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From many-body quantum dynamics to the Hartree–Fock and Vlasov equations with singular potentials

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Abstract. In a combined mean-field and semiclassical regime, we consider the time evolution of N fermions interacting through singular pair interaction potentials of the form $\pm|x-y|^{-a}$, which includes the Coulomb and gravitational interactions. We prove that the many-body dynamics of mixed states are well approximated by solutions of the Hartree–Fock and Vlasov equations in terms of Schatten norms. The errors in these approximations are expressed in terms of the expected number of particles, N, and the Planck constant, h. For cases where $a \in (0, 1/2)$, we obtain local-in-time results when $N^{-1/2} \ll h \leq N^{-1/3}$. Notably, this leads to the derivation of the Vlasov equation with singular potentials. For cases where $a \in [1/2, 1]$, our results hold only within a small time scale or require an N-dependent cut-off. A fundamental ingredient in our analysis is the propagation of regularity for solutions to the Hartree–Fock equation uniformly in the Planck constant, which holds for $a \in (0, 1]$.

Keywords: mean-field limit, semiclassical limit, Hartree–Fock equation, many-body Schrödinger equation, Vlasov equation, singular interaction.

Contents

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Part I
Introduction

1. Background

1.1. The equations

We consider a system of N identical fermions with unit mass interacting through a pair potential $K(x-y)$. The state of the system at time t is described by an N-body anti-symmetric wave function $\psi_N = \psi_N(t, x_1, \dots, x_N)$ belonging to the Hilbert space $\mathfrak{h} = L^2(\mathbb{R}^{3N}, \mathbb{C})$ of square-integrable complex-valued functions, with evolution given by the N-body Schrödinger equation

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

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) unsuitable for studies. In fact, the high-dimensionality of the problem presents a formidable barrier for understanding qualitative behaviors of the many-body dynamics from the wave function at the microscopic scale. Instead, one could consider the problem at a macroscopic 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. In particular, we consider scales where the dynamics of a large number of interacting particles can be approximated by the *Vlasov equation*

$$\partial_t f + \xi \cdot \nabla_x f + E_f \cdot \nabla_\xi f = 0, \tag{2}$$

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

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

To explore the connection between the microscopic and macroscopic scales of the system, we consider an intermediate mean-field quantum equation. Roughly speaking, we approximate the many-body effects exerted by the system on each particle 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 classical mechanics, one could 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

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

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 statistics, a more accurate description of their evolution is given by the *Hartree–Fock equation*

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

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

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

1.2. Mean-field and semiclassical scalings

Our goal in this paper is to study simultaneously the *mean-field limit*, corresponding to the approximations made when the number N of particles is large and each pair interaction is weak, and the *semiclassical limit*, corresponding to a change of scales where the Planck constant h becomes negligible. Let us elaborate more on the two scalings.

To understand the dynamics generated by the many-body Schrödinger equation (1) at different scales, it is convenient to recast the equation in its dimensionless form. Suppose L is some characteristic length of the problem and T is some characteristic time scale. Then we define the dimensionless variables

$$\widetilde{x} := x/L \quad \text{and} \quad \widetilde{T} := t/T.$$

We also recast the interaction potential in its dimensionless form via the change of scale

$$\widetilde{K}(\widetilde{x}) := \frac{NT^2}{mL^2}K(x) = \frac{NT^2}{mL^2}K(L\widetilde{x}),$$

where m denotes the mass which we set to 1. If we define the rescaled dimensionless parameter

$$\widetilde{\hbar} = \frac{\hbar T}{mL^2}$$

and the new rescaled wave function

$$\widetilde{\psi}_N(\widetilde{t},\widetilde{x}_1,\dots,\widetilde{x}_N) := L^{dN/2}\psi_N(t,x_1,\dots,x_N),$$

then multiplying (1) by $\frac{T^2}{mL^2}$ yields the dimensionless equation

$$i\widetilde{\hbar}\partial_{\widetilde{t}}\widetilde{\psi}_N = \sum_{k=1}^{N} -\frac{\widetilde{\hbar}^2}{2}\Delta_{\widetilde{x}_k}\widetilde{\psi}_N + \frac{1}{N}\sum_{1\le k<l\le N}\widetilde{K}(\widetilde{x}_k-\widetilde{x}_l)\widetilde{\psi}_N.$$

Moreover, in the case of a homogeneous interaction of the form $K(x) = \kappa|x|^{-a}$ for some parameter $\kappa \in \mathbb{R}$, this gives $\widetilde{K}(\widetilde{x}) = \widetilde{\kappa}|\widetilde{x}|^{-a}$ where $\widetilde{\kappa} = \kappa NT^2/(mL^{2+a})$. From now on, we consider the case of space-time scales where $\widetilde{\kappa}$ is of order 1 and we simply set $\widetilde{\kappa} = 1$. This provides an N^{-1} prefactor in front of the interaction potential which is usually referred to as the *mean-field scaling*. In this class of scales, the dimensionless parameter $\widetilde{\hbar}$ is of the order $L^a/(\kappa NT)$. Furthermore, we shall refer to the scale where $\widetilde{\hbar}$ becomes negligible as the *semiclassical regime*. For convenience, let us express L and T in terms of the parameters N, κ and $\widetilde{\hbar}$:

$$L = \left(\frac{\hbar^2}{m\kappa N\widetilde{\hbar}^2}\right)^{\frac{1}{2-a}}, \quad T = \frac{\widetilde{\hbar}m}{\hbar}\left(\frac{\hbar^2}{m\kappa N\widetilde{\hbar}^2}\right)^{\frac{2}{2-a}}. \tag{7}$$

From now on, we impose the condition $N\widetilde{\hbar}^2 \ll \kappa^{-1}$ to guarantee that $L \gg 1$. In particular, we could set $\kappa = N^{-1}$.

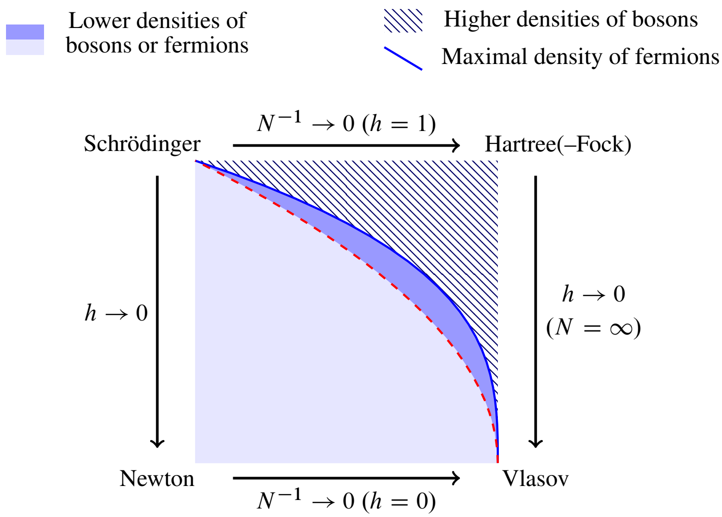

Fig. 1. The different scalings for the combined mean-field and semiclassical limits. The dashed (red) curve corresponds to the equation $h = N^{-1/2}$ and the continuous (blue) curve to $h = N^{-1/3}$.

While $\hbar$ and N can a priori be considered as independent parameters, certain constraints arise when dealing with fermions. In Section 1.4, it is explained that the Pauli principle imposes a limitation on Nh^3, which must remain bounded to ensure convergence of the one-particle density operator to a nonzero function on the phase space. This is in contrast to bosonic systems, which are systems of particles that have permutation symmetry as opposed to the anti-permutation symmetry of fermions, where the Pauli principle does not apply.

In addition, observe that the particle density, defined as the number of particles per unit of characteristic volume, scales as NL^{-3}, where N is the total number of particles. By using the scaling given by (7), we can express the density as

$$N/L^3 \simeq N^{\frac{5-a}{2-a}} h^{\frac{6}{2-a}} \kappa^{\frac{3}{2-a}}.$$

This explains why the region of Figure 1 closer to the Hartree–Fock equation corner corresponds to relatively high densities, while the region below corresponds to relatively low densities. Moreover, note that in this work, we consider h satisfying the constraint $N^{-1/2} \ll h \leq CN^{-1/3}$, which corresponds to the dark shaded region in the figure. It should be noted that the constraint $N^{-1/2} \ll h$, meaning $Nh^2 \to \infty$, could be technical and it arises in the proof of the main result (see Proposition 10.1).

