p}|^a\|_2 \, .$$

By Hölder's inequality, this leads to

$$\|\mathsf{X}_{\tilde{\boldsymbol{\mu}}} \, \boldsymbol{\mu}\|_2^2 \leq C_a \, h^{-a} \, \|\tilde{\boldsymbol{\mu}}\|_2 \, \|\mathsf{X}_{\tilde{\boldsymbol{\mu}}} \, \boldsymbol{\mu}\|_2 \, \|\boldsymbol{\mu}^* \, |\boldsymbol{p}|^a\|_\infty \, .$$

We deduce the result by dividing both sides by $\|\mathsf{X}_{\tilde{\boldsymbol{\mu}}} \, \boldsymbol{\mu}\|_2$ and then using the fact that for $q \geq 2$, $\|\mathsf{X}_{\tilde{\boldsymbol{\mu}}} \, \boldsymbol{\mu}\|_q \leq \|\mathsf{X}_{\tilde{\boldsymbol{\mu}}} \, \boldsymbol{\mu}\|_2$. $\qquad \square$

The following lemma will allow us to replace the Hilbert–Schmidt norm on the right-hand side of Inequality (117) by another Schatten norm with higher index at the expense of using a less sharp power on $|\boldsymbol{p}|$.

Lemma 6.9. *Let $\boldsymbol{\mu}$ be a compact operator. Then for any $\alpha > a$ and any $q \in [2, \infty]$, it holds*

$$(120) \qquad \|\mathsf{X}_{\boldsymbol{\mu}}\|_q \leq C\, h^{-\alpha}\, \|\boldsymbol{\mu}\,(1 + |\boldsymbol{p}|^{\alpha})\|_q\,,$$

for a constant C depending only on a and α.

Proof. Take $(\varphi, \phi) \in (L^2)^2$. Then one has

$$\langle \varphi \,|\, \mathsf{X}_{\boldsymbol{\mu}}\, \phi \rangle_{L^2} = \iint_{\mathbb{R}^6} \frac{\boldsymbol{\mu}(x,y)\, \overline{\varphi(x)}\, \phi(y)}{|x-y|^a}\, \mathrm{d}x\, \mathrm{d}y = (2\pi)^{3-a}\, C_a\, \mathrm{Tr}\Big(\boldsymbol{\mu}\, \varphi\, (-\Delta)^{\frac{a-3}{2}}\, \phi \Big),$$

where φ and ϕ are seen as multiplication operators and $C_a = \frac{\omega_a}{\omega_{3-a}}$. By the definition of $\boldsymbol{p}$, this can be written

$$\langle \varphi \,|\, \mathsf{X}_{\boldsymbol{\mu}}\, \phi \rangle_{L^2} = C_a h^{3-a}\, \mathrm{Tr}\Big(\boldsymbol{\mu}\, \varphi\, |\boldsymbol{p}|^{a-3}\, \phi \Big) = C_a h^{3-a}\, \mathrm{Tr}\big(m\, \boldsymbol{\mu}\, m\, m^{-1} \varphi\, g(\boldsymbol{p})\, \phi\, m^{-1} \big),$$

with $g(x) = |x|^{a-3}$ and $m = 1 + |\boldsymbol{p}|^{\alpha}$. Now taking $1 \leq \frac{3}{\alpha} < p'_0 < \frac{3}{a} < p'_1 \leq \infty$ such that $\frac{1}{p'_0} + \frac{1}{p'_1} = \frac{a}{3}$, we have $g \in L^{p_0} + L^{p_1}$, hence we can write $g = g_0 + g_1$ with $(g_0, g_1) \in L^{p_0} \times L^{p_1}$. Let $\tilde{g} = g_0$ or $\tilde{g} = g_1$, or more generally, take $\tilde{g} \in L^p$ for some $p \geq 1$ verifying $p' > \frac{3}{\alpha}$. Then, by Hölder's inequality for Schatten norms, Lemma 6.4 and the Kato-Seiler-Simon Inequality (21), we have

$$h^3 \left| \mathrm{Tr}\Big(m^{\frac{1}{2}}\, \boldsymbol{\mu}\, m^{\frac{1}{2}}\, m^{-\frac{1}{2}} \varphi\, \tilde{g}(\boldsymbol{p})\, \phi\, m^{-\frac{1}{2}} \Big) \right|$$

$$\leq \left\| m^{\frac{1}{2}}\, \boldsymbol{\mu}\, m^{\frac{1}{2}} \right\|_{\infty} \left\| m^{-\frac{1}{2}} \varphi^{\frac{1}{p'}} \right\|_{\mathcal{L}^{2p'}} \left\| \varphi^{\frac{1}{p}} \tilde{g}(\boldsymbol{p})^{\frac{1}{2}} \right\|_{\mathcal{L}^{2p}} \left\| \tilde{g}(\boldsymbol{p})^{\frac{1}{2}} \phi^{\frac{1}{p}} \right\|_{\mathcal{L}^{2p}} \left\| \phi^{\frac{1}{p'}} m^{-\frac{1}{2}} \right\|_{\mathcal{L}^{2p'}}$$

$$\leq C_p^{\frac{1}{p'}}\, \|\boldsymbol{\mu}\, m\|_{\infty}\, \|\varphi\|_{L^2}\, \|\tilde{g}\|_{L^p}\, \|\phi\|_{L^2}\,,$$

where we used the notation $z^b = |z|^{b-1} z$ and with $C_p = \int_{\mathbb{R}^3} \frac{\mathrm{d}y}{(1+|y|^{\alpha})^{p'}}$. This constant is finite since $\alpha p' > 3$. This proves Inequality (120) when $q = \infty$. When $q = 2$, the inequality follows from Formula (119). The other cases follow by complex interpolation. $\qquad\square$

6.5. **Commutators Involving the Exchange Term.**

Proposition 6.8. *Let $a \in [0, 1]$. Then there exists $C > 0$ such that for any compact self-adjoint operators $\boldsymbol{\rho}$ and $\boldsymbol{\mu}$, any $q \in [1, \infty]$ and any integer $n \geq 2a - 1$*

$$\frac{1}{\hbar} \left\| [h^3 \mathsf{X}_{\boldsymbol{\rho}}, \boldsymbol{p}_{\mathrm{j}}^n]\, \boldsymbol{\mu} \right\|_{\mathcal{L}^q} \leq 3^n\, h^{\frac{3}{2}-a}\, C\, \left\| \boldsymbol{\nabla}_{x_{\mathrm{j}}} \boldsymbol{\rho}\, m \right\|_{\mathcal{L}^2} \|\boldsymbol{\mu}\, m\|_{\mathcal{L}^q}\,,$$

where $m = 1 + |\boldsymbol{p}|^n$.

Proof. By Formula (116), and the triangle inequality, we have

$$\left\| [\mathsf{X}_{\boldsymbol{\rho}}, \boldsymbol{p}_{\mathrm{j}}^n]\, \boldsymbol{\mu} \right\|_q \leq \sum_{k=1}^{n} \binom{n}{k} \left\| \mathsf{X}_{\mathrm{ad}_{\boldsymbol{p}_{\mathrm{j}}}^k(\boldsymbol{\rho})}\, \boldsymbol{p}_{\mathrm{j}}^{n-k}\, \boldsymbol{\mu} \right\|_q\,.$$

Now, Lemma 6.8 gives the bound

$$\left\| \mathsf{X}_{\mathrm{ad}_{\boldsymbol{p}_{\mathrm{j}}}^k(\boldsymbol{\rho})}\, \boldsymbol{p}_{\mathrm{j}}^{n-k}\, \boldsymbol{\mu} \right\|_q \leq C_a\, h^{-a}\, \left\| \mathrm{ad}_{\boldsymbol{p}_{\mathrm{j}}}^k(\boldsymbol{\rho})\, |\boldsymbol{p}|^{a(1-\theta)} \right\|_2 \left\| \boldsymbol{\mu}\, \boldsymbol{p}_{\mathrm{j}}^{n-k}\, |\boldsymbol{p}|^{\theta a} \right\|_{\infty}\,.$$

Using the fact that $\mathrm{ad}_{\boldsymbol{p}_{\mathrm{j}}}(\boldsymbol{\rho}) = -i\hbar\boldsymbol{\nabla}_{x_{\mathrm{j}}}\boldsymbol{\rho}$ and expanding the $k-1$ commutators in $\mathrm{ad}_{\boldsymbol{p}_{\mathrm{j}}}^{k-1}$ by Lemma 6.5, we get

$$\left\| \mathrm{ad}_{\boldsymbol{p}_{\mathrm{j}}}^{k}(\boldsymbol{\rho})\,|\boldsymbol{p}|^{a(1-\theta)} \right\|_{2} \le 2^{k}\hbar\left\| \boldsymbol{\nabla}_{x_{\mathrm{j}}}\boldsymbol{\rho}\,|\boldsymbol{p}|^{a(1-\theta)+k-1} \right\|_{2}.$$

Now when $k \ge a$, we take $\theta = 1$ so that $n - k + \theta a \le n$ and $a(1-\theta) + k - 1 = k - 1 \le n$. When $k < a$, we take $\theta = 0$ so that $n - k + \theta a = n - k \le n$ and $a(1-\theta) + k - 1 \le 2a - 1 \le n$. In all the cases, this leads to

$$\frac{1}{\hbar}\left\| [\mathsf{X}_{\boldsymbol{\rho}},\boldsymbol{p}_{\mathrm{j}}^{n}]\,\boldsymbol{\mu} \right\|_{q} \le C\,h^{-a}\sum_{k=1}^{n}\binom{n}{k}2^{k}\left\| \boldsymbol{\nabla}_{x_{\mathrm{j}}}\boldsymbol{\rho}\,m \right\|_{2}\left\| \boldsymbol{\mu}\,m \right\|_{\infty}.$$

We conclude using the fact that $\|\boldsymbol{\mu}\,m\|_{\infty} \le \|\boldsymbol{\mu}\,m\|_{q}$ and the definition (19) of the $\mathcal{L}^{2}$ norm. $\qquad\square$

Proposition 6.9. *Let* $a \in [0,1]$, $\mathfrak{b} = \frac{3}{a+1}$ *and* $n \in \mathbb{N}$ *verifying* $n \ge 2a$. *Then for any* $\alpha \in (a, n-a]$ *and any* $q \in [2,\infty]$

$$(121)\quad \frac{1}{\hbar}\left\| [h^{3}\mathsf{X}_{\boldsymbol{\mu}},\boldsymbol{\rho}]\,\boldsymbol{p}_{\mathrm{j}}^{n} \right\|_{\mathcal{L}^{q}} \le 3^{n}\,C\,h^{3\left(\frac{1}{q}+\frac{1}{2}-\frac{1}{\mathfrak{b}}\right)}\left\| \boldsymbol{\rho}\,m \right\|_{\mathcal{L}^{\infty}}\left\| \boldsymbol{\mu}\,m \right\|_{\mathcal{L}^{2}}$$

$$(122)\quad \frac{1}{\hbar}\left\| [h^{3}\mathsf{X}_{\boldsymbol{\mu}},\boldsymbol{\rho}]\,\boldsymbol{p}_{\mathrm{j}}^{n} \right\|_{\mathcal{L}^{q}} \le 3^{n}\,C\,\| \boldsymbol{\rho}\,m \|_{\mathcal{L}^{\infty}}\left(h^{\frac{3}{\beta'}}\| \boldsymbol{\mu}\,m \|_{\mathcal{L}^{q}} + h^{\frac{3}{2}-a}\left\| \boldsymbol{\nabla}_{x_{\mathrm{j}}}\boldsymbol{\mu}\,m \right\|_{\mathcal{L}^{2}} \right),$$

where $m = 1 + |\boldsymbol{p}|^{n}$ *and* $\beta = \frac{3}{\alpha+1}$.

Note that the power of h in the first formula is nonnegative only for $q \le q_{a}$ with $\frac{1}{q_{a}} = \frac{1}{\mathfrak{b}} - \frac{1}{2}$. In the second formula, this is true for every q but involves a semiclassical derivative of $\boldsymbol{\mu}$.

Proof of Proposition 6.9. Since the exchange term is vanishing when $\hbar \to 0$, we can estimate the two parts of the commutator separately by writing

$$\left\| [\mathsf{X}_{\boldsymbol{\mu}},\boldsymbol{\rho}]\,\boldsymbol{p}_{\mathrm{j}}^{n} \right\|_{q} = \left\| \boldsymbol{p}_{\mathrm{j}}^{n}\,[\mathsf{X}_{\boldsymbol{\mu}},\boldsymbol{\rho}] \right\|_{q} \le \left\| \boldsymbol{p}_{\mathrm{j}}^{n}\,\boldsymbol{\rho}\,\mathsf{X}_{\boldsymbol{\mu}} \right\|_{q} + \left\| \boldsymbol{p}_{\mathrm{j}}^{n}\,\mathsf{X}_{\boldsymbol{\mu}}\,\boldsymbol{\rho} \right\|_{q}.$$

The first term in the right-hand side can be bounded using Hölder's inequality for Schatten norms and Lemma 6.8 with $\theta = 0$, leading to

$$(123)\quad \left\| \boldsymbol{p}_{\mathrm{j}}^{n}\,\boldsymbol{\rho}\,\mathsf{X}_{\boldsymbol{\mu}} \right\|_{q} \le C\,h^{-a}\left\| \boldsymbol{p}_{\mathrm{j}}^{n}\,\boldsymbol{\rho} \right\|_{\infty}\left\| \boldsymbol{\mu}\,|\boldsymbol{p}|^{a} \right\|_{2} \le C\,h^{-a}\left\| \boldsymbol{\rho}\,m \right\|_{\infty}\left\| \boldsymbol{\mu}\,m \right\|_{2}.$$

We can also use Lemma 6.9 with $\alpha \in (a,n]$, to get

$$(124)\quad \left\| \boldsymbol{p}_{\mathrm{j}}^{n}\,\boldsymbol{\rho}\,\mathsf{X}_{\boldsymbol{\mu}} \right\|_{q} \le C\,h^{-\alpha}\left\| \boldsymbol{p}_{\mathrm{j}}^{n}\,\boldsymbol{\rho} \right\|_{\infty}\left\| \boldsymbol{\mu}\,(1+|\boldsymbol{p}|^{\alpha}) \right\|_{q} \le C\,h^{-\alpha}\left\| \boldsymbol{\rho}\,m \right\|_{\infty}\left\| \boldsymbol{\mu}\,m \right\|_{q}.$$

To treat the second term, we want to put the first weight m either on $\boldsymbol{\mu}$ either on $\boldsymbol{\rho}$. To obtain this effect, we use Formula (115) to get

$$(125)\quad \left\| \boldsymbol{p}_{\mathrm{j}}^{n}\,\mathsf{X}_{\boldsymbol{\mu}}\,\boldsymbol{\rho} \right\|_{q} \le \sum_{k=0}^{n}\binom{n}{k}\left\| \mathsf{X}_{\mathrm{ad}_{\boldsymbol{p}_{\mathrm{j}}}^{k}(\boldsymbol{\mu})}\,\boldsymbol{p}_{\mathrm{j}}^{n-k}\,\boldsymbol{\rho} \right\|_{q}.$$

Now we use Lemma 6.8 and then expand the commutators by Lemma 6.5 to get for any $\theta \in \{0,1\}$

$$\left\| \mathsf{X}_{\mathrm{ad}_{\boldsymbol{p}_{\mathrm{j}}}^{k}(\boldsymbol{\mu})}\,\boldsymbol{p}_{\mathrm{j}}^{n-k}\,\boldsymbol{\rho} \right\|_{q} \le C\,h^{-a}\left\| \mathrm{ad}_{\boldsymbol{p}_{\mathrm{j}}}^{k}(\boldsymbol{\mu})\,|\boldsymbol{p}|^{a(1-\theta)} \right\|_{2}\left\| \boldsymbol{\rho}\,\boldsymbol{p}_{\mathrm{j}}^{n-k}\,|\boldsymbol{p}|^{\theta a} \right\|_{\infty}$$

$$\le 2^{k}\,C\,h^{-a}\left\| \boldsymbol{\mu}\left(1+|\boldsymbol{p}|^{k+a(1-\theta)}\right) \right\|_{2}\left\| \boldsymbol{\rho}\left(1+|\boldsymbol{p}|^{n-k+\theta a}\right) \right\|_{\infty},$$

and similarly as in the proof of Proposition 6.8, if $k \geq a$, we take $\theta = 1$ and if $k \leq a$, we take $\theta = 0$ and use the fact that $2a \leq n$. In any cases, the power on $|\boldsymbol{p}|$ is smaller than n. Therefore, recalling Inequality (125), we obtain

$$(126) \qquad \left\| \boldsymbol{p}_{\mathsf{j}}^n \, \mathsf{X}_{\boldsymbol{\mu}} \, \boldsymbol{\rho} \right\|_q \leq 3^n \, C \, h^{-a} \, \left\| \boldsymbol{\rho} \, m \right\|_\infty \left\| \boldsymbol{\mu} \, m \right\|_2 .$$

Combining inequalities (123) and (126) and using the definition (19) of $\mathcal{L}^q$ norms yield Formula (121).

To get Formula (122), we start back from Inequality (125). If $k > a$, so that in particular $k \geq 1$, we use again Lemma 6.8 and Lemma 6.5 but we use first the fact that $\mathrm{ad}_{\boldsymbol{p}_j}(\boldsymbol{\mu}) = -i\hbar \, \boldsymbol{\nabla}_{x_j} \boldsymbol{\mu}$ to get an additional $\hbar$. This yields

$$\left\| \mathsf{X}_{\mathrm{ad}_{\boldsymbol{p}_j}^k(\boldsymbol{\mu})} \, \boldsymbol{p}_{\mathsf{j}}^{n-k} \, \boldsymbol{\rho} \right\|_q \leq 2^k \, C \, h^{1-a} \left\| \boldsymbol{\nabla}_{x_j} \boldsymbol{\mu} \left(1 + |\boldsymbol{p}|^{k-1} \right) \right\|_2 \left\| \boldsymbol{\rho} \left(1 + |\boldsymbol{p}|^{n-k+a} \right) \right\|_\infty ,$$

If $k \leq a$, then we use Lemma 6.9 with $\alpha \in (a, n-a]$ to get

$$\left\| \mathsf{X}_{\mathrm{ad}_{\boldsymbol{p}_j}^k(\boldsymbol{\mu})} \, \boldsymbol{p}_{\mathsf{j}}^{n-k} \, \boldsymbol{\rho} \right\|_q \leq 2^k \, C \, h^{-\alpha} \left\| \boldsymbol{\mu} \left(1 + |\boldsymbol{p}|^{k+\alpha} \right) \right\|_q \left\| \boldsymbol{\rho} \left(1 + |\boldsymbol{p}|^{n-k} \right) \right\|_\infty .$$

Therefore, Inequality (125) implies

$$(127) \qquad \left\| \boldsymbol{p}_{\mathsf{j}}^n \, \mathsf{X}_{\boldsymbol{\mu}} \, \boldsymbol{\rho} \right\|_q \leq 3^n \, C \, \left\| \boldsymbol{\rho} \, m \right\|_\infty \left(h^{-\alpha} \left\| \boldsymbol{\mu} \, m \right\|_q + h^{1-a} \left\| \boldsymbol{\nabla}_{x_j} \boldsymbol{\mu} \, m \right\|_2 \right),$$

and together with Inequality (123) and the definition of the $\mathcal{L}^q$ norm, this implies Formula (122). $\qquad \square$

6.6. **Proof of the Propagation of Regularity.**

Proof of Proposition 6.1. The strategy to prove Proposition 6.1 is to look at Equations (96), (97) and (98) and find a Grönwall-type inequality on $\|\boldsymbol{\rho}\|_{\mathcal{W}^{1,q}(m)}$. In particular we will see that to close the Grönwall argument for $q = 2$, we need to estimate $\|\boldsymbol{\rho}\|_{\mathcal{W}^{1,q}(m)}$ for $q \in (2,4)$. We will therefore proceed by interpolation and define

$$M_2(t) := \|\boldsymbol{\rho}\|_{\mathcal{W}^{1,2}(m)}, \quad M_4(t) := \|\boldsymbol{\rho}\|_{\mathcal{W}^{1,4}(m)}, \quad M_\infty(t) := \|\boldsymbol{\rho} \, m\|_{\mathcal{L}^\infty} .$$

For $a \in \left[\frac{1}{2}, 1 \right]$ we will find a Grönwall-type inequality on $M_2(t) + M_4(t) + M_\infty(t)$, whereas for $a \in \left[0, \frac{1}{2} \right)$ it suffices to apply Grönwall's Lemma to $M_2(t) + M_4(t)$.

We now look at Equation (96). By Proposition 6.7 we have that

$$\frac{1}{\hbar} \left\| [V_{\boldsymbol{\rho}}, m] \, \boldsymbol{\rho} \right\|_{\mathcal{L}^q} \leq C \left\| \boldsymbol{\rho} \, m \right\|_{\mathcal{L}^r} \left\| \boldsymbol{\rho} \, m \right\|_{\mathcal{L}^{r_1}} .$$

The contribution given by the exchange term in the right-hand side of (96) can be bounded by Proposition 6.8 with $\boldsymbol{\mu} = \boldsymbol{\rho}$. Therefore, we obtain the following bounds on the right-hand side of Equation (96)

$$\frac{\mathrm{d}}{\mathrm{d}t} \left\| \boldsymbol{\rho} \, m \right\|_{\mathcal{L}^q} \leq C \left\| \boldsymbol{\rho} \, m \right\|_{\mathcal{L}^r} \left\| \boldsymbol{\rho} \, m \right\|_{\mathcal{L}^{r_1}} + h^{\frac{3}{2}-a} \left\| \boldsymbol{\nabla}_x \boldsymbol{\rho} \, m \right\|_{\mathcal{L}^2} \left\| \boldsymbol{\rho} \, m \right\|_{\mathcal{L}^q} .$$

In particular, for $q = \infty$ we get

$$\frac{\mathrm{d}}{\mathrm{d}t} \left\| \boldsymbol{\rho} \, m \right\|_{\mathcal{L}^\infty} \leq C \left\| \boldsymbol{\rho} \, m \right\|_{\mathcal{L}^{\frac{3}{2-a}}} \left\| \boldsymbol{\rho} \, m \right\|_{\mathcal{L}^\infty} + h^{\frac{3}{2}-a} \left\| \boldsymbol{\nabla}_x \boldsymbol{\rho} \, m \right\|_{\mathcal{L}^2} \left\| \boldsymbol{\rho} \, m \right\|_{\mathcal{L}^\infty} .$$

Note that we cannot close the Grönwall's inequality and we will need bounds on $\boldsymbol{\nabla}_x\boldsymbol{\rho}$ and $\boldsymbol{\nabla}_\xi\boldsymbol{\rho}$. To this end, we look at Equation (97) and Equation (98). We start bounding the right-hand side of Equation (97). By Proposition 6.7 we obtain

$$(128) \qquad \frac{1}{\hbar}\left\|[V_{\boldsymbol{\rho}},m]\,\boldsymbol{\nabla}_x\boldsymbol{\rho}\right\|_{\mathcal{L}^q} \leq \left\|\boldsymbol{\rho}\,m\right\|_{\mathcal{L}^r}\left\|\boldsymbol{\nabla}_x\boldsymbol{\rho}\,m\right\|_{\mathcal{L}^{r_1}}.$$

By writing $[E_{\boldsymbol{\rho}},\boldsymbol{\rho}]\,m = [E_{\boldsymbol{\rho}},\boldsymbol{\rho}\,m] + \boldsymbol{\rho}\,[E_{\boldsymbol{\rho}},m]$, applying Proposition 6.5 with $\boldsymbol{\rho}_2 = \boldsymbol{\rho}\,m$ and Proposition 6.6 with $\boldsymbol{\mu} = \boldsymbol{\rho}$, we get

$$(129) \quad \frac{1}{\hbar}\left\|[E_{\boldsymbol{\rho}},\boldsymbol{\rho}]\,m\right\|_{\mathcal{L}^q} \leq C\,\|\rho\|_{L^r}^{1-s}\,\|\rho\|_{W^{1,r}}^{s}\,\left\|\boldsymbol{\nabla}_\xi\boldsymbol{\rho}\,m\right\|_{\mathcal{L}^q} + C\left\|\boldsymbol{\nabla}_x\boldsymbol{\rho}\,m\right\|_{\mathcal{L}^r}\left\|\boldsymbol{\rho}\,m\right\|_{\mathcal{L}^{r_1}}$$

for $q > 2$ and $s = 1 - 3\left(\frac{1}{r'} - \frac{1}{\flat'}\right)$, where we used the interpolation of Besov spaces stated in Corollary 6.1.

For $q = 2$, we have

$$(130) \qquad \frac{1}{\hbar}\left\|[E_{\boldsymbol{\rho}},\boldsymbol{\rho}]\,m\right\|_{\mathcal{L}^2} \leq C\,\|\nabla\rho\|_{L^{\flat',1}}\left\|\boldsymbol{\nabla}_\xi\boldsymbol{\rho}\,m\right\|_{\mathcal{L}^2} + C\left\|\boldsymbol{\nabla}_x\boldsymbol{\rho}\,m\right\|_{\mathcal{L}^r}\left\|\boldsymbol{\rho}\,m\right\|_{\mathcal{L}^{r_1}}$$

for $a \in \left[\frac{1}{2},1\right]$, and

$$(131) \qquad \frac{1}{\hbar}\left\|[E_{\boldsymbol{\rho}},\boldsymbol{\rho}]\,m\right\|_{\mathcal{L}^2} \leq C\,\|\rho\|_{L^{\frac{3}{1-a}},1}\left\|\boldsymbol{\nabla}_\xi\boldsymbol{\rho}\,m\right\|_{\mathcal{L}^2} + C\left\|\boldsymbol{\nabla}_x\boldsymbol{\rho}\,m\right\|_{\mathcal{L}^r}\left\|\boldsymbol{\rho}\,m\right\|_{\mathcal{L}^{r_1}}$$

for $a \in \left(0,\frac{1}{2}\right)$.

The contributions of the exchange term can be bounded using Proposition 6.8 and Proposition 6.9. Combining them with (129) leads to, for $q > 2$,

$$
\begin{aligned}
(132) \quad \frac{\mathrm{d}}{\mathrm{d}t}\left\|\boldsymbol{\nabla}_x\boldsymbol{\rho}\,m\right\|_{\mathcal{L}^q} \leq\; & C\left\|\boldsymbol{\rho}\,m\right\|_{\mathcal{L}^r}\left\|\boldsymbol{\nabla}_\xi\boldsymbol{\rho}\,m\right\|_{\mathcal{L}^{r_1}} + C\,\|\rho\|_{B_{r,1}^{1-3\left(\frac{1}{r'}-\frac{1}{\flat}\right)}}\left\|\boldsymbol{\nabla}_\xi\boldsymbol{\rho}\,m\right\|_{\mathcal{L}^q} \\
& + C\left\|\boldsymbol{\nabla}_x\boldsymbol{\rho}\,m\right\|_{\mathcal{L}^r}\left\|\boldsymbol{\rho}\,m\right\|_{\mathcal{L}^{r_1}} + Ch^{\frac{3}{2}-a}\left\|\boldsymbol{\nabla}_x\boldsymbol{\rho}\,m\right\|_{\mathcal{L}^2}\left\|\boldsymbol{\nabla}_x\boldsymbol{\rho}\,m\right\|_{\mathcal{L}^q} \\
& + Ch^{3\left(\frac{1}{q}+\frac{1}{2}-\frac{1}{\flat}\right)}\left\|\boldsymbol{\rho}\,m\right\|_{\mathcal{L}^\infty}\left\|\boldsymbol{\nabla}_x\boldsymbol{\rho}\,m\right\|_{\mathcal{L}^2}.
\end{aligned}
$$

To bound the right-hand side of Equation (98), we use Proposition 6.7 for the contribution due to the direct term and Proposition 6.8 and Proposition 6.9 to estimate the contributions of the exchange term. Hence,

$$
\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}t}\left\|\boldsymbol{\nabla}_\xi\boldsymbol{\rho}\,m\right\|_{\mathcal{L}^q} \leq\; & C\left\|\boldsymbol{\rho}\,m\right\|_{\mathcal{L}^r}\left\|\boldsymbol{\nabla}_\xi\boldsymbol{\rho}\,m\right\|_{\mathcal{L}^{r_1}} + C\left\|\boldsymbol{\nabla}_x\boldsymbol{\rho}\,m\right\|_{\mathcal{L}^q} \\
& + Ch^{\frac{3}{2}-a}\left\|\boldsymbol{\nabla}_x\boldsymbol{\rho}\,m\right\|_{\mathcal{L}^2}\left\|\boldsymbol{\nabla}_\xi\boldsymbol{\rho}\,m\right\|_{\mathcal{L}^q} + Ch^{3\left(\frac{1}{q}+\frac{1}{2}-\frac{1}{\flat}\right)}\left\|\boldsymbol{\rho}\,m\right\|_{\mathcal{L}^\infty}\left\|\boldsymbol{\nabla}_\xi\boldsymbol{\rho}\,m\right\|_{\mathcal{L}^2}.
\end{aligned}
$$

To get an estimate in $\mathcal{L}^2$ we need a bound on the $\mathcal{L}^q$ norm for $q \in (2,4)$. Therefore we look for a bound when $q = 4$ and proceed by interpolation.

To establish a Grönwall type inequality for $a \geq \frac{1}{2}$, we consider the sum $M_2(t) + M_4(t) + M_\infty(t)$ and observe that it satisfies

$$
\begin{aligned}
(133) \quad \frac{\mathrm{d}}{\mathrm{d}t}\left[M_2(t) + M_4(t) + M_\infty(t)\right] \leq\; & CM_2(t) + CM_4(t) + CM_\infty(t) \\
& + C\left(1 + h^{\frac{3}{2}-a} + h^{\frac{3}{\flat'}} + h^{3\left(\frac{3}{4}-\frac{1}{\flat}\right)}\right)\left[M_2(t) + M_4(t) + M_\infty(t)\right]^2,
\end{aligned}
$$

where we used interpolation inequality with $\theta \in (0,1)$ and Young's inequality for products to bound

$$\|\boldsymbol{\rho}\,m\|_{\mathcal{L}^r} \leq C \,\|\boldsymbol{\rho}\,m\|_{\mathcal{L}^2}^{\theta} \,\|\boldsymbol{\rho}\,m\|_{\mathcal{L}^4}^{1-\theta} \leq C \,\|\boldsymbol{\rho}\,m\|_{\mathcal{L}^2} + \|\boldsymbol{\rho}\,m\|_{\mathcal{L}^4} \ ,$$

$$\|\boldsymbol{\nabla}_x\boldsymbol{\rho}\,m\|_{\mathcal{L}^r} \leq C \,\|\boldsymbol{\nabla}_x\boldsymbol{\rho}\,m\|_{\mathcal{L}^2}^{\theta} \,\|\boldsymbol{\nabla}_x\boldsymbol{\rho}\,m\|_{\mathcal{L}^4}^{1-\theta} \leq C \,\|\boldsymbol{\nabla}_x\boldsymbol{\rho}\,m\|_{\mathcal{L}^2} + C \,\|\boldsymbol{\nabla}_x\boldsymbol{\rho}\,m\|_{\mathcal{L}^4} \ ,$$

$$\|\boldsymbol{\nabla}_\xi\boldsymbol{\rho}\,m\|_{\mathcal{L}^r} \leq C \,\|\boldsymbol{\nabla}_\xi\boldsymbol{\rho}\,m\|_{\mathcal{L}^2}^{\theta} \,\|\boldsymbol{\nabla}_\xi\boldsymbol{\rho}\,m\|_{\mathcal{L}^4}^{1-\theta} \leq C \,\|\boldsymbol{\nabla}_\xi\boldsymbol{\rho}\,m\|_{\mathcal{L}^2} + C \,\|\boldsymbol{\nabla}_\xi\boldsymbol{\rho}\,m\|_{\mathcal{L}^4} \ ,$$

whenever $r \in (2,4)$. We observe that Equation (133) is a Grönwall-type inequality of the same form as Equation (92). Thus there exists a time $T > 0$, depending only in the initial data, such that $M_2(t) + M_4(t)$ is bounded for all $t \in [0,T]$.