With a little abuse of notation and language, we shall drop the tildes and study the equation

$$i\hbar\partial_t \psi_N = H_N \psi_N, \quad H_N = \sum_{k=1}^{N} -\frac{\hbar^2}{2}\Delta_{x_k} + \frac{1}{N} \sum_{1 \leq k < l \leq N} K(x_k - x_l), \tag{8}$$

where N is large and $\hbar$ is small, and with

$$K(x) = \kappa/|x|^a, \tag{9}$$

where $\kappa \in \mathbb{R}$ is of order 1 and $a \in (0, 1]$.

More precisely, we study the time evolution of N-body fermionic mixed states, which are self-adjoint, positive trace class operators of rank larger than 1. By the spectral theorem, they can be expressed as

$$\boldsymbol{\rho}_N = \sum_{j=1}^{\infty} \lambda_j \, |\psi_j\rangle\langle\psi_j| \quad \text{with } \lambda_j \geq 0, \tag{10}$$

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

$$i\hbar\partial_t \boldsymbol{\rho}_N = [H_N, \boldsymbol{\rho}_N] \tag{11}$$

where the Hamiltonian H_N is given in (8), which is the quantum analogue of the classical Liouville equation, equivalent to the N-body Newton laws.

1.3. State of the art

Both the problems of the mean-field limits and the semiclassical 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 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 considered for twice differentiable potentials in the pioneering works by Neunzert and Wick [58], Braun and Hepp [19], and then by Dobrushin [27] using the Wasserstein–Monge–Kantorovich distance (see also [74] for an introduction to the topic). The class of potentials was then extended to less regular potentials but still locally Hölder continuous by Hauray and Jabin [42,43], which was later improved by Jabin and Wang using entropy methods in [45], where the potential is only required to be bounded.

From another point of view, it was also proved in [17,43] that it is possible to obtain the mean-field limit for potentials with a vanishing cut-off, converging to potentials almost as singular as the Coulomb potential when $N \to \infty$. This is in particular interesting from a numerical point of view. These results were then improved by Lazarovici [50], allowing the cut-off potential to converge to the Coulomb potential, and by Lazarovici and Pickl [51], with N-dependent cut-off 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 obtained by Narnhofer and Sewel [57] in the case of smooth potentials and with $\hbar = N^{-1/3}$. Subsequently, the restriction on the potential was substantially relaxed by Spohn [73] 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 [39] in the case of weak convergence, and more recently by Golse and Paul [36] in the quantum Wasserstein metrics, and by Chen, Lee and Liew for fermions [22] 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 $\hbar = 1$, that is without taking the semiclassical limit, leading to the Hartree and Hartree–Fock equations. In this case, the situation is better understood, even for singular potentials such as the Coulomb and gravitational potentials. For bosons, weak convergence was proved in [8, 10, 30], and explicit rates in stronger norms were obtained in [23, 24, 40, 46, 56, 59, 62, 66]. 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 [5, 34, 60, 61].

Some of these results have been extended by taking into account the semiclassical parameter $\hbar$. For fermions, taking $\hbar = N^{-1/3}$, convergence of the Husimi transform has been proven in [29] for analytic interactions and short times. Schatten norms estimates have been obtained in [13, 14, 61] for at least twice differentiable potentials. Assuming a certain semiclassical structure on the solution of the Hartree equation, a result was obtained in the case of pure states and singular potentials in [63, 67].

For bosons, results were obtained for at least twice differentiable potentials in [35, 37, 38].

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 [54, 55] in weak topology, but including singular potentials such as the Coulomb interaction (see also [32] for the case of quantum Liouville dynamics). Explicit rates in stronger norms were then obtained in [1, 4, 12, 36] for at least twice differentiable potentials, and then in [47–49, 68, 69] for singular interactions.

To our knowledge our work is the first one addressing mixed states (see (10)) in the case of singular interactions of the form (9) and proving in this context the approximation of the mean-field dynamics with the Hartree–Fock equation on time scales of order 1 when $a \in (0, 1/2)$ and up to time scales of order $\sqrt{\hbar}$ when $a \in [1/2, 1]$; see also Remark 3.9.

1.4. Constraints on the scalings

Let $\mathscr{C}_\infty > 0$ be a constant bounded above independently of N and $\hbar$. We restrict ourselves to the class of initial data $\boldsymbol{\rho}$ of the Hartree–Fock equation (5) that satisfies the conditions

$$\begin{aligned} \|\boldsymbol{\rho}\|_\infty &= \mathscr{C}_\infty, \\ \operatorname{Tr}(\boldsymbol{\rho}) &= h^{-3}, \end{aligned} \tag{12}$$

where $\|\cdot\|_\infty$ denotes the operator norm, that is, the largest eigenvalue of $\boldsymbol{\rho}$ is bounded uniformly in $\hbar$ and the sum of its eigenvalues are normalized to h^{-3}. These quantities are invariant under the Hartree–Fock dynamics. As will be clarified in Section 2.1, this choice of normalization makes the connection with classical kinetic theory. In particular, we see that $\int_{\mathbb{R}^3} \rho(x)\,\mathrm{d}x = h^3 \operatorname{Tr}(\boldsymbol{\rho}) = 1$. For such an operator, we define its *Wigner transform* by

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

so that it is a function of the phase space with mass $\iint f_{\boldsymbol{\rho}}\,\mathrm{d}x\,\mathrm{d}\xi = h^3 \operatorname{Tr}(\boldsymbol{\rho}) = 1$. 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. [54]). We refer to [54] for a listing of the properties of the Wigner transform. One of them is

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

where we denote by

$$\|\boldsymbol{\rho}\|_p = (\operatorname{Tr}(|\boldsymbol{\rho}|^p))^{1/p} \tag{14}$$

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 $h^{3/2}\|\boldsymbol{\rho}\|_2 \xrightarrow[h\to 0]{} \|f\|_{L^2(\mathbb{R}^6)}$, so that $\|\boldsymbol{\rho}\|_2$ is of size $h^{-3/2}$.

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

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

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

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

However, in the case of fermions, we also know that (see for instance [53, equation 12.5.12], or [72, Theorem 8.4])

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

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

$$\|\boldsymbol{\rho}_{N:1}\|_2^2 \leq \|\boldsymbol{\rho}_{N:1}\|_1 \|\boldsymbol{\rho}_{N:1}\|_\infty \leq h^{-6}/N. \tag{17}$$

Combining inequality (17) and formula (13) with $\boldsymbol{\rho} = \boldsymbol{\rho}_{N:1}$, we obtain the bound

$$h \leq \mathscr{C}_2^{-2/3} N^{-1/3}, \tag{18}$$

where $\mathscr{C}_2 = \|f_{N:1}\|_{L^2(\mathbb{R}^6)}$ converges to $\|f\|_{L^2(\mathbb{R}^6)}$, which remains of order 1. Hence, we are mainly interested in the case when Nh^3 is bounded above by a constant independent of N and h. In particular, the case when Nh^3 is of order 1 is called the *critical scaling regime*. This corresponds to the blue line in Figure 1.

Notice that our analysis still makes sense if $Nh^3 \to \infty$. 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. Function spaces

2.1. Semiclassical spaces

The Fourier transform is defined by

$$\widehat{g}(\xi) = \int_{\mathbb{R}^3} e^{-2\pi i x\cdot\xi} g(x)\,\mathrm{d}x \tag{19}$$

for $g \in L^2(\mathbb{R}^3)$. 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 scaled Schatten norms:

$$\|\boldsymbol{\rho}\|_{\mathcal{L}^p} = h^{3/p}\|\boldsymbol{\rho}\|_p = h^{3/p}\,\mathrm{Tr}(|\boldsymbol{\rho}|^p)^{1/p}. \tag{20}$$

More generally, given any positive operator m, we define the corresponding weighted spaces by the norm $\|\boldsymbol{\rho}\|_{\mathcal{L}^p(m)} = \|\boldsymbol{\rho} m\|_{\mathcal{L}^p}$. With this choice of scaling of the norm, for any operator $\boldsymbol{\rho} \geq 0$ satisfying the scaling assumptions (12), one obtains

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

One useful property of the norm (20) 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 satisfies, as one would expect, $\|\sqrt{\boldsymbol{\rho}}\|_{\mathcal{L}^2} = 1$ and $\|\sqrt{\boldsymbol{\rho}}\|_{\mathcal{L}^\infty} = \sqrt{\mathscr{C}_\infty}$.

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 [71, Theorem 4.1] reads

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

with equality when $p = 2$, and where $L^p = L^p(\mathbb{R}^3)$. It is the analogue of the identity $\|f(x)g(\xi)\|_{L^p_{x,\xi}} = \|f\|_{L^p}\|g\|_{L^p}$. Another class of examples is the class of Toeplitz operators, namely when $\boldsymbol{\rho}$ is an averaging of coherent states, as presented in Remark 3.3.

We also want to consider the semiclassical version of Sobolev spaces of the phase space. Thus, as in [49], we introduce the operators

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

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

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

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

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

$$\|\boldsymbol{\rho}\|^p_{\dot{\mathcal{W}}^{1,p}(m_n)} := \sum_{\mathrm{j}=1}^{3} \left(\|\boldsymbol{\nabla}_{\xi_\mathrm{j}} \boldsymbol{\rho}\|^p_{\mathcal{L}^p(m_n)} + \|\boldsymbol{\nabla}_{x_\mathrm{j}} \boldsymbol{\rho}\|^p_{\mathcal{L}^p(m_n)}\right),$$
$$\|\boldsymbol{\rho}\|_{\dot{\mathcal{W}}^{1,\infty}(m_n)} := \sup_{\mathrm{j}\in\{1,2,3\}} \left(\|\boldsymbol{\nabla}_{\xi_\mathrm{j}} \boldsymbol{\rho}\|_{\mathcal{L}^\infty(m_n)}, \|\boldsymbol{\nabla}_{x_\mathrm{j}} \boldsymbol{\rho}\|_{\mathcal{L}^\infty(m_n)}\right),$$

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

$$m_n := 1 + |\boldsymbol{p}|^n. \tag{23}$$

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

$$\|\boldsymbol{\rho}\|^p_{\mathcal{W}^{1,p}(m_n)} := \|\boldsymbol{\rho}\|^p_{\mathcal{L}^p(m_n)} + \|\boldsymbol{\rho}\|^p_{\dot{\mathcal{W}}^{1,p}(m_n)}, \tag{24}$$

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

2.2. *Fermionic Fock space*

Let $\mathfrak{h}^{\wedge N} := \mathfrak{h} \wedge \cdots \wedge \mathfrak{h}$ be the n-fold anti-symmetric tensor product of $\mathfrak{h} = L^2(\mathbb{R}^3, \mathbb{C})$. We define the *fermionic* (anti-symmetric) *Fock space* over $\mathfrak{h}$ to be the closure of

$$\mathcal{F}(\mathfrak{h}) = \mathcal{F} := \mathbb{C} \oplus \bigoplus_{n=1}^{\infty} \mathfrak{h}^{\wedge n} \tag{25}$$

with respect to the norm induced by the inner product

$$\langle \psi \mid \varphi \rangle_{\mathcal{F}} = \overline{\psi^{(0)}}\varphi^{(0)} + \sum_{n\geq 1} \int_{\mathbb{R}^{3n}} \overline{\psi^{(n)}(\underline{x}_n)}\, \varphi^{(n)}(\underline{x}_n)\, \mathrm{d}x_1 \cdots \mathrm{d}x_n \tag{26}$$

for any pair of vectors $\psi = (\psi^{(0)}, \psi^{(1)}, \dots)$ and $\varphi = (\varphi^{(0)}, \varphi^{(1)}, \dots)$ in $\mathcal{F}$ where $\underline{x}_k = (x_1, \dots, x_k) \in \mathbb{R}^{3k}$. For simplicity of notation, we will also denote the closure by $\mathcal{F}$. The *vacuum*, defined by the vector

$$\Omega_{\mathcal{F}} = (1, 0, \dots) \in \mathcal{F},$$

describes the state with no particles. We define the *number of particles operator* by

$$\mathcal{N}\psi = (n\psi^{(n)})_{n\in\mathbb{N}} \tag{27}$$

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

$$\boldsymbol{\rho}_N := \sum_{\mathrm{j}\in\mathbb{N}} \lambda_{\mathrm{j}} \, |\psi_{\mathrm{j}}\rangle\langle\psi_{\mathrm{j}}| \tag{28}$$

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

$$\mathrm{Tr}(\boldsymbol{\rho}_N) = \sum_{\mathrm{j}} \lambda_{\mathrm{j}} = h^{-3} \quad \text{and} \quad h^3 \, \mathrm{Tr}(\mathcal{N}\boldsymbol{\rho}_N) = N. \tag{29}$$

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

$$\boldsymbol{\rho}_N^{(n,m)}(\underline{x}_n, \underline{y}_m) = \sum_{\mathrm{j}\in\mathbb{N}} \lambda_{\mathrm{j}} \psi_{\mathrm{j}}^{(n)}(\underline{x}_n) \, \overline{\psi_{\mathrm{j}}^{(m)}(\underline{y}_m)}. \tag{30}$$

As in the case of the one-particle operator given in (20), we define the Fock space semi-classical Schatten norms by

$$\|\boldsymbol{\rho}_N\|_{\mathcal{L}^p(\mathcal{F})} := h^{3/p} \, \mathrm{Tr}_{\mathcal{F}}(|\boldsymbol{\rho}_N|^p)^{1/p}, \tag{31}$$

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 one-particle marginal, by

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

where $\mathrm{Tr}_{2,\dots,n}$ 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 regularity of the solution to the Hartree–Fock equation (5). Let us notice that there are no constraints on the scaling here since we are only considering the mean-field equation. Moreover, this result also holds uniformly in $\hbar$ in the case of the Coulomb potential.

Recall that we work exclusively with the singular interaction potential $K(x) = \kappa|\cdot|^{-a}$ for $0 < a \leq 1$. We define the parameter

$$\mathfrak{b} := \frac{3}{a+1}, \tag{32}$$

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

Theorem 3.1 (Propagation of regularity). *Let $a \in (0,1]$ and $m_n = 1 + |\boldsymbol{p}|^n$ with $n \in 2\mathbb{N}$ satisfying $n \geq 6$, and let $\boldsymbol{\rho}$ be a solution to the Hartree–Fock equation (5) with initial condition $\boldsymbol{\rho}^{\text{in}} \in \mathcal{L}^\infty(m_n)$ satisfying (12) and such that*

$$\boldsymbol{\rho}^{\text{in}} \in \mathcal{W}^{1,2}(m_n) \cap \mathcal{W}^{1,4}(m_{n-2}). \tag{33}$$

Then there exists $T > 0$ such that

$$\boldsymbol{\rho} \in L^\infty([0,T], \mathcal{W}^{1,2}(m_n) \cap \mathcal{W}^{1,4}(m_{n-2})) \tag{34}$$

uniformly in $\hbar \in (0,1)$.

Remark 3.2. When $a \in (0, 1/2)$, we further extend in [25] the local-in-time and uniform-in-$\hbar$ propagation of regularity result of Theorem 3.1 to a global-in-time result.

Remark 3.3 (On the initial data of the Hartree equation). Define $\varphi(x) = e^{-\pi|x|^2/2}$ and $\varphi_{x,\xi}(y) := \frac{1}{h^{9/4}}\varphi(\frac{y-x}{\sqrt{h}})e^{iy\cdot\xi/\hbar}$. 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 a Toeplitz operator (see e.g. [35, 36]) or Wick quantization (see e.g. [52]), as the operator

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

This defines a positive compact operator such that

$$\|\tilde{\boldsymbol{\rho}}_g\|_{\mathcal{L}^\infty} \leq \|g\|_{L^\infty(\mathbb{R}^6)}, \quad \|\tilde{\boldsymbol{\rho}}_g\|_{\mathcal{L}^2} \leq \|g\|_{L^2(\mathbb{R}^6)},$$

and more generally, as proved for example in [54], such that for any convex function Φ with $\Phi(0) = 0$ we have

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

In particular, in Theorem 3.1, we can take $\boldsymbol{\rho}^{\text{in}} = \tilde{\boldsymbol{\rho}}_g$ with $\|g\|_{L^2(\mathbb{R}^6)} = 1$ and $\|g\|_{L^\infty(\mathbb{R}^6)} = \mathcal{C}_\infty^{1/2}$, and then $\boldsymbol{\rho}^{\text{in}}$ satisfies the assumptions (12).

However, we can consider more general operators than simply the averaging of coherent states. Given a function g on the phase space, one can take the inverse of the Wigner transform, called the *Weyl quantization*, to define $\boldsymbol{\rho}_g$ as the operator with integral kernel

$$\boldsymbol{\rho}_g(x,y) = \int_{\mathbb{R}^3} e^{-2i\pi(y-x)\cdot\xi} g\left(\frac{x+y}{2}, h\xi\right) \mathrm{d}\xi. \tag{35}$$

This operator satisfies the hypotheses on the initial condition of Theorem 3.1 if g is sufficiently smooth and decays at infinity, as proved for example in [49, Section 3].