For $a < \frac{1}{2}$, we consider the quantity $M_2(t) + M_4(t)$ and use that

$$\|\boldsymbol{\rho}\,m\|_{\mathcal{L}^\infty} \leq C h^{-\frac{3}{q}} \,\|\boldsymbol{\rho}\,m\|_{\mathcal{L}^q} \ .$$

Hence

$$\frac{\mathrm{d}}{\mathrm{d}t} \left(M_2(t) + M_4(t) \right)$$
$$\leq C \left(M_2(t) + M_4(t) \right) + C \left(1 + h^{\frac{3}{2}-a} + h^{3\left(\frac{1}{b'}-\frac{1}{2}\right)} \right) \left(M_2(t) + M_4(t) \right)^2 \ .$$

Therefore there exists $T > 0$, depending only in the initial data, such that $M_2(t) + M_4(t)$ is bounded for all $t \in [0,T]$, thus $\boldsymbol{\rho} \in L^\infty((0,T), \mathcal{W}^{1,2}(m) \cap \mathcal{W}^{1,4}(m) \cap \mathcal{L}^\infty(m))$. Moreover, $\rho \in L^\infty((0,T), H^1 \cap W^{1,4} \cap L^1 \cap L^\infty)$ thanks to Proposition 6.4 and the bounds on $M_2(t)$, $M_4(t)$ and $M_\infty(t)$. $\qquad\square$

Proof of Proposition 6.2. Similarly to what we have done for the first-order quantum gradients, we can compute the time derivative of the second order quantum gradients of $\boldsymbol{\rho}$

(134)
$$i\hbar\,\partial_t\,\boldsymbol{\nabla}_x^2\boldsymbol{\rho} = \left[H, \boldsymbol{\nabla}_x^2\boldsymbol{\rho}\right] - 2\left[E_{\boldsymbol{\rho}}, \boldsymbol{\nabla}_x\boldsymbol{\rho}\right] - \left[\boldsymbol{\nabla}_x E_{\boldsymbol{\rho}}, \boldsymbol{\rho}\right] - 2\left[h^3\mathsf{X}_{\boldsymbol{\nabla}_x\boldsymbol{\rho}}, \boldsymbol{\nabla}_x\boldsymbol{\rho}\right] - \left[h^3\mathsf{X}_{\boldsymbol{\nabla}_x^2\boldsymbol{\rho}}, \boldsymbol{\rho}\right]$$

$$i\hbar\,\partial_t\,\boldsymbol{\nabla}_\xi^2\boldsymbol{\rho} = \left[H, \boldsymbol{\nabla}_\xi^2\boldsymbol{\rho}\right] - i\hbar\boldsymbol{\nabla}_\xi\boldsymbol{\nabla}_x\boldsymbol{\rho} - 2\left[h^3\mathsf{X}_{\boldsymbol{\nabla}_\xi\boldsymbol{\rho}}, \boldsymbol{\nabla}_\xi\boldsymbol{\rho}\right] - \left[h^3\mathsf{X}_{\boldsymbol{\nabla}_\xi^2\boldsymbol{\rho}}, \boldsymbol{\rho}\right]$$

$$i\hbar\,\partial_t\,\boldsymbol{\nabla}_\xi\boldsymbol{\nabla}_x\boldsymbol{\rho} = \left[H, \boldsymbol{\nabla}_\xi\boldsymbol{\nabla}_x\boldsymbol{\rho}\right] - i\hbar\boldsymbol{\nabla}_x^2\boldsymbol{\rho} - \left[E_{\boldsymbol{\rho}}, \boldsymbol{\nabla}_\xi\boldsymbol{\rho}\right] - \left[h^3\mathsf{X}_{\boldsymbol{\nabla}_\xi\boldsymbol{\nabla}_x\boldsymbol{\rho}}, \boldsymbol{\rho}\right] - \left[h^3\mathsf{X}_{\boldsymbol{\nabla}_x\boldsymbol{\rho}}, \boldsymbol{\nabla}_\xi\boldsymbol{\rho}\right] \ ,$$

that are of the form

(135)
$$i\hbar\,\partial_t\boldsymbol{\mu} = [\mathsf{A}, \boldsymbol{\mu}] + [\mathsf{B}, \boldsymbol{\nabla}_x\boldsymbol{\rho}] + [\mathsf{C}, \boldsymbol{\rho}] \ ,$$

with A, B and C being self-adjoint operators. The proof of Lemma 6.2 proves also the following statement.

Lemma 6.10 (Lemma 6.2 bis). *Let $\boldsymbol{\rho}$, A, B, C be self-adjoint operators and $\boldsymbol{\mu} = \boldsymbol{\mu}(t)$ be a family of self-adjoint operators verifying* (135). *Then, formally, for any even integer $q \geq 2$ we have*

$$\frac{\mathrm{d}}{\mathrm{d}t} \|\boldsymbol{\mu}\,m\|_q \leq \frac{1}{\hbar} \|[\mathsf{A}, m]\,\boldsymbol{\mu}\|_q + \frac{1}{\hbar} \|[\mathsf{B}, \boldsymbol{\nabla}_x\boldsymbol{\rho}]\,m\|_q + \frac{1}{\hbar} \|[\mathsf{C}, \boldsymbol{\rho}]\,m\|_q \ .$$

We consider the Identities (134) and bound them by Lemma 6.10. This yields

(136)
$$\hbar\,\frac{\mathrm{d}}{\mathrm{d}t} \left\|\boldsymbol{\nabla}_x^2\boldsymbol{\rho}\,m\right\|_q \leq C \left\|[V_{\boldsymbol{\rho}}, m]\,\boldsymbol{\nabla}_x^2\boldsymbol{\rho}\right\|_q + C \left\|[E_{\boldsymbol{\rho}}, \boldsymbol{\nabla}_x\boldsymbol{\rho}]\,m\right\|_q + C \left\|[\boldsymbol{\nabla}_x E_{\boldsymbol{\rho}}, \boldsymbol{\rho}]\,m\right\|_q$$
$$+ C \left\|[h^3\mathsf{X}_{\boldsymbol{\rho}}, m]\,\boldsymbol{\nabla}_x^2\boldsymbol{\rho}\right\|_q + C \left\|[h^3\mathsf{X}_{\boldsymbol{\nabla}_x\boldsymbol{\rho}}, \boldsymbol{\nabla}_x\boldsymbol{\rho}]\,m\right\|_q + C \left\|[h^3\mathsf{X}_{\boldsymbol{\nabla}_x^2\boldsymbol{\rho}}, \boldsymbol{\rho}]\,m\right\|_q$$

$$(137) \quad \begin{aligned} \hbar \frac{\mathrm{d}}{\mathrm{d}t} \left\| \boldsymbol{\nabla}_\xi^2 \boldsymbol{\rho} \, m \right\|_q &\leq C \left\| [V_{\boldsymbol{\rho}}, m] \, \boldsymbol{\nabla}_\xi^2 \boldsymbol{\rho} \right\|_q + C \left\| \boldsymbol{\nabla}_\xi \boldsymbol{\nabla}_x \boldsymbol{\rho} \, m \right\|_q \\ &+ C \left\| [h^3 \mathsf{X}_{\boldsymbol{\rho}}, m] \, \boldsymbol{\nabla}_\xi^2 \boldsymbol{\rho} \right\|_q + C \left\| [h^3 \mathsf{X}_{\boldsymbol{\nabla}_\xi \boldsymbol{\rho}}, \boldsymbol{\nabla}_\xi \boldsymbol{\rho}] \, m \right\|_q + C \left\| \left[h^3 \mathsf{X}_{\boldsymbol{\nabla}_\xi^2 \boldsymbol{\rho}}, \boldsymbol{\rho} \right] m \right\|_q \end{aligned}$$

$$(138) \quad \begin{aligned} \hbar \frac{\mathrm{d}}{\mathrm{d}t} \left\| \boldsymbol{\nabla}_\xi \boldsymbol{\nabla}_x \boldsymbol{\rho} \, m \right\|_q &\leq C \left\| [V_{\boldsymbol{\rho}}, m] \, \boldsymbol{\nabla}_\xi \boldsymbol{\nabla}_x \boldsymbol{\rho} \right\|_q + C \left\| [E_{\boldsymbol{\rho}}, \boldsymbol{\nabla}_\xi \boldsymbol{\rho}] \, m \right\|_q \\ &+ C \left\| \boldsymbol{\nabla}_x^2 \boldsymbol{\rho} \, m \right\|_q + C \left\| [h^3 \mathsf{X}_{\boldsymbol{\rho}}, m] \, \boldsymbol{\nabla}_\xi \boldsymbol{\nabla}_x \boldsymbol{\rho} \right\|_q \\ &+ C \left\| [h^3 \mathsf{X}_{\boldsymbol{\nabla}_x \boldsymbol{\rho}}, \boldsymbol{\nabla}_\xi \boldsymbol{\rho}] \, m \right\|_q + C \left\| [h^3 \mathsf{X}_{\boldsymbol{\nabla}_\xi \boldsymbol{\nabla}_x \boldsymbol{\rho}}, \boldsymbol{\rho}] \, m \right\|_q . \end{aligned}$$

We now estimate the right-hand side of Equation (136). The first three contributions are related to the direct term in the Hartree equation, whereas in the others the exchange operator appears. By Proposition 6.7 we have

$$(139) \quad \frac{1}{\hbar} \left\| [V_{\boldsymbol{\rho}}, m] \, \boldsymbol{\nabla}_x^2 \boldsymbol{\rho} \right\|_{\mathcal{L}^q} \leq C \left\| \boldsymbol{\rho} \, m \right\|_{\mathcal{L}^r} \left\| \boldsymbol{\nabla}_x^2 \boldsymbol{\rho} \, m \right\|_{\mathcal{L}^{r_1}}$$

where $\frac{1}{r} + \frac{1}{r_1} = \frac{1}{q} + \frac{1}{\mathfrak{b}'}$. As for the second term on the right-hand side of Equation (136), we rewrite it as follows:

$$\frac{1}{\hbar} \left\| [E_{\boldsymbol{\rho}}, \boldsymbol{\nabla}_x \boldsymbol{\rho}] \, m \right\|_{\mathcal{L}^q} = \frac{1}{\hbar} \left\| [E_{\boldsymbol{\rho}}, \boldsymbol{\nabla}_x \boldsymbol{\rho} \, m] \right\|_{\mathcal{L}^q} + \frac{1}{\hbar} \left\| [E_{\boldsymbol{\rho}}, m] \, \boldsymbol{\nabla}_x \boldsymbol{\rho} \right\|_{\mathcal{L}^q} .$$

By Proposition 6.5 and Corollary 6.1, we get

$$\frac{1}{\hbar} \left\| [E_{\boldsymbol{\rho}}, \boldsymbol{\nabla}_x \boldsymbol{\rho} \, m] \right\|_{\mathcal{L}^q} \leq C \left\| \rho \right\|_{L^r}^{1-s} \left\| \rho \right\|_{W^{1,r}}^{s} \left\| \boldsymbol{\nabla}_\xi \boldsymbol{\nabla}_x \boldsymbol{\rho} \, m \right\|_{\mathcal{L}^q} ,$$

for $\frac{1}{r} + \frac{1}{q} = \frac{1}{2}$ and $s = 1 - 3 \left(\frac{1}{r'} - \frac{1}{\mathfrak{b}} \right)$. By Proposition 6.6, for $\frac{1}{r} + \frac{1}{r_1} = \frac{1}{q} + \frac{1}{\mathfrak{b}'}$ we have

$$\frac{1}{\hbar} \left\| [E_{\boldsymbol{\rho}}, m] \, \boldsymbol{\nabla}_x \boldsymbol{\rho} \right\|_{\mathcal{L}^q} \leq C \left\| \boldsymbol{\nabla}_x \boldsymbol{\rho} \, m \right\|_{\mathcal{L}^r} \left\| \boldsymbol{\nabla}_x \boldsymbol{\rho} \, m \right\|_{\mathcal{L}^{r_1}} .$$

Whence, the second term in the right-hand side of Equation (136) is bounded by

$$\frac{1}{\hbar} \left\| [E_{\boldsymbol{\rho}}, \boldsymbol{\nabla}_x \boldsymbol{\rho}] \, m \right\|_{\mathcal{L}^q} \leq C \left\| \rho \right\|_{L^r}^{1-s} \left\| \rho \right\|_{W^{1,r}}^{s} \left\| \boldsymbol{\nabla}_\xi \boldsymbol{\nabla}_x \boldsymbol{\rho} \, m \right\|_{\mathcal{L}^q} + C \left\| \boldsymbol{\nabla}_x \boldsymbol{\rho} \, m \right\|_{\mathcal{L}^r} \left\| \boldsymbol{\nabla}_x \boldsymbol{\rho} \, m \right\|_{\mathcal{L}^{r_1}} .$$

The third term on the right-hand side of Equation (136) can be dealt in an analogously manner as to the second term by using that $\boldsymbol{\nabla}_x E_{\boldsymbol{\rho}} = E_{\boldsymbol{\nabla}_x \boldsymbol{\rho}}$ and Proposition 6.6. This gives

$$\frac{1}{\hbar} \left\| [\boldsymbol{\nabla}_x E_{\boldsymbol{\rho}}, \boldsymbol{\rho}] \, m \right\|_{\mathcal{L}^q} \leq C \left\| \nabla \rho \right\|_{L^r}^{1-s} \left\| \nabla \rho \right\|_{W^{1,r}}^{s} \left\| \boldsymbol{\nabla}_\xi \boldsymbol{\rho} \, m \right\|_{\mathcal{L}^q} + C \left\| \boldsymbol{\nabla}_x^2 \boldsymbol{\rho} \, m \right\|_{\mathcal{L}^r} \left\| \boldsymbol{\rho} \, m \right\|_{\mathcal{L}^{r_1}} .$$

We now turn to terms in which the contribution of the exchange term appears. By Proposition 6.8 we obtain

$$(140) \quad \frac{1}{\hbar} \left\| [h^3 \mathsf{X}_{\boldsymbol{\rho}}, m] \, \boldsymbol{\nabla}_x^2 \boldsymbol{\rho} \right\|_{\mathcal{L}^q} \leq C \hbar^{\frac{3}{2} - a} \left\| \boldsymbol{\nabla}_x \boldsymbol{\rho} \, m \right\|_{\mathcal{L}^2} \left\| \boldsymbol{\nabla}_x^2 \boldsymbol{\rho} \, m \right\|_{\mathcal{L}^q} .$$

By Proposition 6.9 we get the bound

$$(141) \quad \frac{1}{\hbar} \left\| [h^3 \mathsf{X}_{\boldsymbol{\nabla}_x \boldsymbol{\rho}}, \boldsymbol{\nabla}_x \boldsymbol{\rho}] \, m \right\|_{\mathcal{L}^q} \leq C \hbar^{3 \left(\frac{1}{q} + \frac{1}{2} - \frac{1}{\mathfrak{b}} \right)} \left\| \boldsymbol{\nabla}_x \boldsymbol{\rho} \, m \right\|_{\mathcal{L}^2} \left\| \boldsymbol{\nabla}_x \boldsymbol{\rho} \, m \right\|_{\mathcal{L}^\infty} .$$

Finally, by noticing that $\boldsymbol{\nabla}_x \mathsf{X}_{\boldsymbol{\nabla}_x \boldsymbol{\rho}} = \mathsf{X}_{\boldsymbol{\nabla}_x^2 \boldsymbol{\rho}}$, we apply Proposition 6.9 to the last term on the right-hand side in Equation (136):

$$(142) \quad \frac{1}{\hbar} \left\| [h^3 \mathsf{X}_{\boldsymbol{\nabla}_x^2 \boldsymbol{\rho}}, \boldsymbol{\rho}] \, m \right\|_{\mathcal{L}^q} \leq C \hbar^{3 \left(\frac{1}{q} + \frac{1}{2} - \frac{1}{\mathfrak{b}} \right)} \left\| \boldsymbol{\rho} \, m \right\|_{\mathcal{L}^\infty} \left\| \boldsymbol{\nabla}_x^2 \boldsymbol{\rho} \, m \right\|_{\mathcal{L}^2} .$$

Therefore, using Proposition 6.1 and estimates (139)–(142) we obtain

$$
\begin{aligned}
(143) \quad \frac{\mathrm{d}}{\mathrm{d}t} \left\| \boldsymbol{\nabla}_x^2 \boldsymbol{\rho}\, m \right\|_{\mathcal{L}^q} &\leq C \left\| \boldsymbol{\nabla}_x^2 \boldsymbol{\rho}\, m \right\|_{\mathcal{L}^{r_1}} + C \left\| \boldsymbol{\nabla}_\xi \boldsymbol{\nabla}_x \boldsymbol{\rho}\, m \right\|_{\mathcal{L}^q} \\
&\quad + \left\| \nabla \rho \right\|_{W^{1,r}}^s + \left\| \boldsymbol{\nabla}_x^2 \boldsymbol{\rho}\, m \right\|_{\mathcal{L}^r} + \hbar^{\frac{3}{2}-a} \left\| \boldsymbol{\nabla}_x^2 \boldsymbol{\rho}\, m \right\|_{\mathcal{L}^q} \\
&\quad + \hbar^{3\left(\frac{1}{q}+\frac{1}{2}-\frac{1}{\mathfrak{b}}\right)} \left\| \boldsymbol{\nabla}_x \boldsymbol{\rho}\, m \right\|_{\mathcal{L}^\infty} + \hbar^{3\left(\frac{1}{q}+\frac{1}{2}-\frac{1}{\mathfrak{b}}\right)} \left\| \boldsymbol{\nabla}_x^2 \boldsymbol{\rho}\, m \right\|_{\mathcal{L}^2}
\end{aligned}
$$

for $s = 1 - 3\left(\frac{1}{r'} - \frac{1}{\mathfrak{b}}\right)$ and with the constraints $\frac{1}{r} + \frac{1}{r_1} = \frac{1}{q} + \frac{1}{\mathfrak{b}'}$ and $\frac{1}{r} + \frac{1}{q} = \frac{1}{2}$.

We now look at the right-hand side of Equation (137). By using Proposition 6.1, Proposition 6.7, Proposition 6.8, Proposition 6.9 and by Proposition 6.9 with $\boldsymbol{\nabla}_\xi \mathsf{X}_{\boldsymbol{\nabla}_\xi \boldsymbol{\rho}} = \mathsf{X}_{\boldsymbol{\nabla}_\xi^2 \boldsymbol{\rho}}$ we obtain

$$
\begin{aligned}
(144) \quad \frac{\mathrm{d}}{\mathrm{d}t} \left\| \boldsymbol{\nabla}_\xi^2 \boldsymbol{\rho}\, m \right\|_{\mathcal{L}^q} &\leq C \left\| \boldsymbol{\nabla}_\xi^2 \boldsymbol{\rho}\, m \right\|_{\mathcal{L}^{r_1}} + C\hbar^{\frac{3}{2}-a} \left\| \boldsymbol{\nabla}_\xi^2 \boldsymbol{\rho}\, m \right\|_{\mathcal{L}^q} \\
&\quad + C\hbar^{3\left(\frac{1}{q}+\frac{1}{2}-\frac{1}{\mathfrak{b}}\right)} \left\| \boldsymbol{\nabla}_\xi \boldsymbol{\rho}\, m \right\|_{\mathcal{L}^\infty} + C\hbar^{3\left(\frac{1}{q}+\frac{1}{2}-\frac{1}{\mathfrak{b}}\right)} \left\| \boldsymbol{\nabla}_\xi^2 \boldsymbol{\rho}\, m \right\|_{\mathcal{L}^2}
\end{aligned}
$$

for $s = 1 - 3\left(\frac{1}{r'} - \frac{1}{\mathfrak{b}}\right)$ and with the constraints $\frac{1}{r} + \frac{1}{r_1} = \frac{1}{q} + \frac{1}{\mathfrak{b}'}$ and $\frac{1}{r} + \frac{1}{q} = \frac{1}{2}$.

As for the mixed term (138), its right-hand side can be bounded as follows. By Proposition 6.7 we get

$$
(145) \qquad \frac{1}{\hbar} \left\| [V_{\boldsymbol{\rho}}, m] \boldsymbol{\nabla}_\xi \boldsymbol{\nabla}_x \boldsymbol{\rho} \right\|_{\mathcal{L}^q} \leq C \left\| \boldsymbol{\rho}\, m \right\|_{\mathcal{L}^r} \left\| \boldsymbol{\nabla}_\xi \boldsymbol{\nabla}_x \boldsymbol{\rho}\, m \right\|_{\mathcal{L}^{r_1}}
$$

where $\frac{1}{r} + \frac{1}{r_1} = \frac{1}{q} + \frac{1}{\mathfrak{b}'}$. As for the second term on the right-hand side of Equation (138), we rewrite it as follows:

$$
\frac{1}{\hbar} \left\| [E_{\boldsymbol{\rho}}, \boldsymbol{\nabla}_\xi \boldsymbol{\rho}]\, m \right\|_{\mathcal{L}^q} = \frac{1}{\hbar} \left\| [E_{\boldsymbol{\rho}}, \boldsymbol{\nabla}_\xi \boldsymbol{\rho}\, m] \right\|_{\mathcal{L}^q} + \frac{1}{\hbar} \left\| [E_{\boldsymbol{\rho}}, m] \boldsymbol{\nabla}_\xi \boldsymbol{\rho} \right\|_{\mathcal{L}^q}.
$$

Proposition 6.5 and Corollary 6.1 yield

$$
\frac{1}{\hbar} \left\| [E_{\boldsymbol{\rho}}, \boldsymbol{\nabla}_\xi \boldsymbol{\rho}\, m] \right\|_{\mathcal{L}^q} \leq C \left\| \rho \right\|_{L^r}^{1-s} \left\| \rho \right\|_{W^{1,r}}^s \left\| \boldsymbol{\nabla}_\xi^2 \boldsymbol{\rho}\, m \right\|_{\mathcal{L}^q}.
$$

By Proposition 6.6, we get

$$
\frac{1}{\hbar} \left\| [E_{\boldsymbol{\rho}}, m] \boldsymbol{\nabla}_\xi \boldsymbol{\rho} \right\|_{\mathcal{L}^q} \leq C \left\| \boldsymbol{\nabla}_x \boldsymbol{\rho}\, m \right\|_{\mathcal{L}^r} \left\| \boldsymbol{\nabla}_\xi \boldsymbol{\rho}\, m \right\|_{\mathcal{L}^{r_1}}.
$$

Whence, the second term in the right-hand side of Equation (138) is bounded by

$$
\frac{1}{\hbar} \left\| [E_{\boldsymbol{\rho}}, \boldsymbol{\nabla}_\xi \boldsymbol{\rho}]\, m \right\|_{\mathcal{L}^q} \leq C \left\| \rho \right\|_{L^r}^{1-s} \left\| \rho \right\|_{W^{1,r}}^s \left\| \boldsymbol{\nabla}_\xi^2 \boldsymbol{\rho}\, m \right\|_{\mathcal{L}^q} + C \left\| \boldsymbol{\nabla}_x \boldsymbol{\rho}\, m \right\|_{\mathcal{L}^r} \left\| \boldsymbol{\nabla}_\xi \boldsymbol{\rho}\, m \right\|_{\mathcal{L}^{r_1}}.
$$

We turn now on the terms in which the contribution of the exchange term appears. By Proposition 6.8 we obtain

$$
(146) \qquad \frac{1}{\hbar} \left\| [\mathsf{X}_{\boldsymbol{\rho}}, m] \boldsymbol{\nabla}_\xi \boldsymbol{\nabla}_x \boldsymbol{\rho} \right\|_{\mathcal{L}^q} \leq C\hbar^{\frac{3}{2}-a} \left\| \boldsymbol{\nabla}_x \boldsymbol{\rho}\, m \right\|_{\mathcal{L}^2} \left\| \boldsymbol{\nabla}_\xi \boldsymbol{\nabla}_x \boldsymbol{\rho}\, m \right\|_{\mathcal{L}^q}.
$$

By Proposition 6.9 we get the bounds

$$
(147) \qquad \frac{1}{\hbar} \left\| [\mathsf{X}_{\boldsymbol{\nabla}_x \boldsymbol{\rho}}, \boldsymbol{\nabla}_\xi \boldsymbol{\rho}]\, m \right\|_{\mathcal{L}^q} \leq C\hbar^{3\left(\frac{1}{q}+\frac{1}{2}-\frac{1}{\mathfrak{b}}\right)} \left\| \boldsymbol{\nabla}_\xi \boldsymbol{\rho}\, m \right\|_{\mathcal{L}^\infty} \left\| \boldsymbol{\nabla}_x \boldsymbol{\rho}\, m \right\|_{\mathcal{L}^2}.
$$

$$
(148) \qquad \frac{1}{\hbar} \left\| [\mathsf{X}_{\boldsymbol{\nabla}_\xi \boldsymbol{\nabla}_x \boldsymbol{\rho}}, \boldsymbol{\nabla}_x \boldsymbol{\rho}]\, m \right\|_{\mathcal{L}^q} \leq C\hbar^{3\left(\frac{1}{q}+\frac{1}{2}-\frac{1}{\mathfrak{b}}\right)} \left\| \boldsymbol{\nabla}_x \boldsymbol{\rho}\, m \right\|_{\mathcal{L}^\infty} \left\| \boldsymbol{\nabla}_\xi \boldsymbol{\nabla}_x \boldsymbol{\rho}\, m \right\|_{\mathcal{L}^2}.
$$

Therefore, using Proposition 6.1 and estimates (145)–(148), we obtain

$$\frac{\mathrm{d}}{\mathrm{d}t} \left\| \boldsymbol{\nabla}_\xi \boldsymbol{\nabla}_x \boldsymbol{\rho}\, m \right\|_{\mathcal{L}^q} \leq C \left\| \boldsymbol{\nabla}_\xi \boldsymbol{\nabla}_x \boldsymbol{\rho}\, m \right\|_{\mathcal{L}^{r_1}} + C \left\| \boldsymbol{\nabla}_\xi^2 \boldsymbol{\rho}\, m \right\|_{\mathcal{L}^q} + C\, \hbar^{\frac{3}{2}-a} \left\| \boldsymbol{\nabla}_\xi \boldsymbol{\nabla}_x \boldsymbol{\rho}\, m \right\|_{\mathcal{L}^q}$$
$$+ C\, \hbar^{3\left(\frac{1}{q}+\frac{1}{2}-\frac{1}{6}\right)} \left\| \boldsymbol{\nabla}_\xi \boldsymbol{\rho}\, m \right\|_{\mathcal{L}^\infty} + C\, \hbar^{3\left(\frac{1}{q}+\frac{1}{2}-\frac{1}{6}\right)} \left\| \boldsymbol{\nabla}_\xi \boldsymbol{\nabla}_x \boldsymbol{\rho}\, m \right\|_{\mathcal{L}^2}$$

for $s = 1 - 3\left(\frac{1}{r'} - \frac{1}{6}\right)$ and with the constraints $\frac{1}{r} + \frac{1}{r_1} = \frac{1}{q} + \frac{1}{b'}$ and $\frac{1}{r} + \frac{1}{q} = \frac{1}{2}$. Now we define

$$N_{x,q}(t) := \left\| \boldsymbol{\nabla}_x^2 \boldsymbol{\rho}\, m \right\|_{\mathcal{L}^q}, \quad N_{v,q}(t) := \left\| \boldsymbol{\nabla}_\xi^2 \boldsymbol{\rho}\, m \right\|_{\mathcal{L}^q}, \quad N_{xv,q}(t) := \left\| \boldsymbol{\nabla}_\xi \boldsymbol{\nabla}_x \boldsymbol{\rho}\, m \right\|_{\mathcal{L}^q}$$

and denote by $N_q(t)$ the quantity

$$N_q(t) = N_{x,q}(t) + N_{v,q}(t) + N_{xv,q}(t).$$

Then we proceed as for the first-order gradients. Using Proposition 6.1, we obtain

$$(149) \qquad \begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t} N_{x,q}(t) &\leq C\, N_{r_1}(t) + C\, N_q(t) + C\, N_r(t) + C\, h^{\frac{3}{2}-a} N_q(t) \\ &\quad + C\, h^{3\left(\frac{1}{q}+\frac{1}{2}-\frac{1}{6}\right)} \left(N_2(t) + \left\| \boldsymbol{\nabla}_x \boldsymbol{\rho}\, m \right\|_{\mathcal{L}^\infty} \right). \end{aligned}$$

$$(150) \qquad \begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t} N_{v,q}(t) &\leq C\, N_{r_1}(t) + h^{\frac{3}{2}-a} N_q(t) \\ &\quad + C\, h^{3\left(\frac{1}{q}+\frac{1}{2}-\frac{1}{6}\right)} \left(N_2(t) + \left\| \boldsymbol{\nabla}_\xi \boldsymbol{\rho}\, m \right\|_{\mathcal{L}^\infty} \right). \end{aligned}$$

$$(151) \qquad \begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t} N_{vx,q}(t) &\leq C\, N_{r_1}(t) + C\, N_q(t) + C\, h^{\frac{3}{2}-a} N_q(t) \\ &\quad + C\, h^{3\left(\frac{1}{q}+\frac{1}{2}-\frac{1}{6}\right)} \left(N_2(t) + \left\| \boldsymbol{\nabla}_\xi \boldsymbol{\rho}\, m \right\|_{\mathcal{L}^\infty} \right). \end{aligned}$$

For $a \in \left[\frac{1}{2}, 1\right]$, we consider the quantity $F_{q,\infty}(t) := N_q(t) + \left\| \boldsymbol{\rho}\, m \right\|_{\mathcal{W}^{1,\infty}}$ and look for a Grönwall type inequality. From Equation (97) and Equation (98) with $q = \infty$, we obtain

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t} F_{q,\infty}(t) &\leq C\, F_{r_1,\infty}(t) + C\, F_{q,\infty}(t) + C\, F_{r,\infty}(t) \\ &\quad + C\, h^{\frac{3}{2}-a} F_{q,\infty}(t) + C\, h^{3\left(\frac{1}{q}+\frac{1}{2}-\frac{1}{6}\right)} F_{2,\infty}(t), \end{aligned}$$

where we used Equation (113) and Proposition 6.4 to show that $\left\| [E_{\boldsymbol{\rho}}, \boldsymbol{\rho}\, m] \right\|_{\mathcal{L}^\infty} \leq C\, \left\| \rho \right\|_{L^2}^{1/2} \left\| \nabla^2 \rho \right\|_{L^2}^{1/2} \leq C\, \left\| \boldsymbol{\nabla}_x^2 \boldsymbol{\rho}\, m \right\|_{\mathcal{L}^2}^{1/2}$. Since $(r, r_1) \in [2,4]^2$ standard interpolation allows to conclude by Grönwall's Lemma.