3.2. *Mean-field and semiclassical limits*

To state our mean-field results, we assume there exists a constant $C > 0$ independent of N and $\hbar$ such that

$$N^{-1/2} \ll h \le CN^{-1/3}, \tag{36}$$

where $a \ll b$ means that $a/b \to 0$ as $N \to \infty$. We further assume that the constant $\mathcal{C}_\infty > 0$ satisfies the bound

$$\mathcal{C}_\infty < (Nh^3)^{-1}. \tag{37}$$

We define the following trace class norm over the Fock space weighted by the number operator:

$$\|\boldsymbol{\rho}_N\|_{\mathcal{L}^1_k(\mathcal{F})} := \|(\mathcal{N} + N)^k \boldsymbol{\rho}_N\|_{\mathcal{L}^1(\mathcal{F})}. \tag{38}$$

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

$$\int_{\mathbb{R}^3} \rho^{\mathrm{in}}(x)(1+|x|)^3 \,\mathrm{d}x \le C,$$

where C may depend on h.

Theorem 3.4 (Mean-field limit). *Let $a \in (0, 1/2)$ and assume that conditions (36) and (37) are satisfied. Let $n \in 2\mathbb{N}$ satisfy $n \ge 6$. Let $\boldsymbol{\rho}$ be a solution to the Hartree–Fock equation (5) with initial condition $\boldsymbol{\rho}^{\mathrm{in}} \in \mathcal{L}^\infty(m_n)$ satisfying (12) and such that*

$$\boldsymbol{\rho}^{\mathrm{in}} \in \mathcal{W}^{2,2}(m_n) \cap \mathcal{W}^{2,4}(m_{n-2}), \tag{39a}$$

$$\sqrt{\boldsymbol{\rho}^{\mathrm{in}}} \in \mathcal{W}^{1,2}(m_n) \cap \mathcal{W}^{1,q}(m_{n-2}), \tag{39b}$$

with $q \in [\frac{6}{1-2a}, \infty]$. Then there exist $T > 0$, $\boldsymbol{\rho}^{\mathrm{in}}_{N,\boldsymbol{\rho}} \in \mathcal{L}^1(\mathcal{F})$, $\lambda > 0$ and $C > 0$ such that for any solution $\boldsymbol{\rho}_N$ of the second quantized version of (11) (see (51) below) with initial condition $\boldsymbol{\rho}^{\mathrm{in}}_N \in \mathcal{L}^1(\mathcal{F})$ commuting with $\mathcal{N}$, for any $t \in [0, T]$ and $p \in [1, \infty]$,

$$\|\boldsymbol{\rho}_{N:1} - \boldsymbol{\rho}\|_{\mathcal{L}^p} \le \frac{Ce^{\lambda t}}{\min(N^{1/2}, Nh^{3/p'})} (1 + \|\boldsymbol{\rho}^{\mathrm{in}}_N - \boldsymbol{\rho}^{\mathrm{in}}_{N,\boldsymbol{\rho}}\|_{\mathcal{L}^1_k(\mathcal{F})})$$

for any $k \ge \frac{1}{2p} + \frac{3}{2}\lceil \frac{\ln N}{p \ln(Nh^2)} \rceil$ where $p' = p/(p-1)$ is the Hölder conjugate of p.

Remark 3.5. The N-body operator $\boldsymbol{\rho}^{\mathrm{in}}_{N,\boldsymbol{\rho}}$ is explicitly created from $\boldsymbol{\rho}^{\mathrm{in}}$ via the Bogolyubov transformation (see (77) in Section 4.3). In particular, $\boldsymbol{\rho}^{\mathrm{in}}_{N,\boldsymbol{\rho}}$ is so constructed that its one-particle reduced density matrix coincides with the initial data $\boldsymbol{\rho}^{\mathrm{in}}$ of the Hartree–Fock equation.

Remark 3.6. If $h = N^{-1/3}$, $\|\boldsymbol{\rho}_N^{\mathrm{in}} - \boldsymbol{\rho}_{N,\boldsymbol{\rho}}^{\mathrm{in}}\|_{\mathfrak{L}^1(\mathcal{F})} \leq CN^{-4}$, and $\|\mathcal{N}^4(\boldsymbol{\rho}_N - \boldsymbol{\rho}_{N,\boldsymbol{\rho}})\|_{\mathfrak{L}^1(\mathcal{F})} \leq C$, then for any $t \in [0, T]$, one obtains

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

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

One can combine the above theorem with the result proved in [49] by two of the present 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 3.7 (Combined mean-field and semiclassical limits). *Under the assumptions of Theorem 3.4, assume that f is a positive solution of the Vlasov equation (2) with initial condition satisfying*

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

Moreover, assume $\boldsymbol{\rho}_N^{\mathrm{in}} \in \mathfrak{L}^1(\mathcal{F})$ is such that $[\mathcal{N}, \boldsymbol{\rho}_N^{\mathrm{in}}] = 0$. Then, for any $p \in [1, 2]$, there exist $T > 0$, $C_T > 0$ and an operator $\boldsymbol{\rho}_{N,f}^{\mathrm{in}} \in \mathfrak{L}^1(\mathcal{F})$ such that for any solution $\boldsymbol{\rho}_N$ to the second quantized version of (11) (see (51) below) with initial condition $\boldsymbol{\rho}_N^{\mathrm{in}}$, the estimate

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

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 3.8. In particular, if $\|\boldsymbol{\rho}_N^{\mathrm{in}} - \boldsymbol{\rho}_{N,f}\|_{\mathfrak{L}^1_k(\mathcal{F})} \leq C$ and $p = 2$, then, by (13), we again obtain L^2 convergence with the quantitative bound

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

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

In our result, 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 optimal in terms of the number of particles, while the rate is of order $h = N^{-1/3}$ in the critical scaling. However, we do not claim our results yield the optimal rates.

Remark 3.9. In the case of the Coulomb potential, we can still obtain an estimate for small times or with an N-dependent cut-off (see Theorem 4.1 and Remark 4.3). Our results are summarized in the following table.

Time of validity

	$a \in (0, 1/2)$	$a \in [1/2, 1]$
Semiclassical regularity	$t < T$	$t < T$
Mean-field	$t < T$	$t \ll h^{a-1/2}$ or cut-off
Mean-field + semiclassical	$t < T$	$t \ll h^{a-1/2}$ or cut-off

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 (11) with a mixed state initial data on $\mathfrak{h}^{\wedge N}$ as a problem on the Fock space $\mathscr{F}$. We briefly present the method of second quantization and state the corresponding Hamiltonian evolution problem on $\mathscr{F}$. We refer the interested reader to [6, 15, 26, 33, 65] 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 $\mathscr{F}$ by their actions on the n-sector of $\mathscr{F}$:

$$(a^*(f)\psi)^{(n)}(\underline{x}_n) := \frac{1}{\sqrt{n}} \sum_{j=1}^{n} (-1)^{j-1} f(x_j)\psi^{(n-1)}(\underline{x}_{n\setminus j}),$$
$$(a(f)\psi)^{(n)}(\underline{x}_n) := \sqrt{n+1} \int_{\mathbb{R}^3} \overline{f(x)}\, \psi^{(n+1)}(x, \underline{x}_n)\, \mathrm{d}x,$$

where $\underline{x}_{n\setminus j} := (x_1, \ldots, \not{x}_j, \ldots, x_n)$. Moreover, the action of the annihilation operator on the vacuum of $\mathscr{F}$ is defined to be $a(f)\Omega_{\mathscr{F}} = 0$. Then, we extend the operators linearly to the whole $\mathscr{F}$. It can be easily checked that the collection of creation and annihilation operators on $\mathscr{F}$ satisfies the *canonical anti-commutation relations* (CAR)

$$[a(f), a^*(g)]_+ = \langle f, g\rangle_{\mathfrak{h}}, \quad [a(f), a(g)]_+ = [a^*(f), a^*(g)]_+ = 0 \tag{40}$$

for all $f, g \in \mathfrak{h}$ where $[A, B]_+ = AB + BA$ is the *anti-commutator* of the operators A, B. Moreover, from (40), we have the identity

$$\|a(f)\psi\|^2_{\mathscr{F}} = \|a^*(f)\psi\|^2_{\mathscr{F}} = \|f\|^2_{\mathfrak{h}}\|\psi\|^2_{\mathscr{F}}, \quad \text{so} \quad \|a^\sharp(f)\|_\infty = \|f\|_{\mathfrak{h}} \tag{41}$$

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 $\mathscr{F}$.