For $a \in \left(0, \frac{1}{2}\right)$, using that $\boldsymbol{\rho} \in \mathcal{W}^{1,4}(m)$ by Proposition 6.1 and that

$$\left\| \boldsymbol{\nabla}_x \boldsymbol{\rho}\, m \right\|_{\mathcal{L}^\infty} \leq C\, h^{-\frac{3}{4}} \left\| \boldsymbol{\nabla}_x \boldsymbol{\rho}\, m \right\|_{\mathcal{L}^4}, \qquad \left\| \boldsymbol{\nabla}_\xi \boldsymbol{\rho}\, m \right\|_{\mathcal{L}^\infty} \leq C h^{-\frac{3}{4}} \left\| \boldsymbol{\nabla}_\xi \boldsymbol{\rho}\, m \right\|_{\mathcal{L}^4},$$

we get

$$(152) \qquad \begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t} N_{x,q}(t) &\leq C\, N_{r_1}(t) + C\, N_q(t) + C\, N_r(t) + C\, h^{\frac{3}{2}-a} N_q(t) \\ &\quad + C\, h^{3\left(\frac{1}{q}+\frac{1}{2}-\frac{1}{6}\right)} N_2(t) + C\, h^{3\left(\frac{1}{q}+\frac{1}{2}-\frac{1}{6}-\frac{1}{4}\right)} M_4(t), \end{aligned}$$

where $M_4(t)$ is bounded by Proposition 6.1. We proceed analogously for $N_{v,q}$ and $N_{vx,q}$. Hence, as for the first-order gradients, we consider $N_2(t) + N_4(t)$ and close the Grönwall type inequality by observing that $r, r_1 \in [2,4]$ and that we can actually bound $N_{r_1}(t)$ and $N_r(t)$ by interpolation with $N_2(t)$ and $N_4(t)$. Notice that we have the constraint

$$\left(\frac{1}{q} + \frac{1}{2} - \frac{1}{b} - \frac{1}{4} \right) > 0,$$

which leads to $a < \frac{1}{2}$ when $q = 4$. We conclude that $\boldsymbol{\rho} \in \mathcal{W}^{2,2}(m) \cap \mathcal{W}^{2,4}(m)$ for $a \in \left(0, \frac{1}{2}\right)$. $\qquad\square$

Proof of Proposition 6.3. We observe that analogously to (96), (97) and (98), the following bounds hold

$$\frac{\mathrm{d}}{\mathrm{d}t} \left\| \sqrt{\boldsymbol{\rho}}\, m \right\|_q \leq \frac{1}{\hbar} \left\| [V_{\boldsymbol{\rho}}, m]\, \sqrt{\boldsymbol{\rho}} \right\|_q + \frac{1}{\hbar} \left\| \left[h^3 X_{\boldsymbol{\rho}}, m \right] \sqrt{\boldsymbol{\rho}} \right\|_q,$$

$$
\begin{aligned}
(153) \qquad \frac{\mathrm{d}}{\mathrm{d}t} \left\| \boldsymbol{\nabla}_x \sqrt{\boldsymbol{\rho}}\, m \right\|_q &\leq \frac{1}{\hbar} \left\| [V_{\boldsymbol{\rho}}, m]\, \boldsymbol{\nabla}_x \sqrt{\boldsymbol{\rho}} \right\|_q + \frac{1}{\hbar} \left\| [E_{\boldsymbol{\rho}}, \sqrt{\boldsymbol{\rho}}]\, m \right\|_q \\
&\quad + \frac{1}{\hbar} \left\| \left[h^3 X_{\boldsymbol{\rho}}, m \right] \boldsymbol{\nabla}_x \sqrt{\boldsymbol{\rho}} \right\|_q + \frac{1}{\hbar} \left\| \left[h^3 X_{\boldsymbol{\nabla}_x \boldsymbol{\rho}}, \sqrt{\boldsymbol{\rho}} \right] m \right\|_q,
\end{aligned}
$$

and

$$
\begin{aligned}
(154) \qquad \frac{\mathrm{d}}{\mathrm{d}t} \left\| \boldsymbol{\nabla}_\xi \sqrt{\boldsymbol{\rho}}\, m \right\|_q &\leq \frac{1}{\hbar} \left\| [V_{\boldsymbol{\rho}}, m]\, \boldsymbol{\nabla}_\xi \sqrt{\boldsymbol{\rho}} \right\|_q + \left\| \boldsymbol{\nabla}_x \sqrt{\boldsymbol{\rho}}\, m \right\|_q \\
&\quad + \frac{1}{\hbar} \left\| \left[h^3 X_{\boldsymbol{\rho}}, m \right] \boldsymbol{\nabla}_\xi \sqrt{\boldsymbol{\rho}} \right\|_q + \frac{1}{\hbar} \left\| \left[h^3 X_{\boldsymbol{\nabla}_\xi \boldsymbol{\rho}}, \sqrt{\boldsymbol{\rho}} \right] m \right\|_q.
\end{aligned}
$$

As in Proposition 6.1, we look for a Grönwall type inequality. To this end, we define

$$\widetilde{M}_q(t) = \left\| \sqrt{\boldsymbol{\rho}} \right\|_{\mathcal{L}^2(m)} + \left\| \sqrt{\boldsymbol{\rho}} \right\|_{\mathcal{L}^q(m)},$$

for $q \in [2, \infty]$ and notice that, because of Propositions 6.7 and 6.8, we have

$$\frac{\mathrm{d}}{\mathrm{d}t} \widetilde{M}_q(t) \leq C\, M_r\, \widetilde{M}_{\tilde{r}} + C\, M_2\, \widetilde{M}_q,$$

that implies the boundedness of $\widetilde{M}_q(t)$ for $q \in [2, \infty]$ thanks to Proposition 6.1.

We now define the quantity

$$\widetilde{N}_q(t) = \left\| \sqrt{\boldsymbol{\rho}} \right\|_{\dot{\mathcal{W}}^{1,2}(m)} + \left\| \sqrt{\boldsymbol{\rho}} \right\|_{\dot{\mathcal{W}}^{1,q}(m)},$$

for $q \in [2, \infty]$ and using Equations (153) and (154) we compute

$$(155) \qquad\qquad \frac{\mathrm{d}}{\mathrm{d}t} \left(\widetilde{N}_2(t) + \widetilde{N}_q(t) \right).$$

The contributions due to the direct term in (155) can be estimated in terms of M_{r_1} and $\widetilde{N}_{r_2}$ by Proposition 6.7, in terms of $M_r^{1+\theta}$ (for $\theta \in (0,1)$) and $\widetilde{N}_q$ by Proposition 6.5, together with $\widetilde{N}_{r_1}$ and $\widetilde{N}_{r_2}$ by Proposition 6.6. The contributions due to the exchange term in (155) can be estimated in terms of M_2 and $\widetilde{N}_q$ by Proposition 6.8, and in terms of $\widetilde{M}_q$, $\widetilde{N}_q$ and N_2 by Proposition 6.9. Hence, in the same spirit of the proofs of Propositions 6.1 and 6.2, using the results of Proposition 6.1 and Proposition 6.2, we conclude by Grönwall's Lemma obtaining boundedness of $\widetilde{N}_q$ for $q \in [2, \infty]$. $\qquad\square$

Part III. Mean-Field Limit

7. Scaling

In order to define the Bogoliubov rotation as explained in Section 4.3, we define

(156) $$\omega := \lambda\,\boldsymbol{\rho} \quad \text{with } \lambda = N\,h^3$$

so that $\text{Tr}(\omega) = N$ and $0 \leq \omega \leq \lambda\mathcal{C}_\infty \leq 1$. Remark that in the critical scaling $N = C\,h^{-3}$, λ is a constant, while in the other cases when $N = h^{-c}$ with $c < 3$ we have $\lambda \to 0$. We also define

$$v = \sqrt{\omega} \quad \text{and} \quad u = \sqrt{1 - \omega},$$

which are well defined bounded positive operators since $0 \leq \omega \leq 1$. Remark that with these definitions, we obtain the following behavior for the Schatten norms for $p \in [1, \infty]$

$$\|\omega\|_p = \mathcal{C}_p\,N\,h^{\frac{3}{p'}}$$

$$\|v\|_p = \mathcal{C}_{p/2}^{1/2}\,N^{1/2}\,h^{3\left(\frac{1}{2} - \frac{1}{p}\right)},$$

where $\mathcal{C}_p = \|\boldsymbol{\rho}\|_{\mathcal{L}^p}$ and $p' = \frac{p}{p-1}$. The operator u satisfies $\|u\|_\infty \leq 1$, but of course u is not bounded in other Schatten norms. However, it is possible to prove that $0 \leq 1 - u \leq \omega$, hence $1 - u$ is of the same order of magnitude as ω. Since $\boldsymbol{\nabla}_\eta u = -\boldsymbol{\nabla}_\eta(1 - u)$, it explains why we can expect the gradients of u to be of the same order as $\boldsymbol{\nabla}_\eta\omega$, as indicated more precisely in the following lemma.

Lemma 7.1. *Assume* $\|\omega\|_\infty = \lambda\,\mathcal{C}_\infty < 1$. *Then*

$$C\,\|\boldsymbol{\nabla}_\eta u\,m\|_p \leq \|\boldsymbol{\nabla}_\eta\,\omega\,m\|_p + \|\omega\,\boldsymbol{\nabla}_\eta m\|_p\,,$$

with $C = 2\sqrt{1 - \lambda\mathcal{C}_\infty}$. *In particular, it implies that*

$$C\,\|\boldsymbol{\nabla}_\xi u\,m\|_p \leq \mathcal{D}_p\,N\,h^{\frac{3}{p'}}$$

where $\mathcal{D}_p = \|\boldsymbol{\nabla}_\xi\,\boldsymbol{\rho}\,m\|_{\mathcal{L}^p} + \|\boldsymbol{\rho}\,\boldsymbol{\nabla}_\xi m\|_{\mathcal{L}^p}$ *is of order* 1 *in the semiclassical limit.*

Proof. Since $\|\omega\|_\infty < 1$, we can write $u = (1 - \omega)^{\frac{1}{2}} = \sum_{n=0}^\infty \binom{1/2}{n}(-1)^n\,\omega^n$. Therefore, for $\eta \in \{x, \xi\}$, we obtain

$$\|\boldsymbol{\nabla}_\eta u\,m\|_p = \|\boldsymbol{\nabla}_\eta(u - 1)\,m\|_p \leq \sum_{n=1}^\infty \left|\binom{1/2}{n}\right| \|\boldsymbol{\nabla}_\eta(\omega^n\,m)\|_p\,.$$

Expanding the gradient with the product rule for commutators gives

$$\boldsymbol{\nabla}_\eta(\omega^n\,m) = \omega^n\,\boldsymbol{\nabla}_\eta m + \sum_{k=1}^n \omega^{k-1}\,(\boldsymbol{\nabla}_\eta\omega)\,\omega^{n-k}$$

which leads to

$$\|\boldsymbol{\nabla}_\eta u\,m\|_p \leq \sum_{n=1}^\infty \left|\binom{1/2}{n}\right| n\,\|\omega\|_\infty^{n-1}\left(\|\boldsymbol{\nabla}_\eta\,\omega\,m\|_p + \|\omega\,\boldsymbol{\nabla}_\eta m\|_p\right).$$

Moreover, for $n \geq 1$, $\left|\binom{1/2}{n}\right| = (-1)^{n-1}\binom{1/2}{n}$ and $\binom{1/2}{n} = \frac{1}{2n}\binom{-1/2}{n-1}$, from which we deduce

$$\sum_{n=1}^\infty \left|\binom{1/2}{n}\right| n\,\|\omega\|_\infty^{n-1} \leq \frac{1}{2}\sum_{n=1}^\infty \binom{-1/2}{n-1}(-1)^{n-1}\,\|\omega\|_\infty^{n-1} = \frac{1}{2\sqrt{1 - \|\omega\|_\infty}}$$

and the proof follows by combining the two last inequalities.   □

8. Preliminary Inequalities

In this section, we provide estimates which are crucial for controlling the growth of the particle number operator with respect to the fluctuation dynamics in the subsequent sections.

As a preliminary, let us begin by defining some convenient notations. For any pair $(\sigma, \sigma') \in \{l, r\}^2$ and a bounded operator $O : \mathfrak{h}_{\sigma'} \to \mathfrak{h}_\sigma$, we generalize the standard notation of the second quantization of the one-particle operator by

$$(157a) \qquad \mathrm{d}\Gamma_{\sigma,\sigma'}(O) = \int_{\mathbb{R}^6} O(x,y)\, a_{x,\sigma}^* \, a_{y,\sigma'} \, \mathrm{d}x \, \mathrm{d}y$$

$$(157b) \qquad \mathrm{d}\Gamma_{\sigma,\sigma'}^+(O) = \int_{\mathbb{R}^6} O(x,y)\, a_{x,\sigma}^* \, a_{y,\sigma'}^* \, \mathrm{d}x \, \mathrm{d}y$$

$$(157c) \qquad \mathrm{d}\Gamma_{\sigma,\sigma'}^-(O) = \int_{\mathbb{R}^6} O(x,y)\, a_{x,\sigma} \, a_{y,\sigma'} \, \mathrm{d}x \, \mathrm{d}y$$

where the operators are expressed in terms of operator-valued distributions (45). When $\sigma = \sigma'$, we write $\mathrm{d}\Gamma_\sigma^\circ := \mathrm{d}\Gamma_{\sigma,\sigma}^\circ$ where $\circ$ denotes either $+$, $-$, or null. Moreover, we have the relations:

$$(158) \qquad \mathrm{d}\Gamma_{\sigma,\sigma'}(O)^* = \mathrm{d}\Gamma_{\sigma',\sigma}(O^*) \quad \text{and} \quad \mathrm{d}\Gamma_{\sigma,\sigma'}^+(O)^* = \mathrm{d}\Gamma_{\sigma',\sigma}^-(O^*).$$

We begin by extending [11, Lemma 4.2] to the case of Schatten class operators between different Hilbert spaces. See [74, Chapter 7].

Lemma 8.1. *Let $(\sigma', \sigma) \in \{l, r\}^2$ and $O : \mathfrak{h}_{\sigma'} \to \mathfrak{h}_\sigma$ be a compact operator. Then, for every $p \in [1, \infty]$, we have the estimate*

$$(159) \qquad \left\| \mathrm{d}\Gamma_\sigma(O)\Psi \right\|_{\mathcal{G}} \le \|O\|_p \left\| \mathcal{N}^{\frac{1}{p'}} \Psi \right\|_{\mathcal{G}}$$

for every $\Psi \in \mathcal{G}$ where $\mathcal{N} = \mathrm{d}\Gamma_l(1) + \mathrm{d}\Gamma_r(1)$. Moreover, for $p \in [1, 2]$ we have the estimates

$$(160a) \qquad \left\| \mathrm{d}\Gamma_{\sigma,\sigma'}^-(O)\Psi \right\|_{\mathcal{G}} \le \|O\|_p \left\| \mathcal{N}^{\frac{1}{p'}} \Psi \right\|_{\mathcal{G}},$$

$$(160b) \qquad \left\| \mathrm{d}\Gamma_{\sigma,\sigma'}^+(O)\Psi \right\|_{\mathcal{G}} \le \|O\|_p \left\| (\mathcal{N}+2)^{\frac{1}{p'}} \Psi \right\|_{\mathcal{G}}$$

for every $\Psi \in \mathcal{G}$.

Proof. The case of inequality (159) with $p = \infty$ and the case of inequalities (160a) and (160b) with $p = 2$ are proved in [11, Lemma 4.2].

For any compact O, we can write down a singular value decomposition of O, that is, $O = \sum_j \mu_j \langle \phi_j, \cdot \rangle \varphi_j$ where $(\phi_j)_{j \in \mathbb{N}} \subset \mathfrak{h}_{\sigma'}$ and $(\varphi_j)_{j \in \mathbb{N}} \subset \mathfrak{h}_\sigma$ are two orthonormal sets, and $\mu_j \ge 0$ are the singular values of O (see e.g. [74, Theorem 7.6]). Thus, using the notation $a^\sharp$ to denote either a or a^*, we have

$$\left\| \int_{\mathbb{R}^6} O(x,y)\, a_{x,\sigma}^\sharp \, a_{y,\sigma'}^\sharp \, \mathrm{d}x \, \mathrm{d}y \right\|_\infty \le \sum_j \mu_j \left\| a_\sigma^\sharp(\tilde{\phi}_j)\, a_{\sigma'}^\sharp(\tilde{\varphi}_j) \right\|_\infty$$

where $\tilde{\phi}_j$ is either ϕ_j or $\bar{\phi}_j$. Since $\left\| a_\sigma^\sharp(\varphi) \right\|_\infty \le \|\varphi\|_{L^2} = 1$, we obtain the estimate

$$\left\| \int_{\mathbb{R}^6} O(x,y)\, a_{x,\sigma}^\sharp \, a_{y,\sigma'}^\sharp \, \mathrm{d}x \, \mathrm{d}y \right\|_\infty \le \sum_j \mu_j = \|O\|_1 \, .$$

Hence, for any $\circ \in \{+, -, \ \}$, we have the estimate $\left\| d\Gamma^{\circ}_{\sigma,\sigma'}(O)\Psi \right\|_{\mathcal{G}} \leq \|O\|_1 \|\Psi\|_{\mathcal{G}}$. Finally, we deduce the desired result by weighted interpolation. $\qquad \square$

As an immediate application, we can bound the expectation values of the operators (157) in terms of the expectation values of powers of the number operator.

Lemma 8.2. *For any $p \in [1, \infty]$, we have the estimate*

$$(161) \qquad \langle \Psi \,|\, d\Gamma_\sigma(O)\Psi \rangle_{\mathcal{G}} \leq \|O\|_p \left\langle \Psi \,\Big|\, \mathcal{N}^{\frac{1}{p'}}\Psi \right\rangle_{\mathcal{G}}$$

for every $\Psi \in \mathcal{G}$. Similarly, for any $p \in [1, 2]$, we have the estimates

$$(162a) \qquad \left\langle \Psi \,\big|\, d\Gamma^{+}_{\sigma,\sigma'}(O)\Psi \right\rangle_{\mathcal{G}} \leq 2^{\frac{1}{2p'}} \|O\|_p \left\langle \Psi \,\Big|\, (\mathcal{N}+1)^{\frac{1}{p'}}\Psi \right\rangle_{\mathcal{G}}$$

$$(162b) \qquad \left\langle \Psi \,\big|\, d\Gamma^{-}_{\sigma,\sigma'}(O)\Psi \right\rangle_{\mathcal{G}} \leq 2^{\frac{1}{2p'}} \|O\|_p \left\langle \Psi \,\Big|\, (\mathcal{N}+1)^{\frac{1}{p'}}\Psi \right\rangle_{\mathcal{G}}$$

for every $\Psi \in \mathcal{G}$.

Proof. For $\epsilon > 0$, one has the equality

$$\langle \Psi \,|\, d\Gamma(O)\,\Psi \rangle_{\mathcal{G}} = \left\langle (\mathcal{N}+\epsilon)^{\frac{1}{2p'}}\Psi \,\Big|\, (\mathcal{N}+\epsilon)^{-\frac{1}{2p'}}\, d\Gamma(O)\,\Psi \right\rangle_{\mathcal{G}}$$
$$= \left\langle (\mathcal{N}+\epsilon)^{\frac{1}{2p'}}\Psi \,\Big|\, d\Gamma(O)\,(\mathcal{N}+\epsilon)^{-\frac{1}{2p'}}\Psi \right\rangle_{\mathcal{G}}.$$

Applying the Cauchy-Schwarz inequality and Lemma 8.1 yields

$$\langle \Psi \,|\, d\Gamma(O)\,\Psi \rangle_{\mathcal{G}} \leq \|O\|_p \left\| (\mathcal{N}+\epsilon)^{\frac{1}{2p'}}\Psi \right\|_{\mathcal{G}} \left\| \mathcal{N}^{\frac{1}{p'}}\,(\mathcal{N}+\epsilon)^{-\frac{1}{2p'}}\Psi \right\|_{\mathcal{G}}$$
$$\leq \|O\|_p \left\| (\mathcal{N}+\epsilon)^{\frac{1}{2p'}}\Psi \right\|_{\mathcal{G}} \left\| \mathcal{N}^{\frac{1}{2p'}}\Psi \right\|_{\mathcal{G}}.$$

Then inequality (161) follows by passing to the limit $\epsilon \to 0$. With a similar argument and the observation that for any nice function g, $g(\mathcal{N})\,a^* = a^*\,g(\mathcal{N}+1)$, we obtain

$$\left\langle \Psi \,\big|\, d\Gamma^{+}_{\sigma,\sigma'}(O)\Psi \right\rangle_{\mathcal{G}} \leq \|O\|_p \left\| \mathcal{N}^{\frac{1}{2p'}}\Psi \right\|_{\mathcal{G}} \left\| (\mathcal{N}+2)^{\frac{1}{2p'}}\Psi \right\|_{\mathcal{G}}$$

from which we deduce inequality (162a). Inequality (162b) follows immediately from (158). $\qquad \square$

9. Quantum Fluctuations and the Mean-Field Limit

In this section, we prove how the error of the mean-field approximation of the fermionic system can be controlled by the mean number of particles of the fluctuation dynamics about a quasi-free state. To this end, it suffices for us to specialize our study to the state vector

$$(163) \qquad \Psi_{\mathrm{fluc}} = \mathsf{R}^*_{\boldsymbol{\rho}}\Phi_t = \mathsf{R}^*_{\boldsymbol{\rho}}e^{-i(t/\hbar)\mathsf{L}_N}\mathsf{R}_{\boldsymbol{\rho}_0}\Psi^{\mathrm{in}}$$

and consider its mean number of particles

$$\langle \Psi_{\mathrm{fluc}} \,|\, \mathcal{N}\Psi_{\mathrm{fluc}} \rangle_{\mathcal{G}} = \left\| \mathcal{N}^{\frac{1}{2}}\Psi_{\mathrm{fluc}} \right\|^2_{\mathcal{G}}.$$

More specifically, we control the error of the mean-field approximation by the norm

$$(164) \qquad \|\Psi_{\mathrm{fluc}}\|_{\mathcal{G}_k} := \left\| (\mathcal{N}+1)^k\,\Psi_{\mathrm{fluc}} \right\|_{\mathcal{G}}$$

for $k > 0$, which allows us to handle additional small error terms. For the rest of this section, we drop the subscript of the fluctuation vector and the dependence on time to reduce cumbersome notations.

One can see that quantity (164) controls the difference of the one-particle density operators in the sense of the following proposition.

Proposition 9.1. *Define Ψ and $\boldsymbol{\rho}_{N:1}$ as in the Theorem 4.1. Then, for any $p \in [1, \infty]$, we have the estimate*

$$(165) \qquad \|\boldsymbol{\rho}_{N:1} - \boldsymbol{\rho}\|_{\mathcal{L}^p} \leq \frac{C_p}{\min(N^{\frac{1}{2}}, N\,h^{\frac{3}{p'}})} \|\Psi\|_{\mathcal{G}_{\frac{1}{2p}}}^2$$

where $C_p = 2^{2 + \frac{1}{2p}}$ if $p \geq 2$ and $C_p = 2 + 2^{\frac{5}{4}} \mathcal{C}_{\frac{p}{2-p}}^{\frac{1}{2}}$ if $p \leq 2$.

Proof. Following the proof of [14, Proof of Theorem 2.1], we have

$$Nh^3 \boldsymbol{\rho}_{N:1}(x, y) - \omega(x, y) = \left\langle \Psi_N \,\middle|\, a_{y,l}^* a_{x,l} \Psi_N \right\rangle_{\mathcal{G}} = \left\langle \Psi \,\middle|\, \mathsf{R}_{\boldsymbol{\rho}}^* a_{y,l}^* a_{x,l} \mathsf{R}_{\boldsymbol{\rho}} \Psi \right\rangle_{\mathcal{G}}$$

$$= \left\langle \Psi \,\middle|\, \left(a_l^*(u_y)\, a_l(u_x) - a_l^*(u_y)\, a_r^*(\overline{v}_x) \right.\right.$$
$$\left.\left. - a_r(\overline{v}_y)\, a_l(u_x) - a_r^*(\overline{v}_x)\, a_r(\overline{v}_y) \right) \Psi \right\rangle_{\mathcal{G}}.$$

Since $\boldsymbol{\rho} = \frac{1}{Nh^3} \omega$, we deduce

$$(166) \qquad (\boldsymbol{\rho}_{N:1} - \boldsymbol{\rho})(x, y) = \frac{1}{Nh^3} \langle \Psi \,|\, \left(a_l^*(u_y)\, a_l(u_x) - a_l^*(u_y)\, a_r^*(\overline{v}_x) \right.$$
$$\left. - a_r(\overline{v}_y)\, a_l(u_x) - a_r^*(\overline{v}_x)\, a_r(\overline{v}_y) \right) \Psi \rangle_{\mathcal{G}}.$$

In particular, pairing operator (166) with an observable O yields

$$\mathrm{Tr}(O\,(\boldsymbol{\rho}_{N:1} - \boldsymbol{\rho}))$$
$$= \frac{1}{N\,h^d} \left\langle \Psi \,\middle|\, \left(\mathrm{d}\Gamma_l(u\,O\,u) - \mathrm{d}\Gamma_r\left(\overline{v}\,\overline{O}^*v\right) - \mathrm{d}\Gamma_{l,r}^+(v\,O\,u) - \mathrm{d}\Gamma_{r,l}^-(v\,O\,u) \right) \Psi \right\rangle_{\mathcal{G}}.$$

In the case $p \in [2, \infty]$, we apply the fact that $\|u\|_\infty \leq 1, \|v\|_\infty \leq 1$, and Lemma 8.2 to deduce the estimate

$$\mathrm{Tr}(O\,(\boldsymbol{\rho}_{N:1} - \boldsymbol{\rho})) \leq \frac{2^{2 + \frac{1}{2p}}}{N\,h^3} \|O\|_{p'} \left\langle \Psi \,\middle|\, (\mathcal{N} + 1)^{\frac{1}{p}}\, \Psi \right\rangle_{\mathcal{G}}.$$

Then, by duality and the fact that $\|\boldsymbol{\mu}\|_{\mathcal{L}^p} = h^{\frac{3}{p}} \|\boldsymbol{\mu}\|_p$, we obtain the result when $p \geq 2$.

For $p \in [1, 2]$, we can bound the terms with $\mathrm{d}\Gamma_l(u\,O\,u)$ and $\mathrm{d}\Gamma_r\left(\overline{v}\,\overline{O}^*v\right)$ as in the previous case. For the other two terms, we begin by applying Hölder's inequality to get $\|v\,O\,u\|_2 \leq \|v\|_r \|O\|_{p'}$ where $\frac{1}{r} = \frac{1}{2} - \frac{1}{p'}$. Then, by Lemma 8.2, it follows that

$$\left| \left\langle \Psi \,\middle|\, \left(\mathrm{d}\Gamma_{l,r}^+(v\,O\,u) + \mathrm{d}\Gamma_{r,l}^-(v\,O\,u) \right) \Psi \right\rangle_{\mathcal{G}} \right| = 2 \left| \left\langle \Psi \,\middle|\, \mathrm{d}\Gamma_{r,l}^-(v\,O\,u)\Psi \right\rangle_{\mathcal{G}} \right|$$
$$\leq 2^{\frac{5}{4}} \|v\|_r \|O\|_{p'} \left\langle \Psi \,\middle|\, (\mathcal{N} + 1)^{\frac{1}{2}}\, \Psi \right\rangle_{\mathcal{G}}.$$

Since $\|v\|_r = \mathcal{C}_{\frac{r}{2}}^{\frac{1}{2}} N^{\frac{1}{2}} h^{3\left(\frac{1}{2} - \frac{1}{r}\right)}$ and $\frac{1}{2} - \frac{1}{r} = \frac{1}{p'}$, this implies

$$\left| \left\langle \Psi \,\middle|\, \left(\mathrm{d}\Gamma_{l,r}^+(v\,O\,u) + \mathrm{d}\Gamma_{r,l}^-(v\,O\,u) \right) \Psi \right\rangle_{\mathcal{G}} \right| \leq 2^{\frac{5}{4}} \|O\|_{p'} \mathcal{C}_{\frac{r}{2}}^{\frac{1}{2}} N^{\frac{1}{2}} h^{\frac{3}{p'}} \left\langle \Psi \,\middle|\, (\mathcal{N} + 1)^{\frac{1}{2}}\, \Psi \right\rangle_{\mathcal{G}}.$$

So, we have the estimate

$$\mathrm{Tr}(O\left(\boldsymbol{\rho}_{N:1} - \boldsymbol{\rho}\right)) \leq \|O\|_{p'} \left(\frac{2}{N\,h^3} + \frac{2^{\frac{5}{4}} \mathcal{C}_{\frac{r}{2}}^{\frac{1}{2}}}{N^{\frac{1}{2}}\,h^{\frac{3}{p}}} \right) \left\langle \Psi \,\middle|\, (\mathcal{N}+1)^{\frac{1}{p}}\, \Psi \right\rangle_{\mathcal{G}}$$

which yields the desired result. $\qquad\square$

To better understand what it means to have a small number of particles after having performed the Bogoliubov transformation, it is useful to see how this latter acts on the number operator. From the definition (77), we obtain the following formula for $\sigma \in \{\, r, l\, \}$

$$(167) \qquad \mathsf{R}_{\boldsymbol{\rho}} \mathcal{N}_\sigma \mathsf{R}_{\boldsymbol{\rho}}^* = \mathsf{A}_\sigma + \mathsf{C} + \mathsf{C}^*,$$

where

$$\mathsf{A}_\sigma = \mathcal{N}_\sigma + N - \mathrm{d}\Gamma(\omega \oplus \overline{\omega})\,, \qquad\qquad \mathsf{C} = \mathrm{d}\Gamma_{r,l}^+(uv)\,.$$

Since changing v by $-v$ changes $\mathsf{R}_{\boldsymbol{\rho}}$ to $\mathsf{R}_{\boldsymbol{\rho}}^*$, we deduce similarly that

$$(168) \qquad \mathsf{R}_{\boldsymbol{\rho}}^* \mathcal{N}_\sigma \mathsf{R}_{\boldsymbol{\rho}} = \mathsf{A}_\sigma - \mathsf{C} - \mathsf{C}^*.$$

From this formulas, we deduce the following interesting fact: the operator $\boldsymbol{\nu}_{\boldsymbol{\rho}}$ acting on the single Fock space $\mathcal{F}$ and corresponding to the Bogoliubov transform of the vacuum in $\mathcal{G}$ commutes with the number of particles operator .

Lemma 9.1. *Let* $\boldsymbol{\nu}_{\boldsymbol{\rho}} := \mathsf{I}_{\mathcal{G}}^{-1}(\mathsf{R}_{\boldsymbol{\rho}}\,\Omega)$. *Then*

$$[\mathcal{N}, \boldsymbol{\nu}_{\boldsymbol{\rho}}] = 0.$$

This also implies that $\boldsymbol{\rho}_{N,\boldsymbol{\rho}} := |\boldsymbol{\nu}_{\boldsymbol{\rho}}|^2$ *commutes with* $\mathcal{N}$.