At times, it is more convenient to deal with creation and annihilation operators at a given position, say x, 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 x, denoted respectively by a^*_x and a_x, as follows:

$$(a^*_x\psi)^{(n)}(\underline{x}_n) = \frac{1}{\sqrt{n}} \sum_{j=1}^{n} (-1)^{j-1}\delta(x - x_j)\psi^{(n-1)}(\underline{x}_{n\setminus j}), \tag{42a}$$
$$(a_x\psi)^{(n)}(\underline{x}_n) = \sqrt{n+1}\, \psi^{(n+1)}(x, \underline{x}_n). \tag{42b}$$

It is also straightforward to check that a^*_x and a_x satisfy the anti-commutation relations

$$[a_x, a^*_y]_+ = \delta(x - y), \quad [a_x, a_y]_+ = [a^*_x, a^*_y]_+ = 0, \tag{43}$$

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

$$a^*(f) = \int_{\mathbb{R}^3} f(x) a_x^* \, \mathrm{d}x, \quad a(f) = \int_{\mathbb{R}^3} \overline{f(x)} \, a_x \, \mathrm{d}x. \tag{44}$$

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

$$\mathrm{d}\Gamma(O) = 0 \oplus \bigoplus_{n=1}^{\infty} \mathrm{d}\Gamma_n(O), \tag{45}$$

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

$$\mathrm{d}\Gamma_n(O) = \sum_{j=1}^{n} 1_{\mathfrak{h}^{j-1}} \otimes O \otimes 1_{\mathfrak{h}^{n-j}}. \tag{46}$$

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

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

$$\mathrm{d}\Gamma(O) = \int_{\mathbb{R}^6} O(x, y) a_x^* a_y \, \mathrm{d}x \, \mathrm{d}y. \tag{47}$$

In particular, the number operator can be rewritten as

$$\mathcal{N} = \int_{\mathbb{R}^3} a_x^* a_x \, \mathrm{d}x. \tag{48}$$

4.2. *State purification and time evolution*

We define the *Fock space Hamiltonian* by

$$\mathsf{H}_N = \int_{\mathbb{R}^3} a_x^* \left(-\frac{\hbar^2}{2} \Delta_x\right) a_x \, \mathrm{d}x + \frac{1}{2N} \int_{\mathbb{R}^6} K(x-y) a_x^* a_y^* a_y a_x \, \mathrm{d}x \, \mathrm{d}y. \tag{49}$$

By direct computation, 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 for any $\psi \in \mathcal{F}$ by

$$(\mathsf{H}_N \psi)^{(n)} = \mathsf{H}_N^{(n)} \psi^{(n)} = \sum_{k=1}^{n} -\frac{\hbar^2}{2} \Delta_{x_k} \psi^{(n)} + \frac{1}{N} \sum_{k<l}^{n} K(x_l - x_k) \psi^{(n)}, \tag{50}$$

which, on the N-sector of $\mathcal{F}$, coincides with the mean-field Hamiltonian defined in (8). We consider the Cauchy problem

$$i\hbar \partial_t \boldsymbol{\rho}_N = [\mathsf{H}_N, \boldsymbol{\rho}_N] \quad \text{with} \quad \boldsymbol{\rho}_N(t=0) = \boldsymbol{\rho}_N^{\mathrm{in}} = \sum_{\mathrm{j}} \lambda_{\mathrm{j}} \, |\psi_{\mathrm{j}}\rangle\langle\psi_j|, \tag{51}$$

where the data are defined as in (28). Following the idea of [11], we reformulate (51) as an evolution problem of a pure state[1] in the fermionic Fock space

$$\mathcal{G} := \mathcal{F}(\mathfrak{h} \oplus \mathfrak{h}) \tag{52}$$

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 (28) and any orthonormal basis ϕ_j of $\mathcal{F}$, we construct the following Hilbert–Schmidt operator on $\mathcal{F}$:

$$\boldsymbol{\upsilon}_N := \sum_{\mathrm{j}\in\mathbb{N}} \varepsilon_\mathrm{j} \, |\psi_\mathrm{j}\rangle\langle\phi_\mathrm{j}|, \tag{53}$$

where $|\varepsilon_\mathrm{j}|^2 = \lambda_\mathrm{j}$. Then $\boldsymbol{\rho}_N = |\boldsymbol{\upsilon}_N|^2$, which is called the *Schmidt decomposition* of $\boldsymbol{\rho}_N$. In particular, the scaled Hilbert–Schmidt norm of $\boldsymbol{\upsilon}_N$, defined by $\|\boldsymbol{\upsilon}\|^2_{\mathcal{L}^2(\mathcal{F})} = h^3 \operatorname{Tr}(|\boldsymbol{\upsilon}|^2)$, is

$$\|\boldsymbol{\upsilon}_N\|^2_{\mathcal{L}^2(\mathcal{F})} = \|\boldsymbol{\rho}_N\|_{\mathcal{L}^1(\mathcal{F})} = 1. \tag{54}$$

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

Recall that the space $\mathcal{L}^2(\mathcal{F})$ of Hilbert–Schmidt operators 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 $|\psi\rangle\langle\phi| \mapsto h^{-3/2}\overline{\phi} \otimes \psi$. One can then associate to $\boldsymbol{\upsilon}_N$ an element of $\mathcal{F}(\mathfrak{h}) \otimes \mathcal{F}(\mathfrak{h})$ as follows:

$$\mathsf{J}\boldsymbol{\upsilon}_N = h^{-3/2} \sum_{\mathrm{j}\in\mathbb{N}} \varepsilon_\mathrm{j} \, \overline{\phi}_\mathrm{j} \otimes \psi_\mathrm{j}. \tag{55}$$

Furthermore, we can associate to every element (55) a vector in the double Fock space $\mathcal{G}$ via the isomorphism $\mathsf{U} : \mathcal{F} \otimes \mathcal{F} \to \mathcal{G}$ defined by setting, for $F \in \mathfrak{h}^{\wedge n}$ and $G \in \mathfrak{h}^{\wedge m}$,

$$\mathsf{U}(F \otimes G) = \sqrt{\frac{(n+m)!}{n!m!}} \, (J_l^{\otimes n} F) \otimes_a (J_r^{\otimes m} G), \tag{56}$$

where $J_l, J_r : \mathfrak{h} \to \mathfrak{h} \oplus \mathfrak{h}$ are respectively the canonical embeddings of $\mathfrak{h}$ into the *left* and *right* coordinate of $\mathfrak{h} \oplus \mathfrak{h}$, and $\otimes_a$ is the anti-symmetric tensor product. Then we extend the mapping linearly to the entire $\mathcal{F} \otimes \mathcal{F}$. The unitary map U is known as the *exponential law for Fock spaces* and it has the following properties (see [26, Theorem 3.43] or [6, Chapter 3]):

$$\Omega_\mathcal{G} = \mathsf{U}(\Omega_\mathcal{F} \otimes \Omega_\mathcal{F}), \tag{57a}$$

$$a_l^\sharp(f) := a^\sharp(f \oplus 0) = \mathsf{U}(a^\sharp(f) \otimes 1)\mathsf{U}^*, \tag{57b}$$

$$a_r^\sharp(f) := a^\sharp(0 \oplus f) = \mathsf{U}((-1)^\mathcal{N} \otimes a^\sharp(f))\mathsf{U}^*, \tag{57c}$$

[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.

where $a^\sharp$ is either a or a^* and $f \in \mathfrak{h}$. 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 $f, g \in \mathfrak{h}$.

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

$$\begin{aligned}
(a_{x,l}^*\Psi)^{(n,m)}(\underline{x}_n, \underline{y}_m) &:= \frac{1}{\sqrt{n}} \sum_{j=1}^{n} (-1)^{j-1} \delta(x - x_j) \Psi^{(n-1,m)}(\underline{x}_{n\setminus j}, \underline{y}_m),\\
(a_{x,l}\Psi)^{(n,m)}(\underline{x}_n, \underline{y}_m) &:= \sqrt{n+1}\, \Psi^{(n+1,m)}(x, \underline{x}_n, \underline{y}_m),\\
(a_{x,r}^*\Psi)^{(n,m)}(\underline{x}_n, \underline{y}_m) &:= \frac{1}{\sqrt{m}} \sum_{j=1}^{m} (-1)^{n+j-1} \delta(x - y_j) \Psi^{(n,m-1)}(\underline{x}_n, \underline{y}_{m\setminus j}),\\
(a_{x,r}\Psi)^{(n,m)}(\underline{x}_n, \underline{y}_m) &:= (-1)^n \sqrt{m+1}\, \Psi^{(n,m+1)}(\underline{x}_n, x, \underline{y}_m).
\end{aligned}$$

This allows us to express $a_\sigma^\sharp(f)$ for $f \in \mathfrak{h}$ in terms of operator-valued distributions:

$$a_\sigma(f) = \int_{\mathbb{R}^3} \overline{f(x)}\, a_{x,\sigma} \,\mathrm{d}x \quad \text{and} \quad a_\sigma^*(f) = \int_{\mathbb{R}^3} f(x) a_{x,\sigma}^* \,\mathrm{d}x, \tag{58}$$

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

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

$$\begin{aligned}
\mathrm{d}\Gamma_l(O) &:= \mathrm{d}\Gamma(O \oplus 0) = \mathsf{U}(\mathrm{d}\Gamma(O) \otimes 1)\mathsf{U}^* = \int_{\mathbb{R}^6} O(x, y) a_{x,l}^* a_{y,l} \,\mathrm{d}x \,\mathrm{d}y,\\
\mathrm{d}\Gamma_r(O) &:= \mathrm{d}\Gamma(0 \oplus O) = \mathsf{U}(1 \otimes \mathrm{d}\Gamma(O))\mathsf{U}^* = \int_{\mathbb{R}^6} O(x, y) a_{x,r}^* a_{y,r} \,\mathrm{d}x \,\mathrm{d}y.
\end{aligned}$$

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

$$\mathcal{N} = \mathcal{N}_l + \mathcal{N}_r = \mathsf{U}(\mathcal{N} \otimes 1 + 1 \otimes \mathcal{N})\mathsf{U}^*. \tag{59}$$

We shall denote by

$$\mathsf{I}_{\mathcal{G}} := \mathsf{U}\mathsf{J} \tag{60}$$

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 as a Cauchy problem for pure states defined on the double Fock space $\mathcal{G}$. Recall that the solution to the Cauchy problem (51) in the Schrödinger picture is given by

$$\boldsymbol{\rho}_N = e^{-i(t/\hbar)\mathsf{H}_N} \boldsymbol{\rho}_N^{\mathrm{in}} e^{i(t/\hbar)\mathsf{H}_N}. \tag{61}$$

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

$$\boldsymbol{v}_N = e^{-i(t/\hbar)\mathsf{H}_N}\boldsymbol{v}_N^{\text{in}} e^{i(t/\hbar)\mathsf{H}_N}. \tag{62}$$

Then $\boldsymbol{\rho}_N = |\boldsymbol{v}_N|^2$ solves (11) with initial data $\boldsymbol{\rho}_N^{\text{in}} = |\boldsymbol{v}_N^{\text{in}}|^2$. In the double Fock space $\mathscr{G}$, this corresponds to saying that the evolution is given by $\Phi = \Phi(t)$ with

$$\Phi := \mathsf{I}_{\mathscr{G}}(\boldsymbol{v}_N) = e^{-i(t/\hbar)\mathsf{L}_N}\mathsf{I}_{\mathscr{G}}(\boldsymbol{v}_N^{\text{in}}) = e^{-i(t/\hbar)\mathsf{L}_N}\Phi^{\text{in}}, \tag{63}$$

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

$$\operatorname{Tr}_{\mathscr{F}}(\mathsf{O}\boldsymbol{\rho}_N) = \langle \Phi \,|\, (\mathsf{O} \otimes 1)\Phi\rangle_{\mathscr{G}} = \operatorname{Tr}_{\mathscr{G}}((\mathsf{O} \otimes 1)|\Phi\rangle\langle\Phi|), \tag{64}$$

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: the integral kernel of $\boldsymbol{\rho}_{N:1}$ is given by

$$\boldsymbol{\rho}_{N:1}(x, y) = \frac{1}{Nh^3}\langle \Phi \,|\, a_{x,l}^* a_{y,l}\Phi\rangle. \tag{65}$$

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

4.3. Bogolyubov transformation and quasi-free states

In general, we do not know if the evolution of the Cauchy problem (51) can be well-approximated by its mean-field dynamics. Therefore, it is natural to restrict our studies to a subclass of initial data. As stated in [11], equilibrium states at finite positive temperature are believed to be well-approximated by mixed quasi-free states. In the particular case of noninteracting fermions at positive temperature, equilibrium states are exactly described by mixed quasi-free states (see [18]). Furthermore, mixed quasi-free states have the important property that they can be represented by the action of a Bogolyubov transformation on the vacuum of the double Fock space $\mathscr{G}$, 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 Bogolyubov transformation in the framework of the double Fock space $\mathscr{G}$ and construct a class of quasi-free states exhibiting the structure of pure states in $\mathscr{G}$, with average number N of particles and pairing density equal to zero. We follow closely the presentation given in [72].

4.3.1. Bogolyubov 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

$$\begin{aligned} A(f, g) &:= a(f) + a^*(\overline{g}) = a_l(f_1) + a_r(f_2) + a_l^*(\overline{g}_1) + a_r^*(\overline{g}_2), \\ A^*(f, g) &:= (A(f, g))^* = a_l(\overline{g}_1) + a_r(\overline{g}_2) + a_l^*(f_1) + a_r^*(f_2). \end{aligned}$$

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

$$A^*(f, g) = A(C(f, g)) \tag{66}$$

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 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 that the collection of field operators satisfy the anti-commutation relations

$$[A(f, g), A^*(h, k)]_+ = \langle (f, g) \,|\, (h, k) \rangle_{(\mathfrak{h}\oplus\mathfrak{h})\oplus(\mathfrak{h}\oplus\mathfrak{h})}, \quad [A^\sharp(f, g), A^\sharp(h, k)]_+ = 0, \tag{67}$$

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 *Bogolyubov* (canonical) *transformation* of $(\mathfrak{h} \oplus \mathfrak{h}) \oplus (\mathfrak{h} \oplus \mathfrak{h})$ provided it preserves the anti-commutation relations (67), that is,

$$[A(\nu(f, g)), A^*(\nu(h, k))]_+ = \langle (f, g) \,|\, (h, k) \rangle_{(\mathfrak{h}\oplus\mathfrak{h})\oplus(\mathfrak{h}\oplus\mathfrak{h})} \tag{68}$$

for all $f, g, h, k \in \mathfrak{h} \oplus \mathfrak{h}$, and likewise for the other relations. Hence, it follows from (66) and (68) that ν is a Bogolyubov transformation provided it satisfies the conditions

$$\nu C = C \nu \quad \text{and} \quad \nu^* \nu = \nu \nu^* = I, \tag{69}$$

where I is the corresponding identity map.

It is more convenient to express conditions (69) as follows: ν is a Bogolyubov 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

$$U^* U + V^* V = I \quad \text{and} \quad U^* \overline{V} + V^* \overline{U} = 0 \tag{70}$$

such that ν has the form

$$\nu = \begin{pmatrix} U & \overline{V} \\ V & \overline{U} \end{pmatrix}. \tag{71}$$

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

$$\mathsf{R}_\nu^* A(f, g) \mathsf{R}_\nu = A(\nu(f, g)) \tag{72}$$

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 [70]: 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 Bogolyubov transformation. It is common to refer to R_ν as the Bogolyubov transformation on $\mathcal{G}$.

4.3.2. Quasi-free states. A fermionic state $\boldsymbol{\rho}_N$ on $\mathcal{F}$ is said to be *quasi-free* provided it has the following factorization properties:

$$\mathrm{Tr}_{\mathcal{F}} \left(a^{\sharp_1}(f_1) \cdots a^{\sharp_{2n+1}}(f_{2n+1}) \boldsymbol{\rho}_N \right) = 0, \tag{73a}$$

$$\mathrm{Tr}_{\mathcal{F}} \left(a^{\sharp_1}(f_1) \cdots a^{\sharp_{2n}}(f_{2n}) \boldsymbol{\rho}_N \right) = \sum_\sigma (-1)^\sigma \prod_{j=1}^n \mathrm{Tr}_{\mathcal{F}} \left(a^{\sharp_{\sigma(2j-1)}}(f_{\sigma(2j-1)}) a^{\sharp_{\sigma(2j)}}(f_{\sigma(2j)}) \boldsymbol{\rho}_N \right), \tag{73b}$$

where $f_k \in \mathfrak{h}$ and the sum is over all permutations σ of $\{1, \ldots, 2n\}$ satisfying

$$\forall j \in \{1, \ldots, n\}, \quad \sigma(2j-1) < \sigma(2j), \quad \text{and} \quad \sigma(2j-1) < \sigma(2j+1) \text{ if } j < n.$$

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 (73) 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 their generalized one-particle reduced density matrix, it can be shown that a pure quasi-free state Φ on $\mathscr{G}$ can be written as $\Phi = \mathsf{R}_\nu \Omega$ for some Bogolyubov transformation R_ν.