Proof. Let $\Phi_{\boldsymbol{\rho}} := \mathsf{R}_{\boldsymbol{\rho}}\,\Omega = \mathsf{I}_{\mathcal{G}}\boldsymbol{\nu}_{\boldsymbol{\rho}}$. Then we obtain $\mathcal{N}_l \Phi_{\boldsymbol{\rho}} = \mathsf{I}_{\mathcal{G}}(\mathcal{N}\boldsymbol{\nu}_{\boldsymbol{\rho}})$ and $\mathcal{N}_r \Phi_{\boldsymbol{\rho}} = \mathsf{I}_{\mathcal{G}}(\boldsymbol{\nu}_{\boldsymbol{\rho}}\mathcal{N})$, therefore

$$\mathsf{I}_{\mathcal{G}}^{-1}[\mathcal{N}, \boldsymbol{\nu}_{\boldsymbol{\rho}}] = (\mathcal{N}_l - \mathcal{N}_r)\,\Phi_{\boldsymbol{\rho}} = (\mathcal{N}_l - \mathcal{N}_r)\,\mathsf{R}_{\boldsymbol{\rho}}\,\Omega.$$

Now we use Formula (168), yielding

$$(\mathcal{N}_l - \mathcal{N}_r)\,\mathsf{R}_{\boldsymbol{\rho}}\,\Omega = \mathsf{R}_{\boldsymbol{\rho}}\,(\mathsf{A}_l - \mathsf{A}_r)\,\Omega = \mathsf{R}_{\boldsymbol{\rho}}\,(\mathcal{N}_l - \mathcal{N}_r)\,\Omega = 0,$$

which proves the result. $\qquad\square$

Since the number operator on the double Fock space $\mathcal{G}$ is given by $\mathcal{N} = \mathcal{N}_l + \mathcal{N}_r$, Equations (167) and (168) imply

$$(169) \qquad \mathsf{R}_{\boldsymbol{\rho}} \mathcal{N} \mathsf{R}_{\boldsymbol{\rho}}^* = \mathsf{A} + 2\mathsf{C} + 2\mathsf{C}^*$$

$$(170) \qquad \mathsf{R}_{\boldsymbol{\rho}}^* \mathcal{N} \mathsf{R}_{\boldsymbol{\rho}} = \mathsf{A} - 2\mathsf{C} - 2\mathsf{C}^*$$

with $\mathsf{A} = \mathsf{A}_l + \mathsf{A}_r = \mathcal{N} + 2N - 2\,\mathrm{d}\Gamma(\omega \oplus \overline{\omega})$. This allows us to prove the following bounds.

Lemma 9.2. *Let* $k \in \mathbb{N}$. *Then for any* $\Psi \in \mathcal{G}_k$

$$\left\| \mathcal{N}^k \mathsf{R}_{\boldsymbol{\rho}}^* \Psi \right\|_{\mathcal{G}} \leq 3^k \left\| (\mathcal{N} + 2N + 2k)^k\, \Psi \right\|_{\mathcal{G}}$$

$$\left\| \mathcal{N}^k \mathsf{R}_{\boldsymbol{\rho}} \Psi \right\|_{\mathcal{G}} \leq 3^k \left\| (\mathcal{N} + 2N + 2k)^k\, \Psi \right\|_{\mathcal{G}}.$$

Remark 9.1. *With a similar proof, one obtains*

$$\left\|\mathsf{R}_{\boldsymbol{\rho}}^*\Psi\right\|_{\mathcal{G}_{1/2}} \le 3^{\frac{1}{2}} \left\|(\mathcal{N}+2N)^{\frac{1}{2}}\,\Psi\right\|_{\mathcal{G}}$$

and so by interpolation, for any $s \in [0, 1/2]$,

$$(171) \qquad \left\|\mathsf{R}_{\boldsymbol{\rho}}^*\Psi\right\|_{\mathcal{G}_s} \le 3^s \left\|(\mathcal{N}+2N)^s\,\Psi\right\|_{\mathcal{G}}.$$

Proof of Lemma 9.2. Since $\mathsf{R}_{\boldsymbol{\rho}}^*\mathcal{N}\mathsf{R}_{\boldsymbol{\rho}}$ and $\mathsf{R}_{\boldsymbol{\rho}}\mathcal{N}\mathsf{R}_{\boldsymbol{\rho}}^*$ are two positive operators, by doing the sum of the two above identities, we deduce that A is also a positive operator. Therefore, since $\mathrm{d}\Gamma(\omega \oplus \overline{\omega})$ is a positive operator, from the definition of A, we obtain

$$0 \le \mathsf{A} \le \mathcal{N} + 2N,$$

which implies that for any $\Psi \in \mathcal{G}_1$, $\left\|\mathsf{A}^{1/2}\Psi\right\|_{\mathcal{G}} \le \left\|(\mathcal{N}+2N)^{1/2}\,\Psi\right\|_{\mathcal{G}}$. Since A commutes with $\mathcal{N}+2N$, we deduce that

$$\left\|\mathsf{A}\Psi\right\|_{\mathcal{G}} \le \left\|(\mathcal{N}+2N)\,\Psi\right\|_{\mathcal{G}}.$$

On the other hand, by Inequalities (160a) and (160b) and the fact that $\|u\|_\infty \le 1$ and $\|v\|_2 = N^{\frac{1}{2}}$, we have

$$\left\|\mathsf{C}^*\Psi\right\|_{\mathcal{G}} \le \|uv\|_2 \left\|(\mathcal{N}+2)^{1/2}\,\Psi\right\|_{\mathcal{G}} \le \frac{1}{2}\left\|(\mathcal{N}+N+2)\,\Psi\right\|_{\mathcal{G}}$$

and similarly, $\left\|\mathsf{C}\Psi\right\|_{\mathcal{G}} \le \frac{1}{2}\left\|(\mathcal{N}+N)\,\Psi\right\|_{\mathcal{G}}$. From these inequalities, using the fact that A commutes with $\mathcal{N}$ and the fact that $\mathcal{N}\mathsf{C} = \mathsf{C}\,(\mathcal{N}-2)$ and $\mathcal{N}\mathsf{C}^* = \mathsf{C}^*\,(\mathcal{N}+2)$, we deduce that for any $j \in \mathbb{N}$, by defining $c_j := 2N + 2j$, we have

$$\left\|(\mathcal{N}+c_j)^j\,\mathsf{R}_{\boldsymbol{\rho}}\mathcal{N}\mathsf{R}_{\boldsymbol{\rho}}^*\Psi\right\|_{\mathcal{G}}$$
$$\le \left\|\mathsf{A}\,(\mathcal{N}+c_j)^j\,\Psi\right\|_{\mathcal{G}} + 2\left\|\mathsf{C}\,(\mathcal{N}+c_j-2)^j\,\Psi\right\|_{\mathcal{G}} + 2\left\|\mathsf{C}^*\,(\mathcal{N}+c_j+2)^j\,\Psi\right\|_{\mathcal{G}}$$
$$\le 3\left\|(\mathcal{N}+c_{j+1})^{j+1}\,\Psi\right\|_{\mathcal{G}}.$$

By induction, this implies that for any $(j, k) \in \mathbb{N}^2$

$$\left\|(\mathcal{N}+c_j)^j\left(\mathsf{R}_{\boldsymbol{\rho}}\mathcal{N}\mathsf{R}_{\boldsymbol{\rho}}^*\right)^k\Psi\right\|_{\mathcal{G}} \le 3^k\left\|(\mathcal{N}+c_{j+k})^{j+k}\,\Psi\right\|_{\mathcal{G}}.$$

Taking $j = 0$ and using the fact that $\mathsf{R}_{\boldsymbol{\rho}}$ is unitary $\left(\mathsf{R}_{\boldsymbol{\rho}}\mathcal{N}\mathsf{R}_{\boldsymbol{\rho}}^*\right)^k = \mathsf{R}_{\boldsymbol{\rho}}\mathcal{N}^k\mathsf{R}_{\boldsymbol{\rho}}^*$, we get

$$\left\|\mathcal{N}^k\mathsf{R}_{\boldsymbol{\rho}}^*\Psi\right\|_{\mathcal{G}} = \left\|\left(\mathsf{R}_{\boldsymbol{\rho}}\mathcal{N}\mathsf{R}_{\boldsymbol{\rho}}^*\right)^k\Psi\right\|_{\mathcal{G}} \le 3^k\left\|(\mathcal{N}+c_k)^k\,\Psi\right\|_{\mathcal{G}}.$$

The case of $\mathcal{N}^k\mathsf{R}_{\boldsymbol{\rho}}$ can be handled in the same way. $\qquad\square$

10. The Fluctuation Dynamics

With the scaling provided in (156), we have that $\rho(x) = N^{-1}\,\omega(x, x)$. Let us define $X_\omega(x, y) := N^{-1}\,K(x-y)\,\omega(x, y)$, then this gives us the relation $X_\omega = h^3\,\mathsf{X}_{\boldsymbol{\rho}}$. Thus, the Hartree–Fock equation (5) can be rewritten as follows

$$(172) \qquad i\hbar\,\partial_t\omega = [H_\omega, \omega] \quad \text{with} \quad H_\omega = -\frac{\hbar^2}{2}\,\Delta + K * \rho - X_\omega.$$

By [11, Proposition 3.1], we know that the dynamics of Ψ_{fluc} verifies

$$(173) \qquad i\hbar\,\partial_t\mathsf{U}_{t,s} = \mathsf{G}_t\,\mathsf{U}_{t,s} \quad \text{with} \quad \mathsf{U}_{s,s} = 1 \quad \text{for all } s \in \mathbb{R}$$

and the generator G_t is given by

$$(174) \qquad \mathsf{G} = \mathrm{d}\Gamma_l(H_\omega) - \mathrm{d}\Gamma_r\big(\overline{H_\omega}\big) + \mathsf{D} + \mathsf{Q} + \mathsf{Q}^* + \tilde{\mathsf{Q}} + \tilde{\mathsf{Q}}^*$$

where

$$
\begin{aligned}
\mathsf{D} = \frac{1}{2N} \int_{\mathbb{R}^6} K(x-y) \bigg(& a_l^*(u_x)\, a_l^*(u_y)\, a_l(u_y)\, a_l(u_x) - a_r^*(\overline{u_x})\, a_r^*(\overline{u_y})\, a_r(\overline{u_y})\, a_r(\overline{u_x}) \\
& + 2\, a_l^*(u_x)\, a_r^*(v_x)\, a_r(v_y)\, a_l(u_y) - 2\, a_l^*(u_x)\, a_r^*(\overline{v_y})\, a_r(\overline{v_y})\, a_l(u_x) \\
& + 2\, a_r^*(\overline{u_x})\, a_l^*(v_y)\, a_l(v_y)\, a_r(\overline{u_x}) - 2\, a_r^*(\overline{u_x})\, a_l^*(v_x)\, a_l(v_y)\, a_r(\overline{u_y}) \\
& + a_r^*(\overline{v_y})\, a_r^*(\overline{v_x})\, a_r(\overline{v_x})\, a_r(\overline{v_y}) - a_l^*(v_y)\, a_l^*(v_x)\, a_l(v_x)\, a_l(v_y) \bigg) \mathrm{d}x\, \mathrm{d}y
\end{aligned}
$$

$$
\begin{aligned}
\mathsf{Q}^* = \frac{1}{N} \int_{\mathbb{R}^6} K(x-y) \bigg(& a_l^*(u_x)\, a_l^*(u_y)\, a_r^*(\overline{v_x})\, a_l(u_y) - a_r^*(\overline{u_x})\, a_l^*(v_y)\, a_l^*(v_x)\, a_l(v_y) \\
& + a_r^*(\overline{u_x})\, a_r^*(\overline{u_y})\, a_l^*(v_x)\, a_r(\overline{u_y}) - a_l^*(u_x)\, a_r^*(\overline{v_y})\, a_r^*(\overline{v_x})\, a_r(\overline{v_y}) \bigg) \mathrm{d}x\, \mathrm{d}y
\end{aligned}
$$

$$
\tilde{\mathsf{Q}}^* = \frac{1}{2N} \int_{\mathbb{R}^6} K(x-y) \bigg(a_l^*(u_x)\, a_l^*(u_y)\, a_r^*(\overline{v_y})\, a_r^*(\overline{v_x}) - a_r^*(\overline{u_x})\, a_r^*(\overline{u_y})\, a_l^*(v_y)\, a_l^*(v_x) \bigg) \mathrm{d}x\, \mathrm{d}y
$$

with $u_x(y) := u(y,x)$ and $v_x(y) := v(y,x)$. D contains quartic terms that commute with $\mathcal{N} = \mathcal{N}_l + \mathcal{N}_r$, whereas Q^* and $\tilde{\mathsf{Q}}^*$ contain quartic terms that do not commute with $\mathcal{N}$.

10.1. **Bounds on the Fluctuation Dynamics.** In this section, we use the uniform in $\hbar$ regularity of the solution of the Hartree–Fock equation to estimate the growth of mean number of particles for the fluctuation dynamics.

We fix $p \in [1,2]$ with

$$(175) \qquad p < \mathfrak{b} = \frac{3}{a+1}$$

and take $1 \le q_0 < q_1 \le \infty$ such that

$$(176) \qquad \frac{1}{2}\left(\frac{1}{q_1} + \frac{1}{q_0} \right) = \frac{1}{p} - \frac{1}{\mathfrak{b}}.$$

We choose $T > 0$ so that the following two quantities are uniformly bounded on $[0,T]$:

$$(177\mathrm{a}) \qquad \tilde{\mathcal{D}}_{q_0,q_1} := \|\boldsymbol{\nabla}_\xi \sqrt{\boldsymbol{\rho}}\, m\|_{\mathcal{L}^{q_0}}^{\frac{1}{2}}\, \|\boldsymbol{\nabla}_\xi \sqrt{\boldsymbol{\rho}}\, m\|_{\mathcal{L}^{q_1}}^{\frac{1}{2}},$$

$$(177\mathrm{b}) \qquad \mathcal{D}_{q_0,q_1} := \big(\mathcal{D}_{q_0}\mathcal{D}_{q_1}\big)^{\frac{1}{2}},$$

with $\mathcal{D}_q$ defined in Lemma 7.1 and $m = 1 + |\boldsymbol{p}|^n$ with $n > a+1$. The main result of this section is the following inequality.

Proposition 10.1. *Let $(k_0, k) \in [0, 1/2] \times \mathbb{N}$. Then, for any $\Psi \in \mathcal{G}$ and $t \in [0,T]$, we have*

$$(178) \qquad \|\mathsf{U}_{t,0}\Psi\|_{\mathcal{G}_{k_0}} \le C_M\, e^{C_M\, \lambda_\alpha\, t} \left(\|\Psi\|_{\mathcal{G}_{k_0 + \frac{3}{2}k}} + \frac{h^{(\alpha-1)k}}{N^{\frac{k}{2}-k_0}}\, t\, \|\Psi\|_{\mathcal{G}_{\frac{3}{2}k}} \right)$$

where $\alpha := \frac{3}{p} - \frac{3}{2}$, $C_M = C^{k+k_0}\left(1 + N^{-\frac{1}{2}}h^{-1}\right)$ for some constant $C > 0$, and

$$(179) \qquad \lambda_\alpha = C_{p,a,q_0}\, |\kappa|\, h^{-\alpha}\left(1 + \mathcal{C}_\infty^{-\frac{1}{2}}\right) \sup_{[0,T]} \Big(\|\rho(t)\|_{L^{pa}}, \mathcal{D}_{q_0,q_1}(t), \tilde{\mathcal{D}}_{q_0,q_1}(t) \Big)$$

with $p_a = \frac{3}{3-2a}$.

Remark 10.1. *With the cut-off given in Remark 4.2, one obtains*

$$(180) \qquad \|\mathsf{U}_{t,0}\Psi\|_{\mathcal{G}_{k_0}} \le C_M \, e^{C_M \, \lambda_R \, t} \left(\|\Psi\|_{\mathcal{G}_{k_0+\frac{3}{2}k}} + \frac{R^{3\alpha k} \, t}{N^{\frac{k}{2}-k_0} h^k} \, \|\Psi\|_{\mathcal{G}_{\frac{3}{2}k}} \right)$$

with

$$\lambda_R = C_{p,a,q_0} \, |\kappa| \, R^{-3\alpha} \left(1 + \mathcal{C}_\infty^{-\frac{1}{2}} \right) \sup_{[0,T]} (\|\rho(t)\|_{L^{p_a}}, \mathcal{D}_{q_0,q_1}(t), \tilde{\mathcal{D}}_{q_0,q_1}(t)).$$

To prove Proposition 10.1, we will first obtain uniform in $\hbar$ estimates for the generator (174). This is done by proving a series of lemmas. In particular, we will estimate each of the terms of the generator that do not commute with $\mathcal{N}$ separately.

10.1.1. *Bounds for* $\tilde{\mathsf{Q}}$. For convenience, let us begin by recalling the following lemma.

Lemma 10.1 (Proposition 4.3 of [47]). *Let* $a \in (-1, \frac{3}{2})$, $p \in [1, \mathfrak{b})$, *and* q_0, q_1 *verifying* (176). *Then, for* $n > a + 1$, *there exists a constant* $C > 0$ *such that the estimate*

$$(181) \qquad \|[K_x, \boldsymbol{\rho}]\|_p \le C \, h^{1-\frac{3}{\mathfrak{b}}} \, \|\boldsymbol{\nabla}_\xi \boldsymbol{\rho} \, m\|_{q_0}^{\frac{1}{2}} \, \|\boldsymbol{\nabla}_\xi \boldsymbol{\rho} \, m\|_{q_1}^{\frac{1}{2}}$$

holds. Here, K_x *denotes the multiplication operator* $K_x(y) := K(x - y)$.

Then we have the following result.

Lemma 10.2. *Let* $a \in (-1, \frac{3}{2})$ *and* $p \in [1, 2]$ *verifying* $p < \mathfrak{b}$. *Then, for any* $(\Psi_1, \Psi_2) \in \mathcal{G}^2$, *the following inequality holds*

$$(182) \qquad \frac{1}{\hbar} \left\langle \Psi_1 \, | \, \tilde{\mathsf{Q}}^* \Psi_2 \right\rangle_{\mathcal{G}} \le |\kappa| \left(\tilde{C}_1 \, h^{3\left(\frac{1}{2}-\frac{1}{p}\right)} + \tilde{C}_2 \, N^{\frac{1}{2}} h^{\frac{3}{p'}} \right) \|\Psi_1\|_{\mathcal{G}_{\frac{1}{2}}} \|\Psi_2\|_{\mathcal{G}_{\frac{1}{p'}}},$$

where $\tilde{C}_1 = C \, \tilde{\mathcal{D}}_{q_0,q_1}$ *and* $\tilde{C}_2 = C \left(N h^3 \mathcal{C}_\infty \right)^{\frac{1}{2}} \mathcal{D}_{q_0,q_1}$ *for some constant* $C > 0$ *depending only on* a, p *and* q_0.

Proof. Recall the definition of $\tilde{\mathsf{Q}}^*$ given in Formula (174). By the anti-commutation relations (41), the products of creation operators in $\tilde{\mathsf{Q}}^*$ can be written as follows

$$a_l^*(u_x) \, a_l^*(u_y) \, a_r^*(\overline{v_y}) \, a_r^*(\overline{v_x}) = a_l^*(u_x) \, a_r^*(\overline{v_x}) \, a_l^*(u_y) \, a_r^*(\overline{v_y})$$
$$a_r^*(\overline{u_x}) \, a_r^*(\overline{u_y}) \, a_l^*(v_y) \, a_l^*(v_x) = a_l^*(v_x) \, a_r^*(\overline{u_x}) \, a_l^*(v_y) \, a_r^*(\overline{u_y}).$$

Moreover, using the notation (157) and the notation $K_x(y) = K(x - y)$, we have $\mathrm{d}\Gamma_{l,r}^+(u \, K_x v) := \int_{\mathbb{R}^3} K(x - y) \, a_l^*(u_y) \, a_r^*(\overline{v_y}) \, \mathrm{d}y$. Therefore, we can rewrite $\tilde{\mathsf{Q}}^*$ as

$$(183) \qquad \tilde{\mathsf{Q}}^* = \frac{1}{2N} \int_{\mathbb{R}^3} \mathrm{d}\Gamma_{l,r}^+(u \, K_x v) \, \mathrm{d}\Gamma_{l,r}^+(u \, \delta_x v) - \mathrm{d}\Gamma_{l,r}^+(v \, \delta_x u) \, \mathrm{d}\Gamma_{l,r}^+(u \, K_x v) \, \mathrm{d}x.$$

Here, $u \, \delta_x v$ denotes the operator with integral kernel $(u \, \delta_x v)(y, z) = u(y, x) \, v(x, z)$.

As in [11, Proof of Proposition 4.3], we need to exploit the hidden commutator structure in (183) to handle the $\hbar^{-1}$ on the left-hand side of inequality (182). We begin by using the fact that u commutes with v to deduce the identity

$$(184) \qquad u \, K_x v = v \, K_x u + u \, [K_x, v] - v \, [K_x, u] =: v \, K_x u + c_x,$$

for any $x \in \mathbb{R}^3$. Moreover, the symmetry of K allows us to write

$$(185) \qquad \int_{\mathbb{R}^3} \mathrm{d}\Gamma_{l,r}^+(v \, K_x u) \, \mathrm{d}\Gamma_{l,r}^+(u \, \delta_x v) \, \mathrm{d}x = \int_{\mathbb{R}^3} \mathrm{d}\Gamma_{l,r}^+(v \, \delta_x u) \, \mathrm{d}\Gamma_{l,r}^+(u \, K_x v) \, \mathrm{d}x.$$

By identities (184)–(185), we make appear more explicitly the commutator structure

$$(183) = \frac{1}{2N} \int_{\mathbb{R}^3} \mathrm{d}\Gamma^+_{l,r}(v\, K_x u + c_x)\, \mathrm{d}\Gamma^+_{l,r}(u\, \delta_x v) - \mathrm{d}\Gamma^+_{l,r}(v\, \delta_x u)\, \mathrm{d}\Gamma^+_{l,r}(u\, K_x v - c_x)\, \mathrm{d}x$$

$$= \frac{1}{2N} \int_{\mathbb{R}^3} \mathrm{d}\Gamma^+_{l,r}(c_x)\, \mathrm{d}\Gamma^+_{l,r}(u\, \delta_x v) + \mathrm{d}\Gamma^+_{l,r}(v\, \delta_x u)\, \mathrm{d}\Gamma^+_{l,r}(c_x)\, \mathrm{d}x.$$

Again, using the fact that the creation operators anti-commute, we obtain

$$\tilde{\mathsf{Q}}^* = \frac{1}{2N} \int_{\mathbb{R}^3} (a_l^*(u_x)\, a_r^*(\overline{v_x}) + a_l^*(v_x)\, a_r^*(\overline{u_x}))\, \mathrm{d}\Gamma^+_{l,r}(u\,[K_x, v] - v\,[K_x, u])\, \mathrm{d}x.$$

Expanding the product inside the integral gives four terms. We define $\tilde{J}_1$ and $\tilde{J}_2$ as the terms with $[K_x, v]$, and $\tilde{J}_3$ and $\tilde{J}_4$ the terms with $[K_x, u]$. Let us look at $\tilde{J}_1$. By the Cauchy-Schwarz inequality, we obtain the following bound

$$\langle \Psi_1 \,|\, \tilde{J}_1 \Psi_2 \rangle_{\mathcal{G}} = \int_{\mathbb{R}^3} \left\langle a_l(u_x)\, \Psi_1 \,\middle|\, a_r^*(\overline{v_x})\, \mathrm{d}\Gamma^+_{l,r}(u\,[K_x, v])\, \Psi_2 \right\rangle_{\mathcal{G}} \mathrm{d}x$$

$$\leq \left(\int_{\mathbb{R}^3} \|a_l(u_x)\, \Psi_1\|^2_{\mathcal{G}}\, \mathrm{d}x \right)^{\frac{1}{2}} \left(\int_{\mathbb{R}^3} \left\| a_r^*(\overline{v_x})\, \mathrm{d}\Gamma^+_{l,r}(u\,[K_x, v])\, \Psi_2 \right\|^2_{\mathcal{G}}\, \mathrm{d}x \right)^{\frac{1}{2}}.$$

The first factor can be written

$$\int_{\mathbb{R}^3} \|a_l(u_x)\, \Psi_1\|^2_{\mathcal{G}}\, \mathrm{d}x = \left\langle \Psi_1 \,\middle|\, \int_{\mathbb{R}^3} a_l^*(u_x)\, a_l(u_x)\, \mathrm{d}x\, \Psi_1 \right\rangle_{\mathcal{G}} = \langle \Psi_1 \,|\, \mathrm{d}\Gamma_l(1 - \omega)\, \Psi_1 \rangle_{\mathcal{G}},$$

which is smaller than $\langle \Psi_1 \,|\, \mathcal{N}_l\, \Psi_1 \rangle_{\mathcal{G}}$. To estimate the second factor, we use the fact that

$$\|a_r^*(\overline{v_x})\|^2_\infty = \|v_x\|^2_{L^2} = N\rho(x)$$

together with Lemma 8.1 and the fact that $\|u\|_\infty \leq 1$ to get

$$\left\| a_r^*(\overline{v_x})\, \mathrm{d}\Gamma^+_{l,r}(u\,[K_x, v])\, \Psi_2 \right\|_{\mathcal{G}} \leq (N\rho(x))^{\frac{1}{2}}\, \|[K_x, v]\|_p \left\| (\mathcal{N} + 2)^{\frac{1}{p'}}\, \Psi_2 \right\|_{\mathcal{G}}.$$

Combining the above inequalities leads to

$$\langle \Psi_1 \,|\, \tilde{J}_1 \Psi_2 \rangle \leq N^{\frac{1}{2}} \left(\int_{\mathbb{R}^3} \|[K_x, v]\|^2_p\, \rho(x)\, \mathrm{d}x \right)^{\frac{1}{2}} \langle \Psi_1 \,|\, \mathcal{N}\Psi_1 \rangle^{\frac{1}{2}} \left\| (\mathcal{N} + 2)^{\frac{1}{p'}}\, \Psi_2 \right\|_{\mathcal{G}}.$$

Applying Lemma 10.1, since $p < \mathfrak{b}$, and the scaling relation (176), we get that

$$(186) \qquad \|[K_x, v]\|_p \leq C\, |\kappa|\, N^{\frac{1}{2}}\, h^{1 + 3\left(\frac{1}{2} - \frac{1}{p}\right)} \tilde{\mathcal{D}}_{q_0, q_1}.$$

Therefore, we finally obtain the inequality

$$(187) \qquad \frac{1}{N\hbar} \langle \Psi_1 \,|\, \tilde{J}_1 \Psi_2 \rangle \leq C'\, |\kappa|\, \tilde{\mathcal{D}}_{q_0, q_1}\, h^{3\left(\frac{1}{2} - \frac{1}{p}\right)} \|\Psi_1\|_{\mathcal{G}_{\frac{1}{2}}} \|\Psi_2\|_{\mathcal{G}_{\frac{1}{p'}}}.$$

The term $\tilde{J}_2$ is treated similarly leading to the same bound.

The terms $\tilde{J}_3$ and $\tilde{J}_4$ can also be treated in a similar manner. Except in this case, we apply Lemma 7.1 and the fact that $\|v\|_\infty = \mathcal{C}_\infty^{\frac{1}{2}}(Nh^3)^{\frac{1}{2}}$ to get

$$(188) \qquad \|v\,[K_x, u]\|_p \leq C\, |\kappa|\, N^{\frac{3}{2}}\, h^{1 + 3\left(\frac{3}{2} - \frac{1}{p}\right)} \mathcal{C}_\infty^{\frac{1}{2}}\, \mathcal{D}_{q_0, q_1}.$$

So, we obtained the claimed bound for $\tilde{\mathsf{Q}}^*$. $\qquad\square$

Remark 10.2. *In the case of the cut-off potential described in Remark 4.2, we can take $q_0 = q_1 = \infty$ and $p = 2$ in the above inequality, with an extra factor $R^{3\left(\frac{1}{2} - \frac{1}{6}\right)}$, leading to*

$$(189) \qquad \frac{1}{\hbar} \left\langle \Psi_1 \,\middle|\, \tilde{Q}^* \Psi_2 \right\rangle_{\mathcal{G}} \leq |\kappa| \, R^{3\left(\frac{1}{2} - \frac{1}{6}\right)} \left(\tilde{C}_1 + \tilde{C}_2 \, N^{\frac{1}{2}} h^{\frac{3}{2}} \right) \|\Psi_1\|_{\mathcal{G}_{1/2}} \, \|\Psi_2\|_{\mathcal{G}_{1/2}} \,.$$

More precisely, Inequality (189) is a direct consequence of the following estimate

$$(190) \qquad \frac{1}{\hbar} \left\| [K_{R,x}, \boldsymbol{\rho}] \right\|_{\mathcal{L}^2} \leq C \, |\kappa| \, R^{3\left(\frac{1}{2} - \frac{1}{6}\right)} \left\| \boldsymbol{\nabla}_\xi \boldsymbol{\rho} \, m \right\|_{\mathcal{L}^\infty}$$

which follows directly from the proof of Proposition 4.3 in [47].

10.1.2. *Bounds for* Q^*. We label the terms of Q^* given in (174) by

$$(191) \qquad \qquad \qquad Q^* = I_1 + I_2 + I_3 + I_4.$$

Using the fact that the creation operators anti-commute, we get

$$I_1 = -\frac{1}{N} \int_{\mathbb{R}^6} K(x - y) \, a_l^*(u_x) \, a_r^*(\overline{v_x}) \, a_l^*(u_y) \, a_l(u_y) \, \mathrm{d}x \, \mathrm{d}y,$$

$$I_2 = -\frac{1}{N} \int_{\mathbb{R}^6} K(x - y) \, a_l^*(v_x) \, a_r^*(\overline{u_x}) \, a_l^*(v_y) \, a_l(v_y) \, \mathrm{d}x \, \mathrm{d}y.$$

I_3 and I_4 have similar forms with the "l" and "r" labels interchanged and (u, v) replaced by $(\overline{u}, \overline{v})$ (they are in fact the Harmitian conjugates of I_1 and I_2). To reveal hidden commutator structures, which are necessary when estimating Q^* uniformly in $\hbar$, we need to further decompose (191).

Let us start with the following decomposition lemma.

Lemma 10.3. *Let* Q^* *be as in (191). Then, we have the decomposition*

$$I_1 + I_2 = J_1 + J_2 + J_{12} + I_{12}$$

where

$$J_1 = \frac{1}{N} \int_{\mathbb{R}^3} a_r^*(u_x) \, a_l^*(\overline{v_x}) \, \mathrm{d}\Gamma_l(u \, [u, K_x]) \, \mathrm{d}x$$

$$J_2 = \frac{1}{N} \int_{\mathbb{R}^3} a_l^*(v_x) \, a_r^*(\overline{u_x}) \, \mathrm{d}\Gamma_l(v \, [v, K_x]) \, \mathrm{d}x$$

$$J_{12} = \frac{1}{N} \int_{\mathbb{R}^3} \mathrm{d}\Gamma_{l,r}^+([u, K_x] \, v + [K_x, v] \, u) \, a_l^*(\omega_x) \, a_{x,l} \, \mathrm{d}x,$$

and

$$I_{12} = -\frac{1}{N} \int_{\mathbb{R}^3} a_l^*(u_x) \, a_r^*(\overline{v_x}) \, \mathrm{d}\Gamma_l(K_x) \, \mathrm{d}x.$$

We have the same splitting for $I_3 + I_4$, interchanging "l" by "r" and replacing (u, v) by $(\overline{u}, \overline{v})$. Hence, we obtain a decomposition of the form

$$(192) \qquad Q^* = (J_1 + J_2 + J_3 + J_4 + J_{12} + J_{34}) + (I_{12} + I_{34}) =: \tilde{P}^* + P^*.$$

Proof. To simplify our computations, we use the Fefferman–de la Llave formula (cf. [29, 39]) in its smooth version. For the potential K it reads

$$(193) \qquad \qquad K(x - y) = \kappa_a \int_0^\infty \int_{\mathbb{R}^3} s^{\frac{a+1}{2}} \varphi_{s,z}(x) \, \varphi_{s,z}(y) \, \mathrm{d}z \, \mathrm{d}s$$

where $\varphi_{s,z}(x) = \varphi_s(x - z) = e^{-\pi|x-z|^2 s}$ and $\kappa_a = 2^{\frac{3-a}{2}} \frac{\pi^{a/2}}{\Gamma(a/2)} \kappa$. This allows us to rewrite I_1 and I_2 in the following forms

$$I_1 = -\frac{\kappa_a}{N} \int_0^\infty \!\!\int_{\mathbb{R}^3} s^{\frac{a+1}{2}} \, \mathrm{d}\Gamma^+_{l,r}(u\,\varphi_{s,z}\,v)\,\mathrm{d}\Gamma_l(u\,\varphi_{s,z}\,u)\,\mathrm{d}z\,\mathrm{d}s,$$

$$I_2 = -\frac{\kappa_a}{N} \int_0^\infty \!\!\int_{\mathbb{R}^3} s^{\frac{a+1}{2}} \, \mathrm{d}\Gamma^+_{l,r}(v\,\varphi_{s,z}\,u)\,\mathrm{d}\Gamma_l(v\,\varphi_{s,z}\,v)\,\mathrm{d}z\,\mathrm{d}s,$$

where $\varphi_{s,z}$ is seen as a multiplication operator. Since $u^2 = 1 - \omega$, then we have the identity

$$\mathrm{d}\Gamma^+_{l,r}(u\,\varphi\,v)\,\mathrm{d}\Gamma_l(u\,\varphi\,u) = \ \mathrm{d}\Gamma^+_{l,r}(u\,\varphi\,v)\,\mathrm{d}\Gamma_l(u\,[\varphi, u]) + \mathrm{d}\Gamma^+_{l,r}([u, \varphi]\,v)\,\mathrm{d}\Gamma_l((1-\omega)\,\varphi)$$
$$+ \mathrm{d}\Gamma^+_{l,r}(\varphi\,u\,v)\,\mathrm{d}\Gamma_l((1-\omega)\,\varphi)$$

where we used the notation $\varphi = \varphi_{s,z}$. Similarly, since $v^2 = \omega$, then we have

$$\mathrm{d}\Gamma^+_{l,r}(v\,\varphi\,u)\,\mathrm{d}\Gamma_l(v\,\varphi\,v) = \mathrm{d}\Gamma^+_{l,r}(v\,\varphi\,u)\,\mathrm{d}\Gamma_l(v\,[\varphi, v]) + \mathrm{d}\Gamma^+_{l,r}([v, \varphi]\,u)\,\mathrm{d}\Gamma_l(\omega\,\varphi)$$
$$+ \mathrm{d}\Gamma^+_{l,r}(\varphi\,u\,v)\,\mathrm{d}\Gamma_l(\omega\,\varphi)\,.$$

Combining the two identities yields

$$(194) \quad \mathrm{d}\Gamma^+_{l,r}(u\,\varphi\,v)\,\mathrm{d}\Gamma_l(u\,\varphi\,u) + \mathrm{d}\Gamma^+_{l,r}(v\,\varphi\,u)\,\mathrm{d}\Gamma_l(v\,\varphi\,v)$$
$$= \mathrm{d}\Gamma^+_{l,r}(u\,\varphi\,v)\,\mathrm{d}\Gamma_l(u\,[\varphi, u]) + \mathrm{d}\Gamma^+_{l,r}(v\,\varphi\,u)\,\mathrm{d}\Gamma_l(v\,[\varphi, v])$$
$$+ \mathrm{d}\Gamma^+_{l,r}([\varphi, u]\,v + [v, \varphi]\,u)\,\mathrm{d}\Gamma_l(\omega\,\varphi) + \mathrm{d}\Gamma^+_{l,r}(u\,\varphi\,v)\,\mathrm{d}\Gamma_l(\varphi)\,.$$

Thus, using identity (194), we can write $I_1 + I_2 = J_1 + J_2 + J_{12} + I_{12}$ with

$$J_1 := \frac{\kappa_a}{N} \int_0^\infty \!\!\int_{\mathbb{R}^3} s^{\frac{a+1}{2}} \, \mathrm{d}\Gamma^+_{l,r}(u\,\varphi\,v)\,\mathrm{d}\Gamma_l(u\,[u, \varphi])\,\mathrm{d}z\,\mathrm{d}s,$$

$$J_2 := \frac{\kappa_a}{N} \int_0^\infty \!\!\int_{\mathbb{R}^3} s^{\frac{a+1}{2}} \, \mathrm{d}\Gamma^+_{l,r}(v\,\varphi\,u)\,\mathrm{d}\Gamma_l(v\,[v, \varphi])\,\mathrm{d}z\,\mathrm{d}s,$$

$$J_{12} := \frac{\kappa_a}{N} \int_0^\infty \!\!\int_{\mathbb{R}^3} s^{\frac{a+1}{2}} \, \mathrm{d}\Gamma^+_{l,r}([u, \varphi]\,v + [\varphi, v]\,u)\,\mathrm{d}\Gamma_l(\omega\,\varphi)\,\mathrm{d}z\,\mathrm{d}s,$$

and

$$I_{12} := -\frac{\kappa_a}{N} \int_0^\infty \!\!\int_{\mathbb{R}^3} s^{\frac{a+1}{2}} \, \mathrm{d}\Gamma^+_{l,r}(u\,\varphi\,v)\,\mathrm{d}\Gamma_l(\varphi)\,\mathrm{d}z\,\mathrm{d}s.$$

Reversing the Fefferman–de la Llave expansion gives us

$$J_1 = \frac{\kappa_a}{N} \int_{\mathbb{R}^3} \int_0^\infty \!\!\int_{\mathbb{R}^3} s^{\frac{a+1}{2}} a_l^*(u_x)\,a_r^*(\overline{v_x})\,\varphi(x)\,\mathrm{d}\Gamma_l(u\,[u, \varphi])\,\mathrm{d}z\,\mathrm{d}s\,\mathrm{d}x$$
$$= \frac{1}{N} \int_{\mathbb{R}^3} a_l^*(u_x)\,a_r^*(\overline{v_x})\,\mathrm{d}\Gamma_l(u\,[u, K_x])\,\mathrm{d}x.$$

The same is true for J_2. Lastly, we have that

$$J_{12} = \frac{\kappa_a}{N} \int_0^\infty \!\!\int_{\mathbb{R}^3} s^{\frac{a+1}{2}} \, \mathrm{d}\Gamma^+_{l,r}([u, \varphi]\,v + [\varphi, v]\,u)\,a_l^*(\omega_x)\,\varphi(x)\,a_{x,l}\,\mathrm{d}z\,\mathrm{d}s$$
$$= \frac{1}{N} \int_{\mathbb{R}^3} \mathrm{d}\Gamma^+_{l,r}([u, K_x]\,v + [K_x, v]\,u)\,a_l^*(\omega_x)\,a_{x,l}\,\mathrm{d}x.$$

This completes the proof of the lemma. $\qquad\qquad\square$

Let us first estimate the J terms, which can be treated in a similar manner as in the $\tilde{\mathsf{Q}}^*$ case. One obtains the following bounds.

Lemma 10.4. *Assuming the same hypotheses as in Lemma 10.2. Then, for any $(\Psi_1, \Psi_2) \in \mathcal{G}^2$, we have the estimates*

(195a)
$$\frac{1}{\hbar} \langle \Psi_1 \,|\, J_1 \,\Psi_2 \rangle \le C_1 \,|\kappa|\, N^{\frac{1}{2}} \, h^{\frac{3}{p'}} \, \|\Psi_1\|_{\mathcal{G}_{\frac{1}{2}}} \, \|\Psi_2\|_{\mathcal{G}_{\frac{1}{p'}}}$$

(195b)
$$\frac{1}{\hbar} \langle \Psi_1 \,|\, J_2 \,\Psi_2 \rangle \le C_2 \,|\kappa|\, N^{\frac{1}{2}} \, h^{\frac{3}{p'}} \, \|\Psi_1\|_{\mathcal{G}_{\frac{1}{2}}} \, \|\Psi_2\|_{\mathcal{G}_{\frac{1}{p'}}}$$

(195c)
$$\frac{1}{\hbar} \langle \Psi_1 \,|\, J_{12} \,\Psi_2 \rangle \le C_{12} \,|\kappa|\, N^{\frac{1}{2}} \, h^{\frac{3}{p'}} \, \|\Psi_1\|_{\mathcal{G}_{\frac{1}{2}}} \, \|\Psi_2\|_{\mathcal{G}_{\frac{1}{p'}}} \,,$$

where $C_1 = C \, \mathcal{D}_{q_0,q_1}$, $C_2 = C \, \mathcal{C}_\infty^{\frac{1}{2}} \, \tilde{\mathcal{D}}_{q_0,q_1}$, and $C_{12} = C \, \mathcal{C}_2 \left(\left(N h^3 \mathcal{C}_\infty\right)^{\frac{1}{2}} \mathcal{D}_{q_0,q_1} + \tilde{\mathcal{D}}_{q_0,q_1} \right)$ for some constant C depending only on p and a. The same inequalities hold respectively for J_3, J_4, J_{34}.

Proof. Applying Lemma 10.1 and the fact that $\|u\|_\infty \le 1$ gives us the estimate

$$\|u\,[K_x, u]\|_p \le C \,|\kappa|\, N \, h^{1+\frac{3}{p'}} \mathcal{D}_{q_0,q_1}.$$

Then following the proof of Lemma 10.2 yields inequality (195a). Similarly, by Lemma 10.1 and the fact that $\|v\|_\infty = \left(\mathcal{C}_\infty \, N \, h^3\right)^{\frac{1}{2}}$, we have that

$$\|v\,[K_x, v]\|_p \le C \,|\kappa|\, N \, h^{1+\frac{3}{p'}} \, \mathcal{C}_\infty^{\frac{1}{2}} \, \tilde{\mathcal{D}}_{q_0,q_1}$$

from which we arrive at inequality (195b). Finally, by direct estimation, we see that

$$\langle \Psi_1 \,|\, J_{12} \,\Psi_2 \rangle \le \frac{1}{N} \left(\int_{\mathbb{R}^3} \left\| a_l(\omega_x) \, \mathrm{d}\Gamma_{r,l}^+(v\,[K_x, u] - u\,[K_x, v]) \, \Psi \right\|_{\mathcal{G}}^2 \mathrm{d}x \right)^{\frac{1}{2}} \left\| \mathcal{N}_l^{\frac{1}{2}} \Psi \right\|_{\mathcal{G}}.$$

Then, inequality (195c) follows from Lemma 8.1 and Lemma 10.1. $\square$

Lastly, let us estimate $\mathsf{P}^* = I_{12} + I_{34}$.

Lemma 10.5. *Let $p_a = \frac{3}{3-2a}$. Then, there exists $C > 0$, depending only on a, such that for any $(\Psi_1, \Psi_2) \in \mathcal{G}^2$ we have the estimate*

(196)
$$\frac{1}{\hbar} \left| \langle \Psi_1 \,|\, \mathsf{P}^* \Psi_2 \rangle_{\mathcal{G}} \right| \le \frac{C \,|\kappa|}{N^{\frac{1}{2}} h} \, \|\rho\|_{L^p}^{\frac{1}{2}} \, \langle \Psi_1 \,|\, \mathcal{N} \Psi_1 \rangle_{\mathcal{G}}^{\frac{1}{2}} \, \langle \Psi_2 \,|\, \mathcal{N} \Psi_2 \rangle_{\mathcal{G}}^{\frac{1}{2}}.$$

Proof. Let $(\Psi_1, \Psi_2) \in \mathcal{G}^2$. By the Cauchy-Schwarz inequality and the boundedness of a^*, we have that

$$\left| \langle \Psi_1 \,|\, I_{12}\Psi_2 \rangle_{\mathcal{G}} \right| \le \frac{1}{N} \left(\int_{\mathbb{R}^3} \|a_l(u_x)\Psi_1\|_{\mathcal{G}}^2 \, \mathrm{d}x \right)^{\frac{1}{2}} \left(\int_{\mathbb{R}^6} \|a_r^*(\overline{v_x}) \, \mathrm{d}\Gamma_l(K_x) \, \Psi_2\|_{\mathcal{G}}^2 \, \mathrm{d}x \right)^{\frac{1}{2}}$$

$$\le \frac{1}{N^{\frac{1}{2}}} \, \langle \Psi_1 \,|\, \mathcal{N}_l \Psi_1 \rangle_{\mathcal{G}}^{\frac{1}{2}} \left(\int_{\mathbb{R}^3} \rho(x) \, \|\mathrm{d}\Gamma_l(K_x) \, \Psi_2\|_{\mathcal{G}}^2 \, \mathrm{d}x \right)^{\frac{1}{2}}.$$

where we used $\|v_x\|_{L^2}^2 = N\rho(x)$. Moreover, using the fact that

(197)
$$(\mathrm{d}\Gamma_l(K_x) \, \Psi)^{(n,m)}(\underline{x}_n, \underline{y}_m) = \kappa \sum_{j=1}^{n} \frac{\Psi^{(n,m)}(\underline{x}_n, \underline{y}_m)}{|x - x_j|^a},$$

where $\underline{x}_n = (x_1, \ldots, x_n)$, $\underline{y}_m = (y_1, \ldots, y_m)$, it follows

$$\left\| (\mathrm{d}\Gamma_l(K_x)\,\Psi)^{(n,m)} \right\|^2_{L^2(\mathbb{R}^{3(n+m)})} \leq |\kappa|^2\, n^2 \int_{\mathbb{R}^3} \frac{g(y)}{|x-y|^{2a}}\, \mathrm{d}y$$

where we defined $g(x) = \left\| \Psi^{(n,m)}(x, \underline{x}_{n-1}, \underline{y}_m) \right\|^2_{L^2(\mathrm{d}\underline{x}_{n-1}\mathrm{d}\underline{y}_m)}$. Finally, by Hardy–Littlewood–Sobolev inequality, we have that

$$\int_{\mathbb{R}^3} \rho(x) \left\| (\mathrm{d}\Gamma_l(K_x)\,\Psi)^{(n,m)} \right\|^2_{L^2(\mathbb{R}^{3(n+m)})}\, \mathrm{d}x \leq |\kappa|^2\, n^2 \int_{\mathbb{R}^6} \frac{\rho(x)\, g(y)}{|x-y|^{2a}}\, \mathrm{d}x\, \mathrm{d}y$$

$$\leq C_{p_a,a}\, |\kappa|^2\, n^2\, \|\rho\|_{L^{p_a}}\, \|g\|_{L^1}$$

where $\|g\|_{L^1} = \left\| \Psi^{(n,m)} \right\|^2_{L^2}$. This yields the desired estimate. The proof for the estimate on I_{34} is the same. $\qquad\square$

10.2. **Proof of Proposition 10.1.** To control the growth of the fluctuation dynamics in the $\mathcal{G}_k$ norms, the strategy consists of splitting the generator G, defined in (174), into two parts then solving the problem perturbatively. More precisely, we define the splitting $\mathsf{G} = \tilde{\mathsf{G}} + \mathsf{B}$ with

(198a) $$\tilde{\mathsf{G}} = \mathrm{d}\Gamma_l(H_\omega) - \mathrm{d}\Gamma_r(\overline{H_\omega}) + \mathsf{D} + \tilde{\mathsf{Q}} + \tilde{\mathsf{Q}}^* + \tilde{\mathsf{P}} + \tilde{\mathsf{P}}^*$$

(198b) $$\mathsf{B} = \mathsf{P} + \mathsf{P}^*$$

where we recall P and $\tilde{\mathsf{P}}$ are defined by Formula (192). The idea is to view G as a small perturbation of $\tilde{\mathsf{G}}$. This view is justifiable since, when $N^{\frac{1}{2}}h$ is large, the effect of the operator B is small in the following sense.

Lemma 10.6. *Let* $2j \in \mathbb{N}$ *and* $p_a = \frac{3}{3-2a}$. *Then there exists a constant* $C > 0$ *depending only on* a *such that*

(199) $$\frac{1}{\hbar} \|\mathsf{B}\|_{\mathcal{G}_{j+\frac{3}{2}} \to \mathcal{G}_j} \leq C\, \frac{2^j\, |\kappa|}{N^{\frac{1}{2}}\, h}\, \|\rho\|^{\frac{1}{2}}_{L^{p_a}}\, .$$

Proof. This follows from Lemma 10.5. Notice that $(\mathcal{N}+1)^k\, \mathsf{P}^* = \mathsf{P}^*\, (\mathcal{N}+3)^k$, then, by Lemma 10.5, we have that

$$\|\mathsf{P}^*\Psi\|_{\mathcal{G}_j} = \sup_{\|\Psi_1\|_{\mathcal{G}} \leq 1} \left\langle (\mathcal{N}+1)^{-\frac{1}{2}}\,\Psi_1 \,\middle|\, \mathsf{P}^*\,(\mathcal{N}+3)^{j+\frac{1}{2}}\,\Psi \right\rangle_{\mathcal{G}}$$

$$\leq \frac{C_a\, |\kappa|}{N^{\frac{1}{2}}}\, \|\rho\|^{\frac{1}{2}}_{L^{p_a}} \left\| (\mathcal{N}+3)^{k+\frac{1}{2}}\,\mathcal{N}\Psi \right\|_{\mathcal{G}} \leq C_a \frac{2^j\, |\kappa|}{N^{\frac{1}{2}}}\, \|\rho\|^{\frac{1}{2}}_{L^{p_a}}\, \|\Psi\|_{\mathcal{G}_{j+\frac{3}{2}}}\, .$$

The estimate for P also follows immediately from Lemma 10.5, that is,

$$\|\mathsf{P}\Psi\|_{\mathcal{G}_k} = \sup_{\|\Psi_1\|_{\mathcal{G}} \leq 1} \left\langle \mathsf{P}^*\,(\mathcal{N}+1)^{-1}\,\Psi_1 \,\middle|\, (\mathcal{N}-1)^{j+1}\,\Psi \right\rangle_{\mathcal{G}}$$

$$\leq \frac{C_a\, |\kappa|}{N^{\frac{1}{2}}}\, \|\rho\|^{\frac{1}{2}}_{L^{p_a}} \left\| (\mathcal{N}-1)^{j+1}\,\mathcal{N}^{\frac{1}{2}}\Psi \right\|_{\mathcal{G}} \leq \frac{C_a\, |\kappa|}{N^{\frac{1}{2}}}\, \|\rho\|^{\frac{1}{2}}_{L^{p_a}}\, \|\Psi\|_{\mathcal{G}_{j+\frac{3}{2}}}\, .$$

This completes the argument. $\qquad\square$

In light of the above lemma, we define the auxiliary dynamics $\tilde{\mathsf{U}}_{t,s}$ to be the unitary dynamics generated by (198a), that is, for any $(t,s) \in \mathbb{R}^2$, $\tilde{\mathsf{U}}_{t,s}$ verifies the differential equation

(200) $$i\hbar\, \partial_t \tilde{\mathsf{U}}_{t,s}\Psi = \tilde{\mathsf{G}}_t \tilde{\mathsf{U}}_{t,s}\Psi \quad \text{with} \quad \tilde{\mathsf{U}}_{s,s}\Psi = \Psi$$

for Ψ sufficiently smooth. The existence of $\tilde{\mathsf{U}}_{t,s}$ is proven in Appendix A. Let us begin by showing the auxiliary dynamics propagates the $\mathcal{G}_k$ norm under regularity assumptions on the solution of the Hartree equation.

Proposition 10.2. *Let $a \in (-1, \frac{3}{2})$, $p \in [1, 2]$ verifying $p < \mathfrak{b} = \frac{3}{a+1}$, and $\Psi_t = \tilde{\mathsf{U}}_{t,s}\Psi$ is a solution to (200). Then, for any k such that $2k \in \mathbb{N}$, the inequality*

$$(201) \qquad \frac{\mathrm{d}}{\mathrm{d}t} \|\Psi_t\|_{\mathcal{G}_k} \le C_k |\kappa| \left(\tilde{\mathcal{D}}_{q_0,q_1} h^{3\left(\frac{1}{2} - \frac{1}{p}\right)} + C_{\boldsymbol{\rho}} N^{\frac{1}{2}} h^{\frac{3}{p'}} \right) \|\Psi_t\|_{\mathcal{G}_{k+\left(\frac{1}{2}-\frac{1}{p}\right)}}$$

holds for some constants C_k of the form $C_k = C_{p,a,q_0} C^k$ and

$$C_{\boldsymbol{\rho}} = \left(1 + \mathcal{C}_\infty^{\frac{1}{2}}\right) \left(\mathcal{D}_{q_0,q_1} + \tilde{\mathcal{D}}_{q_0,q_1}\right)$$

where $\mathcal{D}_{q_0,q_1}$ and $\tilde{\mathcal{D}}_{q_0,q_1}$ are defined by formulas (177a) and (177b).

Remark 10.3. *Since $N^{\frac{1}{2}} h^{\frac{3}{2}} \le \mathcal{C}_\infty^{-\frac{1}{2}}$, then, by Grönwall's inequality, we deduce that*

$$(202) \qquad \left\|\tilde{\mathsf{U}}_{t,s}\right\|_{\mathcal{G}_k \to \mathcal{G}_k} \le e^{C_{t,s}}$$

where $C_{t,s} = C_k |\kappa| h^{-\alpha} \left(1 + \mathcal{C}_\infty^{-\frac{1}{2}}\right) \int_s^t \mathcal{D}_{q_0,q_1}(\tau) + \tilde{\mathcal{D}}_{q_0,q_1}(\tau) \, \mathrm{d}\tau$ with $\alpha := \frac{3}{p} - \frac{3}{2} \ge 0$ and is 0 if and only if $p = 2$.

Proof. Let $k \in \mathbb{N}$. Using the fact that $\tilde{\mathsf{G}} = \tilde{\mathsf{G}}^*$, we get

$$i\hbar \frac{\mathrm{d}}{\mathrm{d}t} \|\Psi_t\|_{\mathcal{G}_{\frac{k}{2}}}^2 = \left\langle \Psi_t \,\Big|\, \left[(\mathcal{N} + 1)^k, \tilde{\mathsf{G}}\right] \Psi_t \right\rangle_{\mathcal{G}}$$

$$= \sum_{j=1}^k \left\langle \Psi_t \,\Big|\, (\mathcal{N} + 1)^{j-1} \left[\mathcal{N}, \tilde{\mathsf{G}}\right] (\mathcal{N} + 1)^{k-j} \Psi_t \right\rangle_{\mathcal{G}}.$$

Note that the only terms in $\tilde{\mathsf{G}}$ that do not commute with $\mathcal{N}$ are $\tilde{\mathsf{Q}}$, $\tilde{\mathsf{P}}$, and their adjoints. Since $\mathcal{N}_\sigma a_\sigma^* = a_\sigma^* (\mathcal{N}_\sigma + 1)$ for $\sigma \in \{r, l\}$, we obtain

$$\left[\mathcal{N}, \tilde{\mathsf{G}}\right] = \left[\mathcal{N}, \tilde{\mathsf{Q}}^* + \tilde{\mathsf{Q}} + \tilde{\mathsf{P}}^* + \tilde{\mathsf{P}}\right] = 4\left(\tilde{\mathsf{Q}}^* - \tilde{\mathsf{Q}}\right) + \tilde{\mathsf{P}}^* - \tilde{\mathsf{P}},$$

which leads to

$$(203) \quad \frac{\mathrm{d}}{\mathrm{d}t} \|\Psi_t\|_{\mathcal{G}_{\frac{k}{2}}}^2 = \frac{2}{\hbar} \operatorname{Im}\left(\sum_{j=1}^k \left\langle \Psi_t \,\Big|\, (\mathcal{N} + 1)^{j-1} \left(4\tilde{\mathsf{Q}}^* + \tilde{\mathsf{P}}^*\right) (\mathcal{N} + 1)^{k-j} \Psi_t \right\rangle_{\mathcal{G}}\right).$$

Using again the commutation relation between the number operator and the creation operator, we can balance the power of the number operators appearing on the left and on the right of $\tilde{\mathsf{Q}}^*$. More precisely, if $j > \frac{k+1}{2}$, then

$$(\mathcal{N} + 1)^{j-1} \tilde{\mathsf{Q}}^* (\mathcal{N} + 1)^{k-j} = (\mathcal{N} + 1)^{\frac{k-1}{2}} \tilde{\mathsf{Q}}^* (\mathcal{N} + 5)^{j - \frac{k+1}{2}} (\mathcal{N} + 1)^{k-j},$$

$$(\mathcal{N} + 1)^{j-1} \tilde{\mathsf{Q}}^* (\mathcal{N} + 1)^{k-j} = (\mathcal{N} + 1)^{\frac{k-1}{2}} \tilde{\mathsf{Q}}^* (\mathcal{N} + 2)^{j - \frac{k+1}{2}} (\mathcal{N} + 1)^{k-j},$$

and similarly if $j < \frac{k+1}{2}$, using the fact that $\tilde{\mathsf{Q}}^* (\mathcal{N} + 1)^s = (\mathcal{N} - 3)^s \tilde{\mathsf{Q}}^*$. Therefore, applying Lemma 10.2 and Lemma 10.4 on each term of the right-hand side of Equation (203) and the fact that $Nh^3 \mathcal{C}_\infty \le 1$ and $\mathcal{C}_2 \le \mathcal{C}_\infty^{\frac{1}{2}}$, we obtain

$$\frac{1}{2} \frac{\mathrm{d}}{\mathrm{d}t} \|\Psi_t\|_{\mathcal{G}_{\frac{k}{2}}}^2 \le C^k |\kappa| C_{p,a,q_0} \left(\tilde{\mathcal{D}}_{q_0,q_1} h^{3\left(\frac{1}{2} - \frac{1}{p}\right)} + C_{\boldsymbol{\rho}} N^{\frac{1}{2}} h^{\frac{3}{p'}}\right) \|\Psi_t\|_{\mathcal{G}_{\frac{k}{2}}} \|\Psi_t\|_{\mathcal{G}_{\frac{k}{2}+\left(\frac{1}{2}-\frac{1}{p}\right)}}$$

which leads to the desired result. $\qquad\square$

Moreover, by Proposition 9.2 and by weighted interpolation, we deduce that for any $t > 0$, $\mathsf{R}_{\boldsymbol{\rho}_t}$ is a bounded mapping from G_k to G_k. More precisely, for any $k \in [0, 1/2]$, we have a bound of the form (171), and the same bound is valid for $\mathsf{R}_{\boldsymbol{\rho}}^*$. Therefore, recalling that by definition $\mathsf{U}_{t,s} = \mathsf{R}_{\boldsymbol{\rho}_t}^* \, e^{-i\mathsf{L}(t-s)/\hbar} \, \mathsf{R}_{\boldsymbol{\rho}_s}$, and since $e^{-i\mathsf{L}(t-s)/\hbar}$ commutes with the number operator, we obtain for $k \in [0, 1/2]$

$$(204) \qquad \|\mathsf{U}_{t,s}\Psi\|_{\mathcal{G}_k} \leq 3\,\|\Psi\|_{\mathcal{G}_k} + 5\,N^k\,\|\Psi\|_{\mathcal{G}}.$$

Combining these three inequalities (202), (199), (204), and using the Duhamel formula, we obtain the main result of the section.

Proof of Proposition 10.1. Let $\mathsf{B}_h := \frac{1}{i\hbar}\mathsf{B}$. Then the Duhamel formula can be written

$$\mathsf{U}_{t,0} = \tilde{\mathsf{U}}_{t,0} + (\mathsf{U} \star \mathsf{B}_h \tilde{\mathsf{U}})_{t,0}$$

where we used the notation $\star$ for the time convolution of operators $(\mathsf{U} \star \mathsf{V})_{t,s} := \int_s^t \mathsf{U}_{t,s'} \mathsf{V}_{s',s}\,ds'$, and the iterated time convolution is defined by $\mathsf{U}^{(\star 1)} = \mathsf{U}$ and for $k \geq 2$ by $\mathsf{U}^{(\star k)} = \mathsf{U} \star \mathsf{U}^{(\star(k-1))}$. From this we deduce the following iterated Duhamel's formula

$$(205) \qquad \mathsf{U}_{t,0} = \sum_{j=0}^{k-1} (\tilde{\mathsf{U}} \star (\mathsf{B}_h\tilde{\mathsf{U}})^{(\star j)})_{t,0} + (\mathsf{U} \star (\mathsf{B}_h\tilde{\mathsf{U}})^{(\star k)})_{t,0}.$$

and from Inequality (204), we deduce

$$\|\mathsf{U}_{t,0}\Psi\|_{\mathcal{G}_{k_0}} \leq \sum_{j=0}^{k-1} \left\| (\tilde{\mathsf{U}} \star (\mathsf{B}_h\tilde{\mathsf{U}})^{(\star j)})_{t,0}\Psi \right\|_{\mathcal{G}_{k_0}}$$
$$+ \int_0^t \left(3\left\| (\mathsf{B}_h\tilde{\mathsf{U}})_{s,0}^{(\star k)}\Psi \right\|_{\mathcal{G}_{k_0}} + 5N^{k_0}\left\| (\mathsf{B}_h\tilde{\mathsf{U}})_{s,0}^{(\star k)}\Psi \right\|_{\mathcal{G}} \right) ds.$$

Since we know from Part II that $C_T := \sup_{[0,T]}(\|\rho\|_{L^{p_a}}, \mathcal{D}_{q_0,q_1}, \tilde{\mathcal{D}}_{q_0,q_1})$ is bounded, we deduce that $C_{t,s} \leq C_T\, C^{k_0}\, C_{p,a,q_0}\, |\kappa|\, h^{-\alpha}\left(1 + \mathcal{C}_\infty^{-\frac{1}{2}}\right)(t-s) =: \lambda_\alpha\, C^{k_0}\,(t-s).$

From inequalities (199) and (202), we obtain for any $0 \leq s \leq t \leq T$

$$\left\| (\mathsf{B}_h\tilde{\mathsf{U}})_{t,s} \right\|_{\mathcal{G}_{k_0+\frac{3}{2}} \to \mathcal{G}_{k_0}} \leq \frac{2^{k_0}\, C\, \lambda_0}{M}\, e^{\lambda_\alpha\, C^k (t-s)}$$

where $M = N^{\frac{1}{2}}h$, which leads to

$$\left\| (\mathsf{B}_h\tilde{\mathsf{U}})_{t,s}^{(\star j)} \right\|_{\mathcal{G}_{k_0+\frac{3}{2}j} \to \mathcal{G}_{k_0}} \leq \frac{(C\lambda_0)^j\, 2^{(k_0+j)(j+1)}}{M^j\,(j-1)!}\,(t-s)^{j-1}\, e^{\lambda_\alpha\, C^k(t-s)}.$$

Hence, for U, we obtain

$$\|\mathsf{U}_{t,0}\Psi\|_{\mathcal{G}_{k_0}} \leq \sum_{j=0}^{k-1} \frac{(C\lambda_0)^j\, 2^{(k_0+j)(j+1)}}{M^j\,j!}\, t^j e^{\lambda_\alpha\, C^k t}\,\|\Psi\|_{\mathcal{G}_{k_0+\frac{3}{2}j}}$$
$$+ \frac{\left(2^k C\lambda_0\right)^k}{M^k\, k!\, \lambda_\alpha}\, t^k e^{\lambda_\alpha\, C^k t}\left(2^{k_0(k+1)}\,\|\Psi\|_{\mathcal{G}_{k_0+\frac{3}{2}k}} + N^{k_0}\,\|\Psi\|_{\mathcal{G}_{\frac{3}{2}k}} \right)$$
$$\leq C_M\, e^{C_M \lambda_\alpha\, t}\,\|\Psi\|_{\mathcal{G}_{k_0+\frac{3}{2}k}} + \frac{\left(2^k C\right)^k \lambda_0^{k-1}}{k!}\, t^k e^{\lambda_\alpha\, C^k t}\,\frac{N^{k_0}\, h^{3\alpha}}{M^k}\,\|\Psi\|_{\mathcal{G}_{\frac{3}{2}k}}$$

where $C_M = C^{k+k_0} \left(1 + \frac{1}{M}\right)$. Remark that since $\lambda_0 = h^\alpha \lambda_\alpha$, this implies

$$\|\mathsf{U}_{t,0}\Psi\|_{\mathcal{G}_{k_0}} \leq C_M \, e^{C_M \lambda_\alpha t} \|\Psi\|_{\mathcal{G}_{k_0+\frac{3}{2}k}}$$
$$+ \frac{2^k C}{k} \frac{\left(2^k C\right)^{k-1} \lambda_\alpha^{k-1}}{(k-1)!} \, t^{k-1} e^{\lambda_\alpha C^k t} \frac{N^{k_0} \, h^{\alpha k} \, t}{M^k} \|\Psi\|_{\mathcal{G}_{\frac{3}{2}k}}$$

and using the fact that for $x > 0$, $\frac{x^{k-1}}{(k-1)!} \leq e^x$, replacing the constant $C^k + 2^k C$ by C^k for some other numerical constant C in the second exponential and bounding $2^k C/k$ by C^k, we can simplify a bit the result and write

$$\|\mathsf{U}_{t,0}\Psi\|_{\mathcal{G}_{k_0}} \leq C_M \, e^{C_M \lambda_\alpha t} \|\Psi\|_{\mathcal{G}_{k_0+\frac{3}{2}k}} + C^k \, e^{\lambda_\alpha C^k t} \frac{N^{k_0} \, h^{\alpha k} \, t}{M^k} \|\Psi\|_{\mathcal{G}_{\frac{3}{2}k}}$$
$$\leq C_M \, e^{C_M \lambda_\alpha t} \left(\|\Psi\|_{\mathcal{G}_{k_0+\frac{3}{2}k}} + \frac{h^{(\alpha-1)k}}{N^{\frac{k}{2}-k_0}} \, t \, \|\Psi\|_{\mathcal{G}_{\frac{3}{2}k}} \right).$$

$\square$

11. Proofs of the Theorems

We can now prove our general theorem.