Let us now construct the Bogolyubov transformation and its corresponding class of quasi-free states that we will study in Part III. Let ω be a one-particle density operator on $\mathfrak{h}$ with $0 \le \omega \le 1$ and $\operatorname{Tr}(\omega) = N$. Define $\nu : (\mathfrak{h} \oplus \mathfrak{h}) \oplus (\mathfrak{h} \oplus \mathfrak{h}) \to (\mathfrak{h} \oplus \mathfrak{h}) \oplus (\mathfrak{h} \oplus \mathfrak{h})$ by (71) with U and V having the explicit forms

$$U = \begin{pmatrix} u & 0 \\ 0 & \overline{u} \end{pmatrix} \quad \text{and} \quad V = \begin{pmatrix} 0 & \overline{v} \\ -v & 0 \end{pmatrix} \tag{74}$$

with

$$u := \sqrt{1-\omega} \quad \text{and} \quad v := \sqrt{\omega}. \tag{75}$$

Notice that U and V satisfy (70), which means ν is a Bogolyubov transformation. Furthermore, V is a Hilbert–Schmidt operator. Indeed, since $\operatorname{Tr}(V^*V) = 2\operatorname{Tr}(\omega) = 2N$ is clearly finite, it follows that, by the Shale–Stinespring condition [70], ν is implementable. Hence, there exists a unitary map $\mathsf{R}_\nu : \mathscr{G} \to \mathscr{G}$ implementing ν. Consequently, (72) yields the relations

$$\begin{aligned} \mathsf{R}_\nu^* a_{x,l} \mathsf{R}_\nu &= a_l(u_x) - a_r^*(\overline{v}_x), \\ \mathsf{R}_\nu^* a_{x,r} \mathsf{R}_\nu &= a_r(\overline{u}_x) + a_l^*(v_x). \end{aligned}$$

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

Let us now use the Bogolyubov transformation to represent quasi-free mixed states. The construction we present here is an example of the well-known Araki–Wyss representation [2, 3, 26]. More precisely, we are interested in constructing a quasi-free mixed state with one-particle reduced density $\boldsymbol{\rho}$ on the double Fock space $\mathscr{G}$. To this end, we define $\mathsf{R}_{\boldsymbol{\rho}}$ as the Bogolyubov transform with

$$\omega = Nh^3 \boldsymbol{\rho}$$

and let the unitary map $\mathsf{R}_{\boldsymbol{\rho}}$ act on the vacuum $\Omega_{\mathscr{G}}$, i.e.

$$\Phi_{\boldsymbol{\rho}} := \mathsf{R}_{\boldsymbol{\rho}} \Omega_{\mathscr{G}} \in \mathscr{G}. \tag{76}$$

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

$$\begin{aligned} \boldsymbol{\rho}_{N:1}(x,y) &= \frac{1}{Nh^3} \langle \Phi_{\boldsymbol{\rho}} \,|\, a_{l,y}^* a_{l,x} \Phi_{\boldsymbol{\rho}} \rangle = \frac{1}{Nh^3} \langle \Omega_{\mathscr{G}} \,|\, \mathsf{R}_{\boldsymbol{\rho}}^* a_{l,y}^* \mathsf{R}_{\boldsymbol{\rho}} \mathsf{R}_{\boldsymbol{\rho}}^* a_{l,x} \mathsf{R}_{\boldsymbol{\rho}} \Omega_{\mathscr{G}} \rangle \\ &= \frac{1}{Nh^3} \langle \Omega_{\mathscr{G}} \,|\, a_l(\overline{v_y}) a_r^*(\overline{v_x}) \Omega_{\mathscr{G}} \rangle = \frac{1}{Nh^3} (v^* v)(x,y) = \boldsymbol{\rho}(x,y). \end{aligned}$$

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 the *pairing density*, is zero. Indeed,

$$\alpha_{\Phi_{\boldsymbol{\rho}}}(x,y) := \langle \mathsf{R}_{\boldsymbol{\rho}}\Omega_{\mathscr{G}} \,|\, a_{l,y}a_{l,x}\mathsf{R}_{\boldsymbol{\rho}}\Omega_{\mathscr{G}}\rangle = \langle \Omega_{\mathscr{G}} \,|\, a_l(u_y)a_l(\overline{v}_x)\Omega_{\mathscr{G}}\rangle = 0,$$

where we have used $[a_l(u_y), a_r^*(\overline{v_x})]_+ = 0$. 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 3.4, by

$$\boldsymbol{\rho}_{N,\boldsymbol{\rho}} = |\mathsf{I}_{\mathscr{G}}^{-1}(\Phi_{\boldsymbol{\rho}})|^2. \tag{77}$$

4.4. The general result

In this section, we state a more general result from which our main results will follow. The result is obtained by controlling the growth of the weighted norm

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

Theorem 4.1. *Let $a \in [0,1]$ and assume condition (36) is satisfied. Let $(k,n) \in \mathbb{N}^2$ and $\alpha \in [0,1]$ satisfy $n \geq 6$ and $\alpha > a - 1/2$. Let $\boldsymbol{\rho}$ be a solution of the Hartree–Fock equation (5) with initial condition $\boldsymbol{\rho}^{\mathrm{in}} \in \mathcal{L}^\infty(m_n)$ satisfying (12) and such that*

$$\boldsymbol{\rho}^{\mathrm{in}} \in \mathcal{W}^{2,2}(m_n) \cap \mathcal{W}^{2,4}(m_{n-2}), \tag{78}$$

$$\sqrt{\boldsymbol{\rho}^{\mathrm{in}}} \in \mathcal{W}^{1,2}(m_n) \cap \mathcal{W}^{1,q}(m_{n-2}), \tag{79}$$

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

$$3/q \in [2(\alpha - a - 1/4), \alpha - a + 1/2]. \tag{80}$$

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

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

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 have assumed we know the perturbation of the vacuum, Ψ^{in}. As done in (77) for the reference state $\boldsymbol{\rho}_{N,\boldsymbol{\rho}}$, we can associate to Ψ^{in} an operator $\boldsymbol{\rho}_N = |\mathsf{I}_{\mathscr{G}}^{-1}(\mathsf{R}_{\boldsymbol{\rho}}\Psi)|^2$ which solves the Schrödinger equation (51).

Remark 4.2. In particular, notice that

$$\frac{h^{2k(\alpha-1)}}{N^{k-1/p}} \leq 1 \iff k \geq \frac{\ln N}{p\ln(N h^{2(1-\alpha)})}.$$

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

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

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

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

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

Remark 4.3. When $a \geq 1/2$, one can also consider the potential with an h-dependent cut-off. For example, a way to get a potential bounded at distance $|x| \leq R$ is to take

$$K_R(x) = \frac{\omega_a \kappa}{2} \int_0^{R^{-2}} s^{a/2-1} e^{-\pi|x|^2 s} \, \mathrm{d}s \xrightarrow[R\to 0]{} \kappa \frac{1}{|x|^a}, \tag{81}$$

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

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

Thus, one obtains a quantitative convergence result as long as $R > 4\lambda^2 t^2/(\ln N)^2$.

Remark 4.4. Let $\boldsymbol{\rho}_{N,\boldsymbol{\rho}}$ be defined by (77). Then the standard deviation of the number of particles, $\sigma_{\mathcal{N}}^2 := h^3 \operatorname{Tr}(\mathcal{N}^2 \boldsymbol{\rho}_{N,\boldsymbol{\rho}}) - (h^3 \operatorname{Tr}(\mathcal{N} \boldsymbol{\rho}_{N,\boldsymbol{\rho}}))^2$, is given by

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

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

Notice also that $\sigma_{\mathcal{N}} = 0 \Leftrightarrow \omega = \omega^2 \Leftrightarrow \mathcal{C}_2^2 N h^3 = 1$. 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 $N h^3 = \mathcal{C}_2^{-2}$. In this case, the regularity conditions (33) are not expected to hold. However, it is a good question to ask whether it is possible to find a state $\boldsymbol{\rho}_N = |\mathsf{I}_{\mathcal{G}}^{-1}(\mathsf{R}_{\boldsymbol{\rho}} \Psi)|^2$ with a fixed number of particles but still close to $\boldsymbol{\rho}_{N,\boldsymbol{\rho}}$, in the sense that the associated Ψ satisfies $\|\Psi\|_{\mathcal{G}_5} \ll N^{1/2}$.