Proof of Theorem 4.1. In order to get the result, we want to apply Proposition 10.1. Hence, we define

$$\frac{1}{p_\alpha} := \frac{\alpha}{3} + \frac{1}{2}.$$

The assumptions $\alpha \in [0,1]$ and $\alpha > a - \frac{1}{2}$ are equivalent to say that $p_\alpha \in \left[\frac{5}{6}, 2\right]$ and $p_\alpha < \mathfrak{b}$, and imply that (88) is a non-empty condition. Therefore, p_α verifies the assumption (175). Now we define

(206) $$q_1 := q \quad \text{and} \quad \frac{1}{q_0} := 2\left(\frac{1}{p_\alpha} - \frac{1}{\mathfrak{b}}\right) - \frac{1}{q_1}$$

so that Formula (176) holds with $p = p_\alpha$. Assumption (88) can be written

(207) $$\frac{1}{q_1} \in \left[2\left(\frac{1}{p_\alpha} - \frac{1}{\mathfrak{b}}\right) - \frac{1}{2}, \frac{1}{p_\alpha} - \frac{1}{\mathfrak{b}}\right].$$

Definition (206) and Equation (207) together imply that q_0 and q_1 verify $2 \leq q_0 < q_1 \leq \infty$.

Next, we have to check that we have a uniform in h bound for the quantity

$$\sup_{[0,T]} \left(\|\rho(t)\|_{L^{p_a}}, \mathcal{D}_{q_0,q_1}(t), \tilde{\mathcal{D}}_{q_0,q_1}(t) \right)$$

appearing in the growth rate λ_α defined in (179). This is done by using the propagation of regularity results for the Hartree–Fock equation of Part II. First, by our initial regularity assumptions and Proposition 6.1, we deduce that $\|\rho(t)\|_{L^{p_a}}$ is bounded uniformly in h and in $t \in [0,T]$ for some $T = T_{\rho^{\mathrm{in}}}$ depending on the initial condition of the Hartree–Fock Equation (5). Then, by Proposition 6.3 we deduce that $\sqrt{\rho} \in \mathcal{W}^{1,q}(m)$ for any $q \in [2, q_1)$, and so

$$\tilde{\mathcal{D}}_{q_0,q_1} = \|\boldsymbol{\nabla}_\xi \sqrt{\rho} \, m\|_{\mathcal{L}^{q_0}}^{\frac{1}{2}} \|\boldsymbol{\nabla}_\xi \sqrt{\rho} \, m\|_{\mathcal{L}^{q_1}}^{\frac{1}{2}}$$

is uniformly bounded on $[0, T]$. Moreover, by Lemma 6.1, we obtain

$$\mathcal{D}_{q,q_0} = \|\boldsymbol{\nabla}_\xi \boldsymbol{\rho}\, m\|_{\mathcal{L}^{q_0}}^{\frac{1}{2}} \|\boldsymbol{\nabla}_\xi \boldsymbol{\rho}\, m\|_{\mathcal{L}^{q_1}}^{\frac{1}{2}} \leq \tilde{\mathcal{D}}_{q_0,q_1}$$

so $\mathcal{D}_{q,q_0}$ is also uniformly bounded on $[0, T]$. Therefore, by Proposition 10.1, we deduce that

$$(208) \qquad \|\mathsf{U}_{t,0}\Psi\|_{\mathcal{G}_{\frac{1}{2p}}}^2 \leq C_M^2\, e^{C_M\, \lambda\, t/h^\alpha} \left(\|\Psi\|_{\mathcal{G}_{\frac{3k}{2}+\frac{1}{2p}}}^2 + \frac{h^{2k(\alpha-1)}}{N^{k-\frac{1}{p}}}\, t^2\, \|\Psi\|_{\mathcal{G}_{\frac{3k}{2}}}^2 \right)$$

with λ uniformly bounded in $t \in [0, T]$ and in the Planck constant h. Then, by Proposition 9.1, the following inequality holds

$$(209) \qquad \|\boldsymbol{\rho}_{N:1} - \boldsymbol{\rho}\|_{\mathcal{L}^p} \leq \frac{C_p}{\min(N^{\frac{1}{2}}, N\, h^{\frac{3}{p'}})}\, \|\Psi\|_{\mathcal{G}_{\frac{1}{2p}}}^2\;.$$

We conclude the proof by combining Inequality (208) with the above inequality. □

Next, we prove that from our general Theorem 4.1, we can deduce our simplified mean-field results, i.e. Theorem 3.2. To this end, we come back to the setting of density operators over the Fock space by the following Lemma

Lemma 11.1. *Let $\boldsymbol{\rho}_{N,\boldsymbol{\rho}} := \left|\mathsf{I}_{\mathcal{G}}^{-1}(\mathsf{R}_{\boldsymbol{\rho}}\,\Omega)\right|^2$ as defined in (85). Then for any $\boldsymbol{\rho}_N \in \mathcal{L}_s^1(\mathcal{F})$, that commutes with $\mathcal{N}$, there exists $\Psi \in \mathcal{G}$ such that*

$$(210) \qquad \boldsymbol{\rho}_N = \left|\mathsf{I}_{\mathcal{G}}^{-1}(\mathsf{R}_{\boldsymbol{\rho}}\,\Psi)\right|^2$$

and

$$(211) \qquad \|\mathcal{N}^s\Psi\|_{\mathcal{G}}^2 \leq C_s \left\|(\mathcal{N}+2N)^s\left(\boldsymbol{\rho}_N - \boldsymbol{\rho}_{N,\boldsymbol{\rho}}\right)\right\|_{\mathcal{L}^1(\mathcal{F})}$$

with $C_s = 12^s\,(s+1)^s$.

Proof. Let $\Phi_{\boldsymbol{\rho}} = \mathsf{R}_{\boldsymbol{\rho}}\Omega = \mathsf{I}_{\mathcal{G}}(\boldsymbol{v}_{N,\boldsymbol{\rho}})$. Then $|\boldsymbol{v}_{N,\boldsymbol{\rho}}| = \sqrt{\boldsymbol{\rho}_{N,\boldsymbol{\rho}}}$, and by the polar decomposition of $\boldsymbol{v}_{N,\boldsymbol{\rho}}$, there exists a unique operator $U_{N,\boldsymbol{\rho}}$ such that

$$\boldsymbol{v}_{N,\boldsymbol{\rho}} = U_{N,\boldsymbol{\rho}}\,|\boldsymbol{v}_{N,\boldsymbol{\rho}}|\,,$$

with $\|U_{N,\boldsymbol{\rho}}\psi\|_{\mathcal{F}} = \|\psi\|_{\mathcal{F}}$ if $\psi \in (\ker \boldsymbol{v}_{N,\boldsymbol{\rho}})^\perp$ and $\|U_{N,\boldsymbol{\rho}}\psi\|_{\mathcal{F}} = 0$ if $\psi \in \ker \boldsymbol{v}_{N,\boldsymbol{\rho}}$ (see e.g. [62, Theorem VI.10]). Then we define

$$\boldsymbol{v}_N := U_{N,\boldsymbol{\rho}}\left|\sqrt{\boldsymbol{\rho}_N}\right|\,,$$

and $\Phi = \mathsf{I}_{\mathcal{G}}(\boldsymbol{v}_N)$, $\Psi := \mathsf{R}_{\boldsymbol{\rho}}^*\Phi$. In particular, $\boldsymbol{\rho}_N = |\boldsymbol{v}_N|^2$ so Formula (210) is verified. Now from Lemma 9.2, we have

$$\|\mathcal{N}^s\Psi\|_{\mathcal{G}} = \|\mathcal{N}^s(\Psi - \Omega)\|_{\mathcal{G}} \leq 3^s\,\|(\mathcal{N}+2N+2s+2)^s\,(\Phi - \Phi_{\boldsymbol{\rho}})\|_{\mathcal{G}}\,.$$

Using the fact that $\mathsf{I}_{\mathcal{G}}$ is an isometry, $\mathcal{N}_l\Phi = \mathsf{I}_{\mathcal{G}}(\mathcal{N}\boldsymbol{v}_N)$, $\mathcal{N}_r\Phi = \mathsf{I}_{\mathcal{G}}(\boldsymbol{v}_N\mathcal{N})$ and $\boldsymbol{v}_N$ commutes with $\mathcal{N}$, we deduce that

$$\|\mathcal{N}^s\Psi\|_{\mathcal{G}} \leq C_s\,\|(\mathcal{N}+N)^s\,(\boldsymbol{v}_N - \boldsymbol{v}_{N,\boldsymbol{\rho}})\|_{\mathcal{L}^2(\mathcal{F})}\,.$$

By our choice of $U_{N,\boldsymbol{\rho}}$, it holds

$$(\mathcal{N}+N)^s\,(\boldsymbol{v}_N - \boldsymbol{v}_{N,\boldsymbol{\rho}}) = U_{N,\boldsymbol{\rho}}\left(|(\mathcal{N}+N)^s\,\boldsymbol{v}_N| - |(\mathcal{N}+N)^s\,\boldsymbol{v}_{N,\boldsymbol{\rho}}|\right)$$

with $\|U_{N,\boldsymbol{\rho}}\|_\infty \leq 1$. Now recall the Powers-Stormer inequality [61, Lemma 4.1] which tells that if A and B are nonnegative operators, then $\mathrm{Tr}\left(|A-B|^2\right) \leq \mathrm{Tr}\left(|A^2 - B^2|\right)$. Hence,

$$\|\mathcal{N}^s\Psi\|_{\mathcal{G}}^2 \leq C_s^2 \left\| |\boldsymbol{v}_N \, (\mathcal{N}+N)^s|^2 - |\boldsymbol{v}_{N,\boldsymbol{\rho}} \, (\mathcal{N}+N)^s|^2 \right\|_{\mathcal{L}^1(\mathcal{F})}$$
$$\leq C_s^2 \left\| (\mathcal{N}+N)^s \left(\boldsymbol{\rho}_N - \boldsymbol{\rho}_{N,\boldsymbol{\rho}}\right) (\mathcal{N}+N)^s \right\|_{\mathcal{L}^1(\mathcal{F})}.$$

$\square$

Proof of Theorem 3.2. In the setting of Theorem 3.2, since $a < 1/2$, we can take $\alpha = 0$ in Theorem 4.1, and the hypothesis for q implies that condition (88) is verified. With this choice, Theorem 4.1 yields for any $k_1 \in \mathbb{N}$

$$\|\boldsymbol{\rho}_{N:1} - \boldsymbol{\rho}\|_{\mathcal{L}^p} \leq \frac{C\,e^{\lambda t}}{\min(N^{\frac{1}{2}}, N\,h^{\frac{3}{p'}})}\|\Psi\|_{\mathcal{G}_{\frac{3}{2}k_1 + \frac{1}{2p}}}^2 \left(1 + \frac{h^{-2k_1}}{N^{k_1 - \frac{1}{p}}}\right).$$

Taking $k = \frac{3}{2}k_1 + \frac{1}{2p}$, the hypothesis on k implies that $\frac{h^{-2k_1}}{N^{k_1 - \frac{1}{p}}} \leq C$. Finally, we use Lemma 11.1 to get

$$\|\Psi\|_{\mathcal{G}_k}^2 \leq 2^{k+1}\left(\|\Psi\|_{\mathcal{G}}^2 + \|\mathcal{N}^k\Psi\|_{\mathcal{G}}^2\right) \leq C_k\left(1 + \|\boldsymbol{\rho}_N - \boldsymbol{\rho}_{N,\boldsymbol{\rho}}\|_{\mathcal{L}_k^1(\mathcal{F})}\right)$$

for some k dependent constant $C_k > 0$. $\square$

Appendix A. Existence of the Auxiliary Dynamics

The purpose of this appendix is to extend the result on the existence of the auxiliary dynamics for smooth potentials in the interaction picture given in the appendix of [11] to the case of singular interaction potentials of the form $K(x) = |x|^{-a}$ for $0 \leq a \leq 1$.

In this section, $\hbar$ will not play any role in our analysis. Therefore, to simplify the presentation, we set $\hbar \equiv 1$. By Formula (192), the time-dependent operator $\tilde{\mathsf{G}}$ defined in Equation (174) can be written

$$(212) \qquad \tilde{\mathsf{G}} = \mathrm{d}\Gamma_l(H_\omega) - \mathrm{d}\Gamma_r(\overline{H_\omega}) + \tilde{\mathsf{Q}} + \tilde{\mathsf{Q}}^* + \mathsf{D} + \tilde{\mathsf{P}} + \tilde{\mathsf{P}}^*$$

where $\tilde{\mathsf{Q}}^*$ and D are already defined after Equation (174) and

$$\tilde{\mathsf{P}}^* = \frac{1}{N}\int_{\mathbb{R}^6}\left(a_r^*(\bar{v}_x)\,a_l^*(u_x)\,\mathrm{d}\Gamma_l(u\,[K_x, u]) + a_r^*(\bar{u}_x)\,a_l^*(v_x)\,\mathrm{d}\Gamma_l(v\,[K_x, v])\right.$$
$$+ \mathrm{d}\Gamma_{l,r}^+([u, K_x]\,v + [K_x, v]\,u)\,\mathrm{d}\Gamma_l(\omega_x)$$
$$+ a_l^*(v_x)\,a_r^*(\bar{u}_x)\,\mathrm{d}\Gamma_r(\bar{u}\,[K_x, \bar{u}]) + a_l^*(u_x)\,a_r^*(\bar{v}_x)\,\mathrm{d}\Gamma_r(\bar{v}\,[K_x, \bar{v}])$$
$$\left. + \mathrm{d}\Gamma_{r,l}^+([\bar{u}, K_x]\,\bar{v} + [K_x, \bar{v}]\,\bar{u})\,\mathrm{d}\Gamma_r(\bar{\omega}_x)\right)\mathrm{d}x.$$

The goal is to show that the operator $\tilde{\mathsf{G}}$ generates a unitary dynamics $\tilde{\mathsf{U}}_{t,s}$ in Fock space that satisfies the differential equation

$$(213) \qquad i\,\partial_t\tilde{\mathsf{U}}_{t,s}\Psi = \tilde{\mathsf{G}}_t\tilde{\mathsf{U}}_{t,s}\Psi \quad\text{with}\quad \tilde{\mathsf{U}}_{s,s}\Psi = \Psi,$$

for sufficiently smooth $\Psi \in \mathcal{G}$. To this end, it is convenient to consider the dynamics in the interaction picture. More precisely, define the operator

$$\widehat{\mathsf{G}}_t = -\mathsf{L}_0 + \mathsf{U}_t^{(0)*}\tilde{\mathsf{G}}_t\mathsf{U}_t^{(0)}$$

where $\mathsf{L}_0 = d\Gamma_r(\Delta) - d\Gamma_l(\Delta)$ and $\mathsf{U}_t^{(0)} = \mathsf{U}_{t,0}^{(0)}$ is the free evolution, i.e. $\mathsf{U}_{t,s}^{(0)}$ solves

$$i\,\partial_t \mathsf{U}_{t,s}^{(0)}\Psi = \mathsf{L}_0 \mathsf{U}_{t,s}^{(0)}\Psi,$$

with $\mathsf{U}_{s,s}^{(0)}\Psi = \Psi$. We will show that $\widehat{\mathsf{G}}_t$ generates a unitary operator $\widehat{\mathsf{U}}_{t,s}$ in Fock space which in turn allows us to define the auxiliary dynamics by

$$\tilde{\mathsf{U}}_{t,s} := \mathsf{U}_t^{(0)}\widehat{\mathsf{U}}_{t,s}\mathsf{U}_s^{(0)*}.$$

which formally satisfies Equation (213).

Since much of the result in this appendix is similar to that of the appendix of [11], we will only focus on the part of the result that relies explicitly on the regularity of the potential and refer the reader to [11] for a more complete proof of the result. Hence, the rest of this section will be devoted to prove that the mapping $t \mapsto \widehat{\mathsf{G}}_t\Psi$ is Hölder continuous when Ψ is sufficiently smooth. More precisely, we define the homogeneous Sobolev-type double Fock space by the norm

$$(214) \qquad \|\Psi\|_{\dot{\mathcal{H}}_k^s} := \left\|\mathcal{N}^{k-1/2}\,d\Gamma((-\Delta)^s)^{1/2}\Psi\right\|_{\mathcal{G}}.$$

In particular, $\|\Psi\|_{\dot{\mathcal{H}}_k^0} = \left\|\mathcal{N}^k\Psi\right\|_{\mathcal{G}}$. The main proposition of this section is the following result.

Proposition A.1. *Let $\boldsymbol{\rho}$ be a solution to the Hartree–Fock equation with initial condition $\boldsymbol{\rho}^{\mathrm{in}}$ satisfying (40a), (40b), and $\int_{\mathbb{R}^3} \rho^{\mathrm{in}}(x)\,\langle x\rangle^3\,dx \leq C$. Then there exists $T > 0$ and a constant C_T depending on $\boldsymbol{\rho}^{\mathrm{in}}$ such that for any $(t,s) \in [0,T]^2$,*

$$\left\|\left(\widehat{\mathsf{G}}_t - \widehat{\mathsf{G}}_s\right)\Psi\right\|_{\mathcal{G}} \leq C_T\,|t-s|^{\frac{3-2a}{7}}\left(\|\Psi\|_{\mathcal{G}_2} + \|\Psi\|_{\dot{\mathcal{H}}_2^{3/2}}\right).$$

Remark A.1. *For a fixed $\hbar$, the global-in-time well-posedness of solutions to the Hartree–Fock equation is a standard result (see for instance [20]). However, the bounds of the propagated quantity may depend on $\hbar$. In particular, for a general fixed $\hbar$, the constant C_T in the above proposition may depend on $\hbar$.*

Remark A.2. *We know from Part II that the conditions (40a) and (40b) remain satisfied on $[0,T]$. In particular, $\left\|\sqrt{\boldsymbol{\rho}}\right\|_{\mathcal{L}^2(|\boldsymbol{p}|^n)}^2 = \mathrm{Tr}\left(\boldsymbol{\rho}\,|\boldsymbol{p}|^{2n}\right)$ is uniformly bounded on $[0,T]$. To see that the third-order spatial moment $\int_{\mathbb{R}^3} \rho^{\mathrm{in}}(x)\,\langle x\rangle^3\,dx = \mathrm{Tr}\left(\boldsymbol{\rho}\,|x|^3\right)$ remains bounded, one can notice that*

$$i\hbar\,\partial_t \mathrm{Tr}\left(\boldsymbol{\rho}\,|x|^3\right) = \mathrm{Tr}\left(\left[\frac{|\boldsymbol{p}|^2}{2}, |x|^3\right]\boldsymbol{\rho}\right) + \mathrm{Tr}\left(\left[\mathsf{X}_{\boldsymbol{\rho}}, |x|^3\right]\boldsymbol{\rho}\right).$$

The first term is controlled, using [46, Formula (42)], by a term proportional to $\mathrm{Tr}\left(\boldsymbol{\rho}\left(|x|^3 + |\boldsymbol{p}|^3 + 1\right)\right)$. The second term is zero since

$$\mathrm{Tr}\left(\left[\mathsf{X}_{\boldsymbol{\rho}}, |x|^3\right]\boldsymbol{\rho}\right) = \iint_{\mathbb{R}^6} |\boldsymbol{\rho}(x,y)|^2\,\frac{|y|^3 - |x|^3}{|x-y|^a}\,dx\,dy$$

is the integral of an anti-symmetric function of x and y. Then, by the standard Grönwall argument, one obtains the desired result.

It will be convenient to use the fact that the above defined norm (214) controls quantities of the form $\|d\Gamma(A\nabla)\Psi\|_{\mathcal{G}}$ as stated in the following lemma.

Lemma A.1. *Let $A \in \mathcal{L}^\infty$ and $\Psi \in \dot{\mathcal{H}}_1^1$. Then $\|d\Gamma(A\nabla)\Psi\|_{\mathcal{G}} \leq \|A\|_\infty\,\|\Psi\|_{\dot{\mathcal{H}}_1^1}$.*

Proof. Using the fact that A is a bounded operator, we obtain

$$\|\mathrm{d}\Gamma(A\nabla)\Psi\|_{\mathcal{G}}^2 \le \|A\|_{\infty}^2 \sum_{n=1}^{\infty} \left(\sum_{j\le n} \left\| \nabla_{x_j} \Psi^{(n)} \right\|_{L^2} \right)^2.$$

By the Cauchy-Schwarz inequality and integration by parts, the last factor verifies

$$\sum_{n=1}^{\infty} \left(\sum_{j\le n} \left\| \nabla_{x_j} \Psi^{(n)} \right\|_{L^2} \right)^2 \le \left\langle \mathcal{N}_l \Psi^{(n)} \,\middle|\, \mathrm{d}\Gamma_l(-\Delta)\, \Psi^{(n)} \right\rangle_{\mathcal{G}} = \left\| \mathrm{d}\Gamma_l(-\Delta)^{1/2} \mathcal{N}_l^{1/2} \Psi \right\|_{\mathcal{G}}^2$$

which is bounded above by $\|\Psi\|_{\dot{\mathcal{H}}_1^1}$. $\hfill\square$

To simplify some of the calculation, it will also be convenient to employ the following lemma.

Lemma A.2. *For any self-adjoint integral operator A on $\mathfrak{h} = L^2(\mathbb{R}^3)$, we have the identities*

(215a) $$\mathsf{U}_t^{(0)*}\, \mathrm{d}\Gamma_l(A)\, \mathsf{U}_t^{(0)} = \mathrm{d}\Gamma_l(A_I)$$

(215b) $$\mathsf{U}_t^{(0)*}\, \mathrm{d}\Gamma_{l,r}^+(A)\, \mathsf{U}_t^{(0)} = \mathrm{d}\Gamma_{l,r}^+(A_I)$$

where $A_I := e^{-it\Delta}\, A\, e^{it\Delta}$ denotes the operator A in the interaction picture.

Proof. By a direct computation, we see that

(216) $$[\mathsf{L}_0, a_{x,l}] = [\mathrm{d}\Gamma_l(-\Delta), a_{x,l}] = \Delta_x a_{x,l}.$$

Therefore, using the Baker–Campbell–Hausdorff formula

$$e^X Y e^{-X} = Y + [X, Y] + \frac{1}{2!}[X, [X, Y]] + \dots$$

and Equation (216), one can show the conjugation formula

$$\mathsf{U}_t^{(0)*} a_{x,l} \mathsf{U}_t^{(0)} = e^{it\Delta_x} a_{x,l}.$$

Hence, we arrive at the desired identity

$$\mathsf{U}_t^{(0)*}\, \mathrm{d}\Gamma_l(A)\, \mathsf{U}_t^{(0)} = \int_{\mathbb{R}^6} A(z_1, z_2)\, \mathsf{U}_t^{(0)*}\, a_{z_1,l}^*\, a_{z_2,r}\, \mathsf{U}_t^{(0)}\, \mathrm{d}z_1\, \mathrm{d}z_2$$

$$= \int_{\mathbb{R}^6} e^{-it\Delta_{z_1}} A(z_1, z_2)\, e^{it\Delta_{z_2}}\, a_{z_1,l}^*\, a_{z_2,r}\, \mathrm{d}z_1\, \mathrm{d}z_2.$$

This establishes (215a). The proof of Identity (215b) is similar. $\hfill\square$

Proof of Proposition A.1. To prove Proposition A.1, first notice that $\left[\mathsf{U}_t^{(0)}, \mathrm{d}\Gamma(-\Delta)\right] = 0$, which using Formula (212) allows us to write

(217) $$\begin{aligned} \widehat{\mathsf{G}}_t &= \mathsf{U}_t^{(0)*}\left(\mathrm{d}\Gamma_l(V_{\boldsymbol{\rho}} - \mathsf{X}_{\boldsymbol{\rho}}) - \mathrm{d}\Gamma_r(V_{\boldsymbol{\rho}} - \mathsf{X}_{\boldsymbol{\rho}}) \right)\mathsf{U}_t^{(0)} \\ &\quad + \mathsf{U}_t^{(0)*}\left(\tilde{\mathsf{Q}} + \tilde{\mathsf{Q}}^*\right)\mathsf{U}_t^{(0)} + \mathsf{U}_t^{(0)*}\, \mathsf{D}\, \mathsf{U}_t^{(0)} + \mathsf{U}_t^{(0)*}\left(\tilde{\mathsf{P}} + \tilde{\mathsf{P}}^*\right)\mathsf{U}_t^{(0)} \\ &=: \mathrm{I}_t + \mathrm{II}_t + \mathrm{III}_t + \mathrm{IV}_t. \end{aligned}$$

We shall prove the Hölder continuity of $t \mapsto \widehat{\mathsf{G}}_t \Psi$ by proving the property for each term I_t, II_t, III_t, and IV_t. This is the content of the following lemmas A.3, A.4, A.5, A.6. Combining these lemmas leads to the result. $\hfill\square$

Lemma A.3. *Under the conditions of Proposition A.1, there exists a constant C_T depending on the initial conditions such that*

$$\|\partial_t \mathrm{I}_t \Psi\|_{L^\infty((0,T),\mathcal{G})} \le C_T \left(\|\Psi\|_{\mathcal{G}_1} + \|\Psi\|_{\dot{\mathcal{H}}_1^1} \right).$$

Proof of Lemma A.3. It suffices to consider the left contribution since the proof for the right contribution is exactly the same. Let us first handle the term with $V_{\boldsymbol{\rho}}$. Using Identity (215a), we see that

$$i\frac{\mathrm{d}}{\mathrm{d}t}\left(\mathsf{U}_t^{(0)*}\,\mathrm{d}\Gamma_l(V_{\boldsymbol{\rho}})\,\mathsf{U}_t^{(0)} \right) = \mathsf{U}_t^{(0)*}\left(\mathrm{d}\Gamma_l([V_{\boldsymbol{\rho}}, -\Delta]) + \mathrm{d}\Gamma_l(i\partial_t \rho * K) \right) \mathsf{U}_t^{(0)}$$
$$=: \mathsf{J}_1 + \mathsf{J}_2.$$

We start by estimating $\mathsf{J}_1\Psi$. We rewrite the commutator in J_1 by using the fact that

$$\mathrm{d}\Gamma_l([V_{\boldsymbol{\rho}}, -\Delta]) = 2\,\mathrm{d}\Gamma_l(\nabla V_{\boldsymbol{\rho}} \cdot \nabla) + \mathrm{d}\Gamma_l(\Delta V_{\boldsymbol{\rho}})\,.$$

Then, since $\mathsf{U}_t^{(0)}$ is unitary and commutes with ∇, we obtain

$$\left\| \mathsf{U}_t^{(0)*}\,\mathrm{d}\Gamma_l(\nabla V_{\boldsymbol{\rho}} \cdot \nabla)\,\mathsf{U}_t^{(0)}\Psi \right\|_{\mathcal{G}} \le \|\nabla V_{\boldsymbol{\rho}}\|_{L^\infty}\,\|\Psi\|_{\dot{\mathcal{H}}_1^1}\,,$$

where since $\nabla K \in L^{\flat,\infty}$, we have

$$\|\nabla V_{\boldsymbol{\rho}}\|_{L^\infty} \le \sup_{x\in\mathbb{R}^3}\int_{\mathbb{R}^3} |\nabla K(x-y)|\,\rho(y)\,\mathrm{d}y \le \|\nabla K\|_{L^{\flat,\infty}}\,\|\rho\|_{L^{\flat',1}}\,.$$

Similarly, for the second term, by Lemma 8.1 and the fact that $\nabla K \in L^{\flat,\infty}$, we have that

$$\left\| \mathsf{U}_t^{(0)*}\,\mathrm{d}\Gamma_l(\Delta V_{\boldsymbol{\rho}})\,\mathsf{U}_t^{(0)}\Psi \right\|_{\mathcal{G}} \le \|\Delta V_{\boldsymbol{\rho}}\|_{L^\infty}\,\|\Psi\|_{\mathcal{G}_1} \le \|\nabla K\|_{L^{\flat,\infty}}\,\|\nabla\rho\|_{L^{\flat',1}}\,\|\Psi\|_{\mathcal{G}_1}\,.$$

By Proposition 6.1, the norm of ρ in $L^{\flat',1}$ remains bounded for $t \in [0,T]$. When $\flat' \ge 2$, the same holds for $\nabla\rho$. Moreover, since $\hbar = 1$, $\|\nabla\rho\|_{L^1} \le C\,\mathrm{Tr}((1-\Delta)\,\boldsymbol{\rho})$ is also bounded on $[0,T]$ by Proposition 6.1, and so $\nabla\rho$ is in $L^\infty([0,T], L^p)$ for any $p \in [1,4]$. Hence, it follows that

$$\tag{218} \|\mathsf{J}_1\Psi\|_{\mathcal{G}} \le C_T \left(\|\Psi\|_{\mathcal{G}_1} + \|\Psi\|_{\dot{\mathcal{H}}_1^1} \right).$$

For the J_2 term, let us begin by recalling the fact that ρ satisfies the equation

$$\tag{219} \partial_t \rho + \nabla \cdot j_{\boldsymbol{\rho}} = 0$$

where $j_{\boldsymbol{\rho}} = \frac{1}{2}\,\mathrm{diag}(\boldsymbol{\rho}\,\boldsymbol{p} + \boldsymbol{p}\,\boldsymbol{\rho})$ is known as the probability current. Similarly as for J_1, we have the estimate

$$\tag{220} \|\mathsf{J}_2\Psi\|_{\mathcal{G}} = \left\| \mathsf{U}_t^{(0)*}\,\mathrm{d}\Gamma_l(\nabla \cdot (j_{\boldsymbol{\rho}} * K))\,\mathsf{U}_t^{(0)}\Psi \right\|_{\mathcal{G}} \le \|j_{\boldsymbol{\rho}}\|_{L^{\flat',1}}\,\|\nabla K\|_{L^{\flat,\infty}}\,\|\Psi\|_{\mathcal{G}_1}\,.$$

The term $\|j_{\boldsymbol{\rho}}\|_{L^{\flat',1}}$ is bounded as for ρ by Proposition (6.4) and the kinetic energy of $\boldsymbol{\rho}$.

Now let us handle the exchange term $\mathsf{X}_{\boldsymbol{\rho}}$ in term I_t. Note that

$$i\frac{\mathrm{d}}{\mathrm{d}t}\left(\mathsf{U}_t^{(0)*}\,\mathrm{d}\Gamma_l(\mathsf{X}_{\boldsymbol{\rho}})\,\mathsf{U}_t^{(0)} \right) = \mathsf{U}_t^{(0)*}\left(\mathrm{d}\Gamma_l([\mathsf{X}_{\boldsymbol{\rho}}, -\Delta]) + \mathrm{d}\Gamma_l(i\partial_t \mathsf{X}_{\boldsymbol{\rho}}) \right) \mathsf{U}_t^{(0)} =: \mathsf{J}_3 + \mathsf{J}_4.$$

We start by rewriting the J_3 term. Observe we have that

$$\mathrm{d}\Gamma_l([\mathsf{X}_{\boldsymbol{\rho}}, -\Delta]) = 2\,\mathrm{d}\Gamma_l((\mathsf{X}_{\boldsymbol{\nabla}_x \boldsymbol{\rho}}) \cdot \nabla) + \mathrm{d}\Gamma_l(\mathsf{X}_{\boldsymbol{\Delta}_x \boldsymbol{\rho}})\,.$$

The two terms are handled in the same exact manner as before. We will only deal with the second term. By Lemma 8.1 and Inequality (119), we have that

$$(221) \qquad \left\| \mathsf{U}_t^{(0)*} \, \mathrm{d}\Gamma_l(\mathsf{X}_{\boldsymbol{\Delta}_x \boldsymbol{\rho}}) \, \mathsf{U}_t^{(0)} \Psi \right\|_{\mathcal{G}} \leq \left\| \mathsf{X}_{\boldsymbol{\Delta}_x \boldsymbol{\rho}} \right\|_2 \left\| \Psi \right\|_{\mathcal{G}_1} \leq \left\| \boldsymbol{\Delta}_x \boldsymbol{\rho} \, |\boldsymbol{p}|^a \right\|_2 \left\| \Psi \right\|_{\mathcal{G}_1},$$

and since $\hbar = 1$, we have $\boldsymbol{\Delta}_x \boldsymbol{\rho} = - \sum_{j=1}^{3} \left[\boldsymbol{p}_j, \left[\boldsymbol{p}_j, \boldsymbol{\rho} \right] \right]$ and so by Lemma 6.5, $\left\| \boldsymbol{\Delta}_x \boldsymbol{\rho} \, |\boldsymbol{p}|^a \right\|_2 \leq C \left\| \boldsymbol{\rho} \, |\boldsymbol{p}|^{a+2} \right\|_2$ which remains bounded on $[0, T]$ by Proposition 6.1. Hence we have the estimate

$$(222) \qquad \left\| \mathsf{J}_3 \Psi \right\|_{\mathcal{G}} \leq C_T \left(\left\| \Psi \right\|_{\mathcal{G}_1} + \left\| \Psi \right\|_{\dot{\mathcal{H}}_1^1} \right).$$

For the J_4 term, we have that

$$\mathsf{J}_4 = \mathsf{U}_t^{(0)*} \left(\mathrm{d}\Gamma_l \left(\mathsf{X}_{[-\Delta, \boldsymbol{\rho}]} \right) + \mathrm{d}\Gamma_l \left(\mathsf{X}_{[V_{\boldsymbol{\rho}}, \boldsymbol{\rho}]} \right) - \mathrm{d}\Gamma_l \left(\mathsf{X}_{[\mathsf{X}_{\boldsymbol{\rho}}, \boldsymbol{\rho}]} \right) \right) \mathsf{U}_t^{(0)}.$$

To estimate the term with the Laplacian, we proceed as in Inequality (221) and use the fact that since $\hbar = 1$, $[-\Delta, \boldsymbol{\rho}] = |\boldsymbol{p}|^2 \boldsymbol{\rho} - \boldsymbol{\rho} \, |\boldsymbol{p}|^2$. To estimate the second term, we use Inequality (119) to get

$$\left\| \mathsf{X}_{[V_{\boldsymbol{\rho}}, \boldsymbol{\rho}]} \right\|_{\infty} \leq \left\| [V_{\boldsymbol{\rho}}, \boldsymbol{\rho}] \, |\boldsymbol{p}|^a \right\|_{\infty} \leq \left\| [V_{\boldsymbol{\rho}}, \boldsymbol{\rho}] \left(1 + |\boldsymbol{p}|^2 \right) \right\|_{\infty}.$$

Then similarly as in Section 6.3, we write $[V_{\boldsymbol{\rho}}, \boldsymbol{\rho}] \, m = [V_{\boldsymbol{\rho}}, \boldsymbol{\rho} \, m] - [V_{\boldsymbol{\rho}}, m] \, \boldsymbol{\rho}$ and use Proposition 6.5 with $V_{\boldsymbol{\rho}}$ instead of $E_{\boldsymbol{\rho}}$ and Proposition 6.7. Similarly, to bound the last term, we use Inequality (119) and then Proposition 6.9. Hence we have the estimate

$$(223) \qquad \left\| \mathsf{J}_4 \Psi \right\|_{\mathcal{G}} \leq C_T \left\| \Psi \right\|_{\mathcal{G}_1}.$$

The bound on $\partial_t \mathsf{I}_t$ now follows by combining the inequalities for each part, i.e. (218), (220), (222) and (223). $\qquad \square$

Lemma A.4. *Under the conditions of Proposition A.1, there exists a constant C_T depending on the initial conditions such that for any $(t, s) \in [0, T]^2$,*

$$\left\| \left(\mathrm{II}_t - \mathrm{II}_s \right) \Psi \right\|_{\mathcal{G}} \leq C_T \, |t - s|^{\frac{3 - 2a}{7}} \left\| \Psi \right\|_{\mathcal{G}_{3/2}}.$$

Proof of Lemma A.4. To estimate term II, it suffices to focus on the first term of $\tilde{\mathsf{Q}}^*$, which we will denote by $\tilde{\mathsf{Q}}_1^*$. Furthermore, we decompose the singular potential into a long-range part and a singular part as follows

$$(224) \qquad K = K_R^L + K_R^S := C_a \left(\int_0^{R^{-2}} s^{\frac{a}{2} - 1} \varphi_s \, \mathrm{d}s + \int_{R^{-2}}^{\infty} s^{\frac{a}{2} - 1} \varphi_s \, \mathrm{d}s \right).$$

for some R which we will determine shortly, and with $\varphi_s(x) = e^{-\pi |x|^2 s}$. Consequently, we have the decomposition

$$N \, \tilde{\mathsf{Q}}_1^* = \int_{\mathbb{R}^6} \left(K_R^L + K_R^S \right) (x - y) \, \mathrm{d}\Gamma_{l,r}^+ (u \, \delta_x \, v) \, \mathrm{d}\Gamma_{l,r}^+ (u \, \delta_y \, v) \, \mathrm{d}x \, \mathrm{d}y =: \tilde{\mathsf{Q}}_{1,R}^{L*} + \tilde{\mathsf{Q}}_{1,R}^{S*}.$$

For the long-range part, we follow the proof of the bounded potential case as in [11] and show that $\tilde{\mathsf{Q}}_{1,R}^{L*}$ is time differentiable. Applying Lemma A.2 and the operator identity $e^{-it\Delta} A(x) \, e^{it\Delta} = A(x - 2it\nabla)$, we can now rewrite $\tilde{\mathsf{Q}}_{1,R}^L$ as follows

$$\mathsf{U}_t^{(0)*} \tilde{\mathsf{Q}}_{1,R}^{L*} \mathsf{U}_t^{(0)} = \int_{\mathbb{R}^3} \widehat{K_R^L}(y) \, \mathrm{d}\Gamma_{l,r}^+ \left(u_I \, e^{iy \cdot (x - 2it\nabla)} \, v_I \right) \mathrm{d}\Gamma_{l,r}^+ \left(u_I \, e^{-iy \cdot (x - 2it\nabla)} \, v_I \right) \mathrm{d}y,$$

where $A_I := e^{-it\Delta} A \, e^{it\Delta}$ denotes the operator A in the interaction picture. To estimate the time derivative of $\tilde{\mathsf{Q}}_{1,R}^L$, we make the observation that

$$i \, \partial_t(u_I \, e^{iy \cdot (x-2it\nabla)} \, v_I) = e^{-it\Delta} \left(u \left[e^{iy \cdot x}, -\Delta \right] v \right) e^{it\Delta}$$
$$+ e^{-it\Delta} \left([V_{\boldsymbol{\rho}} - \mathsf{X}_{\boldsymbol{\rho}}, u] \, e^{iy \cdot x} v + u \, e^{iy \cdot x} [V_{\boldsymbol{\rho}} - \mathsf{X}_{\boldsymbol{\rho}}, v] \right) e^{it\Delta}.$$

Applying Lemma 8.1, we have the estimates

(225)
$$\left\| \mathrm{d}\Gamma_{l,r}^+ \left(u_I e^{iy \cdot (x-2it\nabla)} v_I \right) \Psi \right\|_{\mathcal{G}} \le 2 \, \|u\|_\infty \, \|v\|_2 \, \|\Psi\|_{\mathcal{G}_1} ,$$
$$\left\| \mathrm{d}\Gamma_{l,r}^+ \left(\partial_t(u_I \, e^{iy \cdot (x-2it\nabla)} \, v_I) \right) \Psi \right\|_{\mathcal{G}} \le C_T \, \langle y \rangle^2 \, \|u\|_\infty \, \|\langle\nabla\rangle \, v\|_2 \, \|\Psi\|_{\mathcal{G}_1} ,$$

where $C_T = C \sup_{t \in [0,T]} \left(1 + \|V_{\boldsymbol{\rho}}\|_{L^\infty} + \|\mathsf{X}_{\boldsymbol{\rho}}\|_\infty \right)$ is finite, and $\langle y \rangle^2 = 1 + |y|^2$. In particular, it follows from (225) that we have the inequality

$$\left\| \frac{\mathrm{d}}{\mathrm{d}t} \mathsf{U}_t^{(0)*} \tilde{\mathsf{Q}}_{1,R}^{L*} \mathsf{U}_t^{(0)} \Psi \right\|_{\mathcal{G}} \le C_T \int_{\mathbb{R}^3} \left| \widehat{K_R^L}(y) \right| \langle y \rangle^2 \, \mathrm{d}y \, \|\Psi\|_{\mathcal{G}_1} .$$

To complete the estimate, we need to compute the L^1-norm of $\widehat{K_R^L}$ to get the explicit dependence of the constant on R. Using the fact that $\widehat{\varphi_s} = s^{-\frac{3}{2}} \varphi_{1/s}$, we have

(226)
$$\int_{\mathbb{R}^3} \left| \widehat{K_R^L} \right| \langle y \rangle^2 \, \mathrm{d}y = \int_0^{R^{-2}} \int_{\mathbb{R}^3} s^{\frac{a-5}{2}} e^{-\frac{\pi}{s}|y|^2} \langle y \rangle^2 \, \mathrm{d}y \, \mathrm{d}s = \frac{3}{\pi} \left(\frac{R^{-(a+2)}}{a+2} + \frac{R^{-a}}{a} \right).$$

Therefore, provided $R < 1$, we obtain the estimate

$$\left\| \frac{\mathrm{d}}{\mathrm{d}t} \left(\mathsf{U}_t^{(0)*} \tilde{\mathsf{Q}}_{1,R}^{L*} \mathsf{U}_t^{(0)} \Psi \right) \right\|_{\mathcal{G}} \le \frac{6}{\pi a} R^{-(a+2)} \|\Psi\|_{\mathcal{G}_1}$$

which implies for any $(t,s) \in [0,T]^2$,

(227)
$$\left\| \left(\mathsf{U}_t^{(0)*} \tilde{\mathsf{Q}}_{1,R}^{L*} \mathsf{U}_t^{(0)} - \mathsf{U}_s^{(0)*} \tilde{\mathsf{Q}}_{1,R}^{L*} \mathsf{U}_s^{(0)} \right) \Psi \right\|_{\mathcal{G}} \le \frac{6}{\pi a} R^{-(a+2)} |t-s| \, \|\Psi\|_{\mathcal{G}_1} .$$

For the singular part, by the Cauchy-Schwarz inequality, we have

$$\left| \langle \Psi_1 \mid \tilde{\mathsf{Q}}_{1,R}^{S*} \Psi_2 \rangle \right| = \left| \int_{\mathbb{R}^3} \left\langle a_l(u_x) \Psi_1 \mid a_r^*(\overline{v_x}) \, \mathrm{d}\Gamma_{l,r}^+ \left(u \, K_{R,x}^S v \right) \Psi_2 \right\rangle \mathrm{d}x \right|$$
$$\le \left(\int_{\mathbb{R}^3} \|a_l(u_x)\Psi_1\|_{\mathcal{G}}^2 \, \mathrm{d}x \right)^{\frac{1}{2}} \left(\int_{\mathbb{R}^3} \left\| a_r^*(\overline{v_x}) \, \mathrm{d}\Gamma_{l,r}^+ \left(u \, K_{R,x}^S v \right) \Psi_2 \right\|_{\mathcal{G}}^2 \, \mathrm{d}x \right)^{\frac{1}{2}} .$$

Applying Lemma 8.1 and the fact that $\|u\|_\infty \le 1$ yields

$$\left\| a_r^*(\overline{v_x}) \, \mathrm{d}\Gamma_{l,r}^+ \left(u \, K_{R,x}^S v \right) \Psi_2 \right\|_{\mathcal{G}} \le (N\rho(x))^{\frac{1}{2}} \left\| K_{R,x}^S v \right\|_2 \|\Psi_2\|_{\mathcal{G}_{1/2}} ,$$

which gives us

$$\left| \langle \Psi_1 \mid \tilde{\mathsf{Q}}_{1,R}^{S*} \Psi_2 \rangle \right| \le C \, N^{\frac{1}{2}} \, \langle \Psi_1 \mid \mathcal{N} \Psi_1 \rangle^{\frac{1}{2}} \left(\int_{\mathbb{R}^3} \rho(x) \left\| K_{R,x}^S v \right\|_2^2 \, \mathrm{d}x \right)^{\frac{1}{2}} \|\Psi_2\|_{\mathcal{G}_{1/2}} .$$

Since $\mathrm{diag}(v^2) = N\,\rho$, we see that

$$\begin{aligned}
\left\|K_{R,x}^S v\right\|_2 &\leq \int_{R^{-2}}^{\infty} s^{\frac{a}{2}-1} \left\|\varphi_{s,x}\, v\right\|_2 \mathrm{d}s \\
&= N^{\frac{1}{2}} \int_{R^{-2}}^{\infty} s^{\frac{a}{2}-1} \left(|\varphi_s|^2 * \rho\right)^{\frac{1}{2}}(x)\, \mathrm{d}s \\
&\leq N^{\frac{1}{2}} \|\rho\|_{L^\infty}^{\frac{1}{2}} \int_{R^{-2}}^{\infty} s^{\frac{a}{2}-1} \|\varphi_s\|_{L^2}\, \mathrm{d}s \leq C_T\, N^{\frac{1}{2}}\, R^{\frac{3}{2}-a}.
\end{aligned}$$

Hence, by duality, it follows that $\left\|\tilde{\mathsf{Q}}_{1,R}^S \Psi\right\|_{\mathcal{G}} \leq R^{\frac{3}{2}-a} \|\Psi\|_{\mathcal{G}_{3/2}}$. By a similar argument, one can also show the same inequality for the dual operator $\tilde{\mathsf{Q}}_{1,R}^{S*}$. Therefore,

$$(228) \qquad\qquad \left\|\tilde{\mathsf{Q}}_{1,R}^{S*}\Psi\right\|_{\mathcal{G}} \leq C_T\, N\, R^{\frac{3}{2}-a} \|\Psi\|_{\mathcal{G}_{3/2}}.$$

Combining (227) and (228), we obtain that for any $(t,s) \in [0,T]^2$ and any $R \in (0,1)$, the following inequality holds

$$\left\|\left(\mathsf{U}_t^{(0)*}\tilde{\mathsf{Q}}_1^*\mathsf{U}_t^{(0)} - \mathsf{U}_s^{(0)*}\tilde{\mathsf{Q}}_1^*\mathsf{U}_s^{(0)}\right)\Psi\right\| \leq C_T \left(R^{-(a+2)}\,|t-s| + R^{\frac{3}{2}-a}\right) \|\Psi\|_{\mathcal{G}_{3/2}}.$$

In particular, if $t \neq s$, one can take $R^{\frac{7}{2}} = \frac{|t-s|}{T} \leq 1$, leading to

$$(229) \qquad \left\|\left(\mathsf{U}_t^{(0)*}\tilde{\mathsf{Q}}_1^*\mathsf{U}_t^{(0)} - \mathsf{U}_s^{(0)*}\tilde{\mathsf{Q}}_1^*\mathsf{U}_s^{(0)}\right)\Psi\right\|_{\mathcal{G}} \leq C_T\,|t-s|^{\frac{3-2a}{7}} \|\Psi\|_{\mathcal{G}_{3/2}}.$$

If $t = s$, we can make $R \to 0$ to obtain the same inequality. $\qquad\square$

Next, let us consider the type III terms.

Lemma A.5. *Under the conditions of Proposition A.1, there exists a constant C_T depending on the initial conditions such that for any $(t,s) \in [0,T]^2$,*

$$\|(\mathrm{III}_t - \mathrm{III}_s)\,\Psi\|_{\mathcal{G}} \leq C_T\,|t-s|^{\frac{3-2a}{7}} \left(\|\Psi\|_{\mathcal{G}_2} + \|\Psi\|_{\dot{\mathcal{H}}_2^{3/2}}\right).$$

Proof of Lemma A.5. Let us focus on the first term of D which we denote by D_1. The proof of Hölder continuity of D_1 is similar to that of $\tilde{\mathsf{Q}}_1$. Using (224), we decompose D_1 into two parts

$$(230) \qquad\qquad 2\,N\,\mathsf{D}_1 = \mathsf{D}_{1,R}^L + \mathsf{D}_{1,R}^S.$$

For the long-range part, we begin by writing

$$\mathsf{U}_t^{(0)*}\mathsf{D}_{1,R}^L\mathsf{U}_t^{(0)} = \int_{\mathbb{R}^3} \widehat{K_R^L}(y)\,\mathrm{d}\Gamma_l\left(u_I\,e^{iy\cdot(x-2it\nabla)}u_I\right)\mathrm{d}\Gamma_l\left(u_I\,e^{-iy\cdot(x-2it\nabla)}u_I\right)\mathrm{d}y.$$

Using the identity

$$(231) \quad i\partial_t(u_I\,e^{iy\cdot(x-2it\nabla)}u_I) = e^{-it\Delta}\left(\eta\,e^{iy\cdot x}u + u\,e^{iy\cdot x}\eta + u\left[e^{iy\cdot x}, -\Delta\right]u\right)e^{it\Delta},$$

where $\eta = [V_{\boldsymbol{\rho}} - \mathsf{X}_{\boldsymbol{\rho}}, u]$, and Lemma 8.1, we deduce the following estimates

$$(232) \qquad \begin{aligned}
\left\|\mathrm{d}\Gamma_l\left(u_I\,e^{iy\cdot(x-2it\nabla)}u_I\right)\Psi\right\|_{\mathcal{G}} &\leq \|\Psi\|_{\mathcal{G}_1} \\
\left\|\mathrm{d}\Gamma_l\left(\partial_t(u_I\,e^{iy\cdot(x-2it\nabla)}u_I)\right)\Psi\right\|_{\mathcal{G}} &\leq \left(\|\eta\|_\infty + |y|^2\right)\|\Psi\|_{\mathcal{G}_1} + |y|\,\|\Psi\|_{\dot{\mathcal{H}}_1^1}.
\end{aligned}$$

By the above inequalities (232) and Formula (226), provided $R \in (0,1)$, we get an estimate of the form

$$\left\|\frac{\mathrm{d}}{\mathrm{d}t}\left(\mathsf{U}_t^{(0)*}\mathsf{D}_{1,R}^L\mathsf{U}_t^{(0)}\right)\Psi\right\|_{\mathcal{G}} \leq C_a\left(1 + \|\eta\|_\infty\right)R^{-(a+2)}\left(\|\Psi\|_{\mathcal{G}_2} + \|\Psi\|_{\dot{\mathcal{H}}_2^1}\right).$$

To handle the singular part, we begin by writing $u = 1 - w$. Then it follows that

$$
\begin{aligned}
\mathsf{D}_{1,R}^S &= \int_{\mathbb{R}^6} K_R^S(x-y)\, a_{x,l}^*\, a_{y,l}^*\, a_l(u_y)\, a_l(u_x)\, \mathrm{d}x\, \mathrm{d}y \\
&\quad + \int_{\mathbb{R}^6} K_R^S(x-y)\, a_l^*(w_x)\, a_l^*(w_y)\, a_l(u_y)\, a_l(u_x)\, \mathrm{d}x\, \mathrm{d}y \\
&\quad - \int_{\mathbb{R}^6} K_R^S(x-y)\, a_{x,l}^*\, a_l^*(w_y)\, a_l(u_y)\, a_l(u_x)\, \mathrm{d}x\, \mathrm{d}y \\
&\quad - \int_{\mathbb{R}^6} K_R^S(x-y)\, a_l^*(w_x)\, a_{y,l}^*\, a_l(u_y)\, a_l(u_x)\, \mathrm{d}x\, \mathrm{d}y \\
&=: \mathsf{I}_1 + \mathsf{I}_2 + \mathsf{I}_3 + \mathsf{I}_4.
\end{aligned}
$$

To estimate I_1, we begin by observing that

$$
(\mathsf{I}_1 \Psi)^{(n,m)}\left(\underline{x}_n, \underline{y}_m\right) = \sum_{1 \le j < k \le n} K_R^S(x_i - x_j)\left(\bar{u}^{(x_j)}\bar{u}^{(x_k)}\Psi^{(n,m)}\right)\left(\underline{x}_n, \underline{y}_m\right)
$$

where $u^{(x_j)}$ is the operator acting on the variable x_j and $\underline{x}_n = (x_1, \ldots, x_n)$. Defining $g(x,y) := \left\| \bar{u}^{(x)}\bar{u}^{(y)}\Psi^{(n,m)}(x, y, \ldots) \right\|_{L^2(\mathbb{R}^{3(n+m-2)})}$, it follows from the triangle inequality and the anti-symmetry of Ψ that

$$
\begin{aligned}
\left\| (\mathsf{I}_1 \Psi)^{(n,m)} \right\|_{L^2} &\le n\,(n-1)\left(\iint_{|z| \le R} \frac{|g(x+z,x)|^2}{|z|^{2a}}\, \mathrm{d}z\, \mathrm{d}x \right)^{\frac{1}{2}} \\
&\le n^2 R^{\frac{3}{2}-a}\left(\int_{\mathbb{R}^3} \left\| \frac{g_{R,x}(z)}{|z|^a} \right\|_{L_z^2(B_1)}^2 \mathrm{d}x \right)^{\frac{1}{2}}
\end{aligned}
$$

where $g_{R,x}(z) = g(x + zR, x)$ and B_1 is the unit ball of $\mathbb{R}^3$. Now let T_{B_1} be the bounded extension operator

$$
T_{B_1} : H^a(B_1) \to H^a(\mathbb{R}^3), \qquad \forall x \in B_1, (T_{B_1}g)(x) = g(x)
$$

which exists as proved for example in [19, Theorem IX.7] when $a \in \mathbb{N}$. One can proceed by interpolation when $a \in \mathbb{R}$. Then one has

$$
\left\| \frac{g_{R,x}(z)}{|z|^a} \right\|_{L_z^2(B_1)} = \left\| \frac{T_{B_1} g_{R,x}(z)}{|z|^a} \right\|_{L_z^2(B_1)} \le \left\| \frac{T_{B_1} g_{R,x}(z)}{|z|^a} \right\|_{L_z^2(\mathbb{R}^3)}
$$

and by Hardy-Rellich's inequality

$$
\left\| \frac{T_{B_1} g_{R,x}(z)}{|z|^a} \right\|_{L_z^2(\mathbb{R}^3)} \le C \left\| (-\Delta)^{\frac{a}{2}} T_{B_1} g_{R,x} \right\|_{L^2(\mathbb{R}^3)} \le C_{T_{B_1}} \left\| g_{R,x} \right\|_{H^a(B_1)}.
$$

For I_1, this leads to

$$
\begin{aligned}
\left\| (\mathsf{I}_1 \Psi)^{(n,m)} \right\|_{L^2} &\le C\, n^2 R^{\frac{3}{2}-a}\left(\iint_{|z| \le 1} \left| (-\Delta)^{\frac{a}{2}} g_{R,x}(z) \right|^2 + |g_{R,x}(z)|^2\, \mathrm{d}x\, \mathrm{d}z \right)^{\frac{1}{2}} \\
&\le C\, n^2 \left(\iint_{|z| \le R} \left| (-\Delta)_z^{\frac{a}{2}} g \right|^2 + \left| R^{-a} g \right|^2 \mathrm{d}z\, \mathrm{d}x \right)^{\frac{1}{2}}.
\end{aligned}
$$

Now by Hölder's inequality and by Sobolev's embedding, for any $\alpha > 0$ and any $f \in H^\alpha$,

$$\int_{|z| \le R} |f(z)|^2 \, \mathrm{d}z \le \|f\|_{L^{2p'}}^2 \|\mathbb{1}_{B_R}\|_{L^p} \le C \, R^{2\alpha} \left\|(-\Delta)^{\alpha/2} f\right\|_{L^2}^2,$$

with $p = \frac{3}{2\alpha}$. In particular, taking $f = (-\Delta)_z^{\frac{a}{2}} g$ and $\alpha = \frac{3}{2} - a$ and taking $f = R^{-a} g$ and $\alpha = \frac{3}{2}$ we obtain for I_1

$$\left\|(\mathsf{I}_1 \Psi)^{(n,m)}\right\|_{L^2} \le C \, n^2 \, R^{\frac{3}{2} - a} \left\|(-\Delta)_x^{3/4} g\right\|_{L^2}.$$

Using the fact that $\|u\|_\infty \le 1$, we can control the L^2 norm on the right-hand side of the above inequality by

$$\left\|(-\Delta)_x^{3/4} g\right\|_{L^2} = \left\|\left(\bar{u}^{(y)} (-\Delta)_x^{3/4} \bar{u}^{(x)} \Psi^{(n,m)}\right)(x, y, \dots)\right\|_{L^2(\mathbb{R}^{3(n+m)})}$$

$$\le \left\|\left((-\Delta)^{3/4} \bar{u}\right)^{(x)} \Psi^{(n,m)}(x, \dots)\right\|_{L^2(\mathbb{R}^{3(n+m)})}$$

and using the fact that $\bar{u} = 1 - \bar{w}$, we finally obtain

$$\|\mathsf{I}_1 \Psi\|_{\mathcal{G}} \le \frac{C}{N} \, R^{\frac{3}{2} - a} \left(\|\Psi\|_{\mathcal{H}_2^{\frac{3}{2}}} + \left\||\boldsymbol{p}|^{\frac{3}{2}} w\right\|_2 \|\Psi\|_{\mathcal{G}_2}\right).$$

The other I_i terms are less singular and treated in the same way, leading to

$$(233) \qquad \left\|\mathsf{U}_t^{(0)*} \mathsf{D}_{1,R}^S \mathsf{U}_t^{(0)} \Psi\right\|_{\mathcal{G}} \le C_T \, R^{\frac{3}{2} - a} \left(\|\mathcal{N}\Psi\|_{\dot{\mathcal{H}}_2^{3/2}} + \|\Psi\|_{\mathcal{G}_2}\right).$$

By the same argument as in the case of $\tilde{\mathsf{Q}}_1$, we see that $\mathsf{U}_t^{(0)*} \mathsf{D}_1 \mathsf{U}_t^{(0)} \Psi$ is also Hölder continuous in time. $\qquad \square$

Finally, let us handle type IV terms.

Lemma A.6. *Under the conditions of Proposition A.1, there exists a constant C_T depending on the initial conditions such that for any $(t, s) \in [0, T]^2$,*

$$\|(\mathrm{IV}_t - \mathrm{IV}_s) \Psi\|_{\mathcal{G}} \le C_T |t - s|^{\frac{3 - 2a}{7}} \left(\|\Psi\|_{\mathcal{H}_2^1} + \|\Psi\|_{\mathcal{G}_2}\right).$$

Proof of Lemma A.6. For this case, it suffices to consider

$$(234) \qquad J_1 = -\int_{\mathbb{R}^3} \mathrm{d}\Gamma_{l,r}^+(u \, \delta_x \, v) \, \mathrm{d}\Gamma_l(u \, [K_x, u]) \, \mathrm{d}x$$

$$(235) \qquad J_{12} = -\int_{\mathbb{R}^3} \mathrm{d}\Gamma_{l,r}^+([K_x, u] \, v + [v, K_x] \, u) \, \mathrm{d}\Gamma_l(\omega_x) \, \mathrm{d}x.$$

Following the same routine as before, we decompose the operators into a long-range part and a singular part using Formula (224). Again, we will denote the decomposition by $J_{1,R}^L + J_{1,R}^S$ and likewise for J_{12}. Applying Lemma A.2, we can now rewrite $J_{1,R}^L$ as follows

$$\mathsf{U}_t^{(0)*} J_{1,R}^L \mathsf{U}_t^{(0)} = \int_{\mathbb{R}^3} \widehat{K_R^L}(y) \, \mathrm{d}\Gamma_{l,r}^+\left(u_I \, e^{-iy \cdot (x - 2it\nabla)} v_I\right) \mathrm{d}\Gamma_l\left(u_I \left[e^{-iy \cdot (x - 2it\nabla)}, w_I\right]\right) \mathrm{d}y.$$

Since we have that

$$i \, \partial_t \left(u_I \left[e^{-iy \cdot (x - 2it\nabla)}, w_I\right]\right) = e^{-it\Delta} \left([V_{\boldsymbol{\rho}} - \mathsf{X}_{\boldsymbol{\rho}}, u] \left[e^{-iy \cdot x}, w\right]\right) e^{it\Delta}$$

$$+ e^{-it\Delta} \left(u \left[\left[e^{iy \cdot x}, -\Delta\right], w\right] + u \left[e^{-iy \cdot x}, [V_{\boldsymbol{\rho}} - \mathsf{X}_{\boldsymbol{\rho}}, w]\right]\right) e^{it\Delta}$$

then by Lemma 8.1, since $\|u\|_\infty \leq 1$ and $\|w\|_\infty \leq 1$, we have the estimate

$$\left\| d\Gamma_l\left(u_I\left[e^{-iy\cdot(x-2it\nabla)}, w_I\right]\right)\Psi \right\|_{\mathcal{G}} \leq 2\|\Psi\|_{\mathcal{G}_1} \tag{236a}$$

$$\left\| d\Gamma_l\left(\partial_t\left(u_I\left[e^{-iy\cdot(x-2it\nabla)}, w_I\right]\right)\right)\Psi \right\|_{\mathcal{G}} \leq \mathcal{C}_T \langle y\rangle^2 \left\|\langle\boldsymbol{p}\rangle^2 w\right\|_2 \|\Psi\|_{\mathcal{G}_1}. \tag{236b}$$

where $\mathcal{C}_T = C\sup_{[0,T]}\left(1 + \|V_{\boldsymbol{\rho}}\|_\infty + \|\mathsf{X}_{\boldsymbol{\rho}}\|_\infty\right)$. In particular, by inequalities (225), (236), and (226), we have that

$$\left\| \frac{d}{dt}\mathsf{U}_t^{(0)*}J_{1,R}^L\mathsf{U}_t^{(0)}\Psi \right\|_{\mathcal{G}} \leq C_T\,R^{-(a+2)}\|\Psi\|_{\mathcal{G}_1}. \tag{237}$$

The singular part follows from Lemma 10.2 and Remark 10.2. More precisely, we have that

$$\left\| \mathsf{U}_t^{(0)*}J_{1,R}^S\mathsf{U}_t^{(0)}\Psi \right\|_{\mathcal{G}} \leq C_T\,R^{\frac{3}{2}-a}\|\Psi\|_{\mathcal{G}_1}. \tag{238}$$

Repeating the argument of $\tilde{\mathsf{Q}}_1$ shows that $\mathsf{U}_t^{(0)*}J_1\mathsf{U}_t^{(0)}\Psi$ is Hölder continuous in time.

Lastly, let us estimate the operator J_{12}. We begin by writing

$$\mathsf{U}_t^{(0)*}J_{12}\mathsf{U}_t^{(0)} = \int_{\mathbb{R}^3} d\Gamma_{l,r}^+([K_{x,I}, w_I]\,v_I)\,d\Gamma_l(\omega_{x,I})\,dx \tag{239a}$$

$$+ \int_{\mathbb{R}^3} d\Gamma_{l,r}^+([K_{x,I}, v_I]\,u_I)\,d\Gamma_l(\omega_{x,I})\,dx. \tag{239b}$$

It suffices to handle Term (239b) since Term (239b) can be treated in a similar manner. Taking its time-derivative yields

$$i\,\partial_t(239\mathrm{b}) = \int_{\mathbb{R}^3} d\Gamma_{l,r}^+(i\partial_t([K_{x,I}, v_I]\,u_I))\,d\Gamma_l(\omega_{x,I})\,dx$$

$$+ \int_{\mathbb{R}^3} d\Gamma_{l,r}^+([K_{x,I}, v_I]\,u_I)\,d\Gamma_l(i\partial_t\omega_{x,I})\,dx =: \mathsf{I}_5 + \mathsf{I}_6.$$

Let us first consider I_6. Notice, we have the identity

$$i\,\partial_t\omega_{x,I} = e^{-it\Delta}\left(2\,\nabla_1\omega_x\cdot\nabla_1 + \Delta_2\omega_x + [V_{\boldsymbol{\rho}} - \mathsf{X}_{\boldsymbol{\rho}}, \omega]_x\right)e^{it\Delta}. \tag{240}$$

In particular, we can write

$$\mathsf{I}_6 = \mathsf{U}_t^{(0)*}\int_{\mathbb{R}^3} d\Gamma_{l,r}^+([K_x, v]\,u)\,d\Gamma_l(2\,\nabla_1\omega_x\cdot\nabla)\,dx\,\mathsf{U}_t^{(0)}$$

$$+ \mathsf{U}_t^{(0)*}\int_{\mathbb{R}^3} d\Gamma_{l,r}^+([K_x, v]\,u)\,d\Gamma_l(\Delta_x\omega_x)\,dx\,\mathsf{U}_t^{(0)}$$

$$+ \mathsf{U}_t^{(0)*}\int_{\mathbb{R}^3} d\Gamma_{l,r}^+([K_x, v]\,u)\,d\Gamma_l\left([V_{\boldsymbol{\rho}} - \mathsf{X}_{\boldsymbol{\rho}}, \omega]_x\right)dx\,\mathsf{U}_t^{(0)}$$

$$=: \mathsf{J}_1 + \mathsf{J}_2 + \mathsf{J}_3.$$

To bound J_1, it suffices to estimate the following quantity

$$\left\| \int_{\mathbb{R}^3}([K_x, v]\,u)(z_1, z_2)\,\nabla_1\omega(x_n, x)\cdot\nabla\Psi^{(n,m)}(\underline{x}_{n-1}, x_n, \underline{y}_n)\,dx \right\|_{L^2(dz_1 dz_2 d\underline{x}_n d\underline{y}_n)} \tag{241}$$

where $\mathrm{d}\underline{x}_n = \mathrm{d}x_1 \ldots \mathrm{d}x_n$. Let us also break the commutator, that is,

$$(241) \leq \left\| \int_{\mathbb{R}^6} \frac{v(z_1, z)\, u(z, z_2)}{|x - z_1|^a} \nabla_1 \omega(x_n, x) \cdot \nabla \Psi^{(n,m)}(\underline{x}_{n-1}, x_n, \underline{y}_n)\, \mathrm{d}x\, \mathrm{d}z \right\|_{L^2(\mathrm{d}z_1 \mathrm{d}z_2 \mathrm{d}\underline{x}_n \mathrm{d}\underline{y}_n)}$$
$$+ \left\| \int_{\mathbb{R}^6} \frac{v(z_1, z)\, u(z, z_2)}{|x - z|^a} \nabla_1 \omega(x_n, x) \cdot \nabla \Psi^{(n,m)}(\underline{x}_{n-1}, x_n, \underline{y}_n)\, \mathrm{d}x\, \mathrm{d}z \right\|_{L^2(\mathrm{d}z_1 \mathrm{d}z_2 \mathrm{d}\underline{x}_n \mathrm{d}\underline{y}_n)}.$$

Since $u = 1 - w$ where w is a Hilbert–Schmidt operator, we will focus on the identity part. Using the fact that $\omega = v^2$ and the Cauchy-Schwarz inequality, we see that

$$\left\| \int_{\mathbb{R}^3} \frac{v(z_1, z_2)}{|x - z_1|^a} \nabla_1 \omega(x_n, x) \cdot \nabla_{x_n} \Psi^{(n,m)}(\underline{x}_{n-1}, x_n, \underline{y}_n)\, \mathrm{d}x \right\|_{L^2(\mathrm{d}z_1 \mathrm{d}z_2 \mathrm{d}\underline{x}_n \mathrm{d}\underline{y}_n)}$$
$$= \left\| \int_{\mathbb{R}^6} \frac{v(z, x)}{|x - z_1|^a} v(z_1, z_2) \nabla_1 v(x_n, z) \cdot \nabla_{x_n} \Psi^{(n,m)}(\underline{x}_{n-1}, x_n, \underline{y}_n)\, \mathrm{d}x\, \mathrm{d}z \right\|_{L^2(\mathrm{d}z_1 \mathrm{d}z_2 \mathrm{d}\underline{x}_n \mathrm{d}\underline{y}_n)}$$
$$\leq \sup_{z_1} \left(\int_{\mathbb{R}^3} \frac{\rho(x)^{\frac{1}{2}}}{|x - z_1|^a}\, \mathrm{d}x \right) \|v\|_2 \|\nabla_1 v\|_{L_x^\infty L_z^2} \left\| \nabla \Psi^{(n)} \right\|_{L^2(\mathrm{d}\underline{x}_n \mathrm{d}\underline{y}_n)},$$

since $\|v_x\|_{L^2} = \rho(x)^{1/2}$. Note that by Young's and Hölder's inequalities,

$$\int_{\mathbb{R}^3} \frac{\rho(x)^{\frac{1}{2}}}{|x - z_1|^a}\, \mathrm{d}x \leq C \left\| \rho^{1/2} \right\|_{L^{\frac{3}{3-a}}} \leq C \int_{\mathbb{R}^3} \rho(x) \langle x \rangle^k\, \mathrm{d}x$$

provided $k > 3 - 2a$. Hence, we have the estimate

$$(242) \qquad\qquad \|\mathsf{J}_1 \Psi\|_{\mathcal{G}} \leq C_T \left(\|\Psi\|_{\mathcal{H}_2^1} + \|\Psi\|_{\mathcal{G}_2} \right).$$

The other two terms J_2 and J_3 can be handled in the same manner since v is sufficiently smooth and $\|V_{\boldsymbol{\rho}}\|_{L^\infty}$ and $\|\mathsf{X}_{\boldsymbol{\rho}}\|_{L_x^\infty L_y^2} \leq C \left\| \boldsymbol{\rho}\, |\boldsymbol{p}|^{2+a} \right\|_2$ are bounded. Thus, it follows that

$$(243) \qquad\qquad \|\mathsf{I}_6 \Psi\|_{\mathcal{G}} \leq C_T \left(\|\Psi\|_{\mathcal{H}_2^1} + \|\Psi\|_{\mathcal{G}_2} \right).$$

Lastly, we handle the I_5 term. Since we have that

$$(244) \qquad \begin{aligned} i\, \partial_t([K_{x,I}, v_I]\, u_I) &= e^{-it\Delta} \left([K_x, v]\, [V_{\boldsymbol{\rho}} - \mathsf{X}_{\boldsymbol{\rho}}, u] \right) e^{it\Delta} \\ &\quad + e^{-it\Delta} \left([[\Delta, K_x], v]\, u + [K_x, [V_{\boldsymbol{\rho}} - \mathsf{X}_{\boldsymbol{\rho}}, v]]\, u \right) e^{it\Delta} \end{aligned}$$

then we can write

$$\begin{aligned} \mathsf{I}_5 &= \mathsf{U}_t^{(0)*} \int_{\mathbb{R}^3} \mathrm{d}\Gamma_{l,r}^+([K_x, v]\, [-V_{\boldsymbol{\rho}} + \mathsf{X}_{\boldsymbol{\rho}}, w])\, \mathrm{d}\Gamma_l(\omega_x)\, \mathrm{d}x\, \mathsf{U}_t^{(0)} \\ &\quad + \mathsf{U}_t^{(0)*} \int_{\mathbb{R}^3} \mathrm{d}\Gamma_{l,r}^+([K_x, [V_{\boldsymbol{\rho}} - \mathsf{X}_{\boldsymbol{\rho}}, v]]\, u)\, \mathrm{d}\Gamma_l(\omega_x)\, \mathrm{d}x\, \mathsf{U}_t^{(0)} \\ &\quad + \mathsf{U}_t^{(0)*} \int_{\mathbb{R}^3} \mathrm{d}\Gamma_{l,r}^+([[\Delta, K_x], v]\, u)\, \mathrm{d}\Gamma_l(\omega_x)\, \mathrm{d}x\, \mathsf{U}_t^{(0)} \\ &=: \mathsf{J}_4 + \mathsf{J}_5 + \mathsf{J}_6. \end{aligned}$$

Term J_4 and J_5 can be estimated in the same manner as in the previous case, since $[-V_{\boldsymbol{\rho}} + \mathsf{X}_{\boldsymbol{\rho}}, w]$ is a bounded operator and $[V_{\boldsymbol{\rho}} - \mathsf{X}_{\boldsymbol{\rho}}, v]$ is a Hilbert–Schmidt operator. Hence, it suffices to estimate J_6.

To bound J_6, it suffices to estimate the following quantity

$$(245) \qquad \left\| \int_{\mathbb{R}^3} [\Delta K_x + 2\nabla K_x \cdot \nabla, v](z_1, z_2) \, \omega(x_n, x) \, \Psi^{(n,m)}(\underline{x}_{n-1}, x_n, \underline{y}_n) \, \mathrm{d}x \right\|_{L^2(\mathrm{d}z_1 \mathrm{d}z_2 \mathrm{d}\underline{x}_n \mathrm{d}\underline{y}_n)}.$$

In the case $a = 1$, we have that

$$(245) \leq C \left\| \int_{\mathbb{R}^3} (v \, \delta_x)(z_1, z_2) \, \omega(x_n, x) \, \Psi^{(n,m)}(\underline{x}_{n-1}, x_n, \underline{y}_n) \, \mathrm{d}x \right\|_{L^2(\mathrm{d}z_1 \mathrm{d}z_2 \mathrm{d}\underline{x}_n \mathrm{d}\underline{y}_n)}$$

$$+ C \left\| \int_{\mathbb{R}^3} \frac{x - z_1}{|x - z_1|^3} \cdot \nabla_1 v(z_1, z_2) \, \omega(x_n, x) \, \Psi^{(n,m)}(\underline{x}_{n-1}, x_n, \underline{y}_n) \, \mathrm{d}x \right\|_{L^2(\mathrm{d}z_1 \mathrm{d}z_2 \mathrm{d}\underline{x}_n \mathrm{d}\underline{y}_n)}.$$

For the first term, we have

$$\left\| v(z_1, z_2) \, \omega(x_n, z_2) \, \Psi^{(n,m)}(\underline{x}_{n-1}, x_n, \underline{y}_n) \right\|_{L^2(\mathrm{d}z_1 \mathrm{d}z_2 \mathrm{d}\underline{x}_n \mathrm{d}\underline{y}_n)}$$

$$\leq \|v\|_{L_x^\infty L_y^2} \|\omega\|_{L_x^\infty L_y^2} \left\| \Psi^{(n)} \right\|_{L^2(\mathrm{d}\underline{x}_n \mathrm{d}\underline{y}_n)} \leq C \|\rho\|_{L^\infty}^{\frac{1}{2}} \left\| \omega \, |\boldsymbol{p}|^2 \right\|_2 \left\| \Psi^{(n)} \right\|_{L^2(\mathrm{d}\underline{x}_n \mathrm{d}\underline{y}_n)}.$$

For the second term, we have

$$\left\| \int_{\mathbb{R}^3} \frac{x - z_1}{|x - z_1|^3} \cdot \nabla_1 v(z_1, z_2) \, \omega(x_n, x) \, \Psi^{(n,m)}(\underline{x}_{n-1}, x_n, \underline{y}_n) \, \mathrm{d}x \right\|_{L^2(\mathrm{d}z_1 \mathrm{d}z_2 \mathrm{d}\underline{x}_n \mathrm{d}\underline{y}_n)}$$

$$\leq C \sup_{z_1} \left(\int_{\mathbb{R}^3} \frac{\rho(x)^{\frac{1}{2}}}{|x - z_1|^2} \, \mathrm{d}x \right) \|\rho\|_{L^\infty}^{\frac{1}{2}} \|\nabla_1 v\|_2 \left\| \Psi^{(n)} \right\|_{L^2(\mathrm{d}\underline{x}_n \mathrm{d}\underline{y}_n)}.$$

where the first integral term is controlled by $\|\rho\|_{L^\infty}^{\frac{1}{2}} + \|\rho\|_{L^1}^{\frac{1}{2}}$. The case when $0 < a < 1$ is similar, except that when $a \leq 1/2$, we need to estimate the last quantity with moments in x. Thus, it follows that

$$(246) \qquad \|\mathsf{I}_5 \Psi\|_{\mathcal{G}} \leq C_T \|\Psi\|_{\mathcal{G}_2}$$

which completes the proof. $\qquad \qquad \square$

References

[1] L. Amour, M. Khodja, and J. Nourrigat. The Semiclassical Limit of the Time Dependent Hartree– Fock Equation: the Weyl Symbol of the Solution. *Analysis & PDE*, 6(7):1649–1674, 2013.

[2] H. Araki. On Quasifree States of CAR and Bogoliubov Automorphisms. *Publications of the Research Institute for Mathematical Sciences*, 6(3):385–442, 1971.

[3] H. Araki and W. Wyss. Representations of canonical anticommutation relations. *Helvetica Physica Acta*, 37(2):136–159, 1964.

[4] A. Athanassoulis, T. Paul, F. Pezzotti, and M. Pulvirenti. Semiclassical Propagation of Coherent States for the Hartree Equation. *Annales Henri Poincaré*, 12(8):1613–1634, 2011.

[5] V. Bach, S. Breteaux, S. Petrat, P. Pickl, and T. Tzaneteas. Kinetic Energy Estimates for the Accuracy of the Time-Dependent Hartree-Fock Approximation with Coulomb Interaction. *Journal de Mathématiques Pures et Appliquées*, 105(1):1–30, Jan. 2016.

[6] J. C. Baez, I. E. Segal, and Z. Zhou. *Introduction to Algebraic and Constructive Quantum Field Theory*. Princeton University Press, July 2014. Publication Title: Introduction to Algebraic and Constructive Quantum Field Theory.

[7] H. Bahouri, J.-Y. Chemin, and R. Danchin. *Fourier Analysis and Nonlinear Partial Differential Equations*, volume 343 of *Grundlehren der mathematischen Wissenschaften*. Springer, Berlin, Heidelberg, Jan. 2011.

[8] C. Bardos, L. Erdös, F. Golse, N. J. Mauser, and H.-T. Yau. Derivation of the Schrödinger–Poisson Equation from the Quantum N-body Problem. *Comptes Rendus Mathematique*, 334(6):515–520, Jan. 2002.

[9] C. Bardos, F. Golse, A. D. Gottlieb, and N. J. Mauser. Mean field dynamics of fermions and the time-dependent Hartree–Fock equation. *Journal de Mathématiques Pures et Appliquées*, 82(6):665–683, June 2003.

[10] C. Bardos, F. Golse, and N. J. Mauser. Weak Coupling Limit of the N-particle Schrödinger Equation. *Methods and Applications of Analysis*, 7(2):275–294, 2000.

[11] N. Benedikter, V. Jaksic, M. Porta, C. Saffirio, and B. Schlein. Mean-Field Evolution of Fermionic Mixed States. *Communications on Pure and Applied Mathematics*, 69(12):2250–2303, 2016.

[12] N. Benedikter, M. Porta, C. Saffirio, and B. Schlein. From the Hartree Dynamics to the Vlasov Equation. *Archive for Rational Mechanics and Analysis*, 221(1):273–334, 2016.

[13] N. Benedikter, M. Porta, and B. Schlein. Mean-field Evolution of Fermionic Systems. *Communications in Mathematical Physics*, 331(3):1087–1131, Nov. 2014.

[14] N. Benedikter, M. Porta, and B. Schlein. Mean-Field Regime for Fermionic Systems. In *Effective Evolution Equations from Quantum Dynamics*, pages 57–78. Springer, 2016.

[15] F. A. Berezin. *The Method of Second Quantization*, volume 24 of *Pure and Applied Physics: a Series of Monographs and Textbooks*. Academic Press, New York, 1966.

[16] J. Bergh and J. Löfström. *Interpolation spaces. An introduction*, volume 223 of *Grundlehren der Mathematischen Wissenschaften*. Springer Berlin Heidelberg, Berlin, Heidelberg, 1976.

[17] N. Boers and P. Pickl. On Mean Field Limits for Dynamical Systems. *Journal of Statistical Physics*, 164(1):1–16, 2015.

[18] W. Braun and K. Hepp. The Vlasov dynamics and its fluctuations in the 1/N limit of interacting classical particles. *Communications in Mathematical Physics*, 56(2):101–113, Jan. 1977.

[19] H. Brezis. *Analyse fonctionnelle : Théorie et applications*. Sciences Sup. Dunod, Paris, nouvelle présentation 2005 edition, May 2005.

[20] J. M. Chadam. The time-dependent Hartree-Fock equations with Coulomb two-body interaction. *Communications in Mathematical Physics*, 46(2):99–104, June 1976.

[21] L. Chen, J. Lee, and M. Liew. Combined Mean-Field and Semiclassical Limits of Large Fermionic Systems. *Journal of Statistical Physics*, 182(2):24, Jan. 2021.

[22] L. Chen, J. O. Lee, and J. Lee. Rate of Convergence towards Hartree Dynamics with Singular Interaction Potential. *Journal of Mathematical Physics*, 59(3):031902, 2018.

[23] L. Chen, J. O. Lee, and B. Schlein. Rate of Convergence Towards Hartree Dynamics. *Journal of Statistical Physics*, 144(4):872–903, 2011.

[24] J. Dereziński and C. Gérard. *Mathematics of Quantization and Quantum Fields*. Cambridge Monographs on Mathematical Physics. Cambridge University Press, Cambridge, Mar. 2013.

[25] R. L. Dobrushin. Vlasov equations. *Functional Analysis and Its Applications*, 13(2):115–123, 1979.

[26] J. Duoandikoetxea. *Fourier Analysis*, volume 29 of *Graduate Studies in Mathematics*. American Mathematical Society, 2001.

[27] A. Elgart, L. Erdős, B. Schlein, and H.-T. Yau. Nonlinear Hartree equation as the mean field limit of weakly coupled fermions. *Journal de Mathématiques Pures et Appliquées*, 83(10):1241–1273, Oct. 2004.

[28] L. Erdös and H.-T. Yau. Derivation of the Nonlinear Schrödinger Equation from a Many Body Coulomb System. *Advances in Theoretical and Mathematical Physics*, 5(6):1169–1205, 2001.

[29] C. Fefferman and R. d. l. Llave. Relativistic stability of matter–I. *Revista Matemática Iberoamericana*, 2(2):119–213, 1986.

[30] A. Figalli, M. Ligabò, and T. Paul. Semiclassical Limit for Mixed States with Singular and Rough Potentials. *Indiana University Mathematics Journal*, 61(1):193–222, 2012.

[31] G. B. Folland. *Harmonic Analysis in Phase Space*, volume 122 of *The Annals of mathematics studies*. Princeton University Press, Princeton, N.J., Mar. 1989. Google-Books-ID: 5rcqrJT9gAgC.

[32] J. Fröhlich and A. Knowles. A Microscopic Derivation of the Time-Dependent Hartree-Fock Equation with Coulomb Two-Body Interaction. *Journal of Statistical Physics*, 145(1):23, Oct. 2011.

[33] F. Golse, C. Mouhot, and T. Paul. On the Mean Field and Classical Limits of Quantum Mechanics. *Communications in Mathematical Physics*, 343(1):165–205, Apr. 2016.

[34] F. Golse and T. Paul. The Schrödinger Equation in the Mean-Field and Semiclassical Regime. *Archive for Rational Mechanics and Analysis*, 223(1):57–94, Jan. 2017.

[35] F. Golse and T. Paul. Empirical Measures and Quantum Mechanics: Application to the Mean-Field Limit. *Communications in Mathematical Physics*, 369(3):1021–1053, Aug. 2019.

[36] F. Golse, T. Paul, and M. Pulvirenti. On the Derivation of the Hartree Equation from the N-Body Schrödinger Equation: Uniformity in the Planck Constant. *Journal of Functional Analysis*, 275(7):1603–1649, Oct. 2018.

[37] S. Graffi, A. Martinez, and M. Pulvirenti. Mean-Field Approximation of Quantum Systems and Classical Limit. *Mathematical Models and Methods in Applied Sciences*, 13(01):59–73, Jan. 2003.

[38] M. G. Grillakis, M. Machedon, and D. Margetis. Second-order corrections to mean field evolution for weakly interacting Bosons. I. *Communications in Mathematical Physics*, 294(1):273–301, Feb. 2010.

[39] C. Hainzl and R. Seiringer. General decomposition of radial functions on R^n and applications to N-body quantum systems. *Letters in Mathematical Physics*, 61:75–84, June 2002.

[40] M. Hauray and P.-E. Jabin. N-particles Approximation of the Vlasov Equations with Singular Potential. *Archive for Rational Mechanics and Analysis*, 183(3):489–524, 2007.

[41] M. Hauray and P.-E. Jabin. Particle approximation of Vlasov equations with singular forces: propagation of chaos. *Annales Scientifiques de l'École Normale Supérieure. Quatrième Série*, 48(4):891–940, 2015.

[42] R. A. Hunt. On L(p, q) spaces. *L'Enseignement Mathématique*, 12:249–276, 1966.

[43] P.-E. Jabin and Z. Wang. Mean Field Limit and Propagation of Chaos for Vlasov Systems with Bounded Forces. *Journal of Functional Analysis*, 271(12):3588–3627, Dec. 2016.

[44] E. Kuz. Rate of Convergence to Mean Field for Interacting Bosons. *Communications in Partial Differential Equations*, 40(10):1831–1854, Oct. 2015.

[45] L. Lafleche. Propagation of Moments and Semiclassical Limit from Hartree to Vlasov Equation. *Journal of Statistical Physics*, 177(1):20–60, July 2019.

[46] L. Lafleche. Global Semiclassical Limit from Hartree to Vlasov Equation for Concentrated Initial Data. *Annales de l'Institut Henri Poincaré C, Analyse non linéaire*, pages 1–26, Feb. 2021.

[47] L. Lafleche and C. Saffirio. Strong Semiclassical Limit from Hartree and Hartree-Fock to Vlasov-Poisson Equation. *arXiv:2003.02926*, pages 1–35, Mar. 2020.

[48] D. Lazarovici. The Vlasov-Poisson Dynamics as the Mean Field Limit of Extended Charges. *Communications in Mathematical Physics*, 347(1):271–289, 2016.

[49] D. Lazarovici and P. Pickl. A Mean Field Limit for the Vlasov–Poisson System. *Archive for Rational Mechanics and Analysis*, 225(3):1201–1231, Sept. 2017.

[50] E. H. Lieb and M. Loss. *Analysis*, volume 14 of *Graduate Studies in Mathematics*. American Mathematical Society, Providence, RI, 2 edition edition, 2001.

[51] P.-L. Lions and T. Paul. Sur les mesures de Wigner. *Revista Matemática Iberoamericana*, 9(3):553–618, 1993.

[52] P. A. Markowich and N. J. Mauser. The Classical Limit of a Self-Consistent Quantum Vlasov Equation. *Mathematical Models and Methods in Applied Sciences*, 3(01):109–124, Feb. 1993.

[53] D. Mitrouskas, S. Petrat, and P. Pickl. Bogoliubov corrections and trace norm convergence for the Hartree dynamics. *Reviews in Mathematical Physics*, page 1950024, Feb. 2019.

[54] H. Narnhofer and G. L. Sewell. Vlasov hydrodynamics of a quantum mechanical model. *Communications in Mathematical Physics*, 79(1):9–24, Mar. 1981.

[55] H. Neunzert and J. Wick. Theoretische und numerische Ergebnisse zur nichtlinearen Vlasov-Gleichung. *Numerische Lösung nichtlinearer partieller Differential- und Integrodifferentialgleichungen*, pages 159–185, 1972. Publisher: Springer, Berlin, Heidelberg.

[56] T. Paul, M. Pulvirenti, and S. Simonella. On the size of chaos in the mean field dynamics. *Archive for Rational Mechanics and Analysis*, 231(1):285–317, Jan. 2019.

[57] S. Petrat. Hartree Corrections in a Mean-field Limit for Fermions with Coulomb Interaction. *Journal of Physics A: Mathematical and Theoretical*, 50(24):244004, 2017.

[58] S. Petrat and P. Pickl. A New Method and a New Scaling for Deriving Fermionic Mean-Field Dynamics. *Mathematical Physics, Analysis and Geometry*, 19(1):3, Mar. 2016.

[59] P. Pickl. A Simple Derivation of Mean Field Limits for Quantum Systems. *Letters in Mathematical Physics*, 97(2):151–164, Aug. 2011.

[60] M. Porta, S. Rademacher, C. Saffirio, and B. Schlein. Mean Field Evolution of Fermions with Coulomb Interaction. *Journal of Statistical Physics*, 166(6):1345–1364, 2017.

[61] R. T. Powers and E. Størmer. Free States of the Canonical Anticommutation Relations. *Communications in Mathematical Physics*, 16(1):1–33, 1970.

[62] M. C. Reed and B. Simon. *Methods of Modern Mathematical Physics: Functional Analysis*, volume 1. Academic Press, New York, revised and enlarged edition, Jan. 1980.

[63] I. Rodnianski and B. Schlein. Quantum Fluctuations and Rate of Convergence Towards Mean Field Dynamics. *Communications in Mathematical Physics*, 291(1):31–61, Oct. 2009.

[64] C. Saffirio. Mean-Field Evolution of Fermions with Singular Interaction. In D. Cadamuro, M. Duell, W. Dybalski, and S. Simonella, editors, *Macroscopic Limits of Quantum Systems*, Springer Proceedings in Mathematics & Statistics, pages 81–99, Cham, 2018. Springer International Publishing.

[65] C. Saffirio. Semiclassical Limit to the Vlasov Equation with Inverse Power Law Potentials. *Communications in Mathematical Physics*, 373(2):571–619, Mar. 2019.

[66] C. Saffirio. From the Hartree equation to the Vlasov-Poisson system: strong convergence for a class of mixed states. *SIAM Journal on Mathematical Analysis*, 52(6):5533–5553, Jan. 2020.

[67] D. Shale and W. F. stinespring. Spinor Representations of Infinite Orthogonal Groups. *Journal of Mathematics and Mechanics*, 14(2):315–322, 1965. Publisher: Indiana University Mathematics Department.

[68] B. Simon. *Trace Ideals and Their Applications: Second Edition*, volume 120 of *Mathematical Surveys and Monographs*. American Mathematical Society, 2 edition edition, 2005.

[69] J. P. Solovej. Many Body Quantum Mechanics. Course notes, University of Vienna, Wien, 2014.

[70] H. Spohn. On the Vlasov hierarchy. *Mathematical Methods in the Applied Sciences*, 3(1):445–455, 1981.

[71] H. Spohn. *Large Scale Dynamics of Interacting Particles*. Texts and monographs in physics. Springer, Berlin, Heidelberg, 1991.

[72] L. Tartar. *An Introduction to Sobolev Spaces and Interpolation Spaces*, volume 3 of *Lecture Notes of the Unione Matematica Italiana*. Springer-Verlag Berlin Heidelberg, Berlin, Heidelberg, 1 edition, 2007.

[73] H. Triebel. *Interpolation Theory, Function Spaces, Differential Operators*. Number 18 in North-Holland Mathematical Library. Elsevier Science, 1978.

[74] J. Weidmann. *Linear Operators in Hilbert Spaces*, volume 68 of *Graduate Texts in Mathematics*. Springer-Verlag, New York, 1980.

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