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 3.4.

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

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

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

$$\partial_t(\nabla_x f) = -\mathsf{T}\nabla_x f - \nabla E \cdot \nabla_\xi f, \quad \partial_t(\nabla_\xi f) = -\mathsf{T}\nabla_\xi f - \nabla_x f. \tag{82}$$

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

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

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 observe that $\mathsf{T}^* = -\mathsf{T}$ and $\mathsf{T}(uv) = u\mathsf{T}(v) + \mathsf{T}(u)v$, so that by writing $u^p := |u|^{p-1}u$, we have

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

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,

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

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

$$\begin{aligned}\iint_{\mathbb{R}^6} (\nabla_x f)^{p-1} \cdot \nabla E \cdot \nabla_\xi f m \,\mathrm{d}x\,\mathrm{d}\xi &\leq \|\nabla K * \nabla\rho\|_{L^\infty} \iint_{\mathbb{R}^6} |\nabla_x f|^{p-1} |\nabla_\xi f| m \,\mathrm{d}x\,\mathrm{d}\xi \\ &\leq (\|F_1\|_{L^{\mathfrak{b}_1}} \|\nabla\rho\|_{L^{\mathfrak{b}_1'}} + \|F_2\|_{L^{\mathfrak{b}_2}} \|\nabla\rho\|_{L^{\mathfrak{b}_2'}}) N_{p,x}^{1-1/p} N_{p,\xi}^{1/p} \\ &\leq B_K (\|\nabla\rho\|_{L^{\mathfrak{b}_1'}} + \|\nabla\rho\|_{L^{\mathfrak{b}_2'}}) N_{p,x}^{1-1/p} N_{p,\xi}^{1/p}\end{aligned}$$

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

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

Therefore, taking respectively $p = \mathfrak{b}_1'$ and $p = \mathfrak{b}_2'$ and using the notation $u_k = u_k(t) := N^{1/\mathfrak{b}_k'}_{\mathfrak{b}_k',x}$ and $v_k = v_k(t) := N^{1/\mathfrak{b}_k'}_{\mathfrak{b}_k',\xi}$ for $k = 1$ and $k = 2$, we obtain

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

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

$$\frac{\mathrm{d}}{\mathrm{d}t}U \leq n\|E\|_{L^\infty}U + \left(B_K + \frac{1}{2}\right)U^2, \tag{83}$$

where we have used the fact that $2uv \leq u^2 + v^2$, and by Grönwall's inequality we find 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

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

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 $c_2 = \mathfrak{b}_2 > 3$. ∎

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 inequality, which we manage to do by propagating at the same time the $\mathcal{L}^\infty(m_n)$, the $\mathcal{W}^{1,2}(m_n)$, and the $\mathcal{W}^{1,q}(m_{n-2})$ norms with $q \geq 2$ and

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

where $n \in 2\mathbb{N}$. This first step allows us to prove that the $\mathcal{W}^{1,q}(m_n)$ 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 $\boldsymbol{\rho}^{\mathrm{in}} \in \mathcal{W}^{1,2}(m_n) \cap \mathcal{W}^{1,4}(m_{n-2}) \cap \mathcal{L}^\infty(m_n)$, then there exists $T > 0$ such that*

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

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 and assuming moreover that $\boldsymbol{\rho}^{\mathrm{in}} \in \mathcal{W}^{2,2}(m_n) \cap \mathcal{W}^{2,4}(m_{n-2})$, we have*

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

Remark 6.3. The propagation of 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 $a \geq 1/2$.

In order to tahe the mean-field limit, we actually need to prove the propagation of these norms for $\sqrt{\boldsymbol{\rho}}$ instead of $\boldsymbol{\rho}$ (cf. (162a)–(162b)), which works in a similar way.

Proposition 6.4. *Under the hypotheses of Proposition 6.2, if $\sqrt{\boldsymbol{\rho}^{\mathrm{in}}} \in \mathcal{W}^{1,q}(m_n)$ for some $q \in [2, \infty]$, then*

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

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

Lemma 6.5. *Let $\boldsymbol{\rho} \geq 0$ be a compact operator. Then for any $q \in [1, \infty]$,*

$$\|\boldsymbol{\rho}\|_{\dot{\mathcal{W}}^{1,q}(m_n)} \leq 2\|\sqrt{\boldsymbol{\rho}}\|_{\mathcal{L}^\infty(m_n)} \|\sqrt{\boldsymbol{\rho}}\|_{\dot{\mathcal{W}}^{1,q}(m_n)}. \tag{84}$$

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

$$\begin{aligned} \|\nabla_\eta \boldsymbol{\rho}\|_{\mathcal{L}^q} &= \left\|\left(\nabla_\eta(\sqrt{\boldsymbol{\rho}})\sqrt{\boldsymbol{\rho}} + \sqrt{\boldsymbol{\rho}}\,\nabla_\eta(\sqrt{\boldsymbol{\rho}})\right)m_n\right\|_{\mathcal{L}^q} \\ &\leq \|\nabla_\eta(\sqrt{\boldsymbol{\rho}})\|_{\mathcal{L}^q} \|\sqrt{\boldsymbol{\rho}}\, m_n\|_{\mathcal{L}^\infty} + \|\sqrt{\boldsymbol{\rho}}\|_{\mathcal{L}^\infty} \|\nabla_\eta \sqrt{\boldsymbol{\rho}}\, m_n\|_{\mathcal{L}^q}, \end{aligned}$$

which implies (84). ■

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 $H = |\boldsymbol{p}|^2/2 + V_{\boldsymbol{\rho}} - h^3\mathsf{X}_{\boldsymbol{\rho}}$ (with $\mathsf{X}_{\boldsymbol{\rho}} = 0$ in the case of the Hartree equation). If we look at the time derivatives of quantum gradients, since $\nabla_x H = \nabla V_{\boldsymbol{\rho}} = -E_{\boldsymbol{\rho}}$ and $\frac{1}{i\hbar}[\nabla_\xi H, \boldsymbol{\rho}] = \frac{1}{i\hbar}[\boldsymbol{p}, \boldsymbol{\rho}] = -\nabla_x \boldsymbol{\rho}$, 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 6.18 below), we obtain

$$\begin{aligned} \partial_t \nabla_x \boldsymbol{\rho} &= \frac{1}{i\hbar}[H, \nabla_x \boldsymbol{\rho}] - \frac{1}{i\hbar}[h^3\mathsf{X}_{\nabla_x\boldsymbol{\rho}}, \boldsymbol{\rho}] - \frac{1}{i\hbar}[E_{\boldsymbol{\rho}}, \boldsymbol{\rho}], \\ \partial_t \nabla_\xi \boldsymbol{\rho} &= \frac{1}{i\hbar}[H, \nabla_\xi \boldsymbol{\rho}] - \frac{1}{i\hbar}[h^3\mathsf{X}_{\nabla_\xi\boldsymbol{\rho}}, \boldsymbol{\rho}] - \nabla_x \boldsymbol{\rho}. \end{aligned} \tag{85}$$

These equations are of the form

$$i\hbar\partial_t \boldsymbol{\mu} = [\mathsf{A}, \boldsymbol{\mu}] + [\mathsf{B}, \boldsymbol{\rho}] \tag{86}$$

with A and B self-adjoint. Our goal is to propagate the weighted Schatten norms for solutions of these equations, where we recall that Schatten norms were defined in (14). Computing the time derivative of such quantities, we get the following result.

Lemma 6.6. *Let $\boldsymbol{\rho}$, A and B be self-adjoint operators and $\boldsymbol{\mu} = \boldsymbol{\mu}(t)$ be a family of self-adjoint operators satisfying* (86)*. Then, formally, for any even integer $q \geq 2$,*

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

Applying this lemma for $\boldsymbol{\mu} = \boldsymbol{\rho}$ solving the Hartree–Fock equation or for $\boldsymbol{\mu} = \nabla_x \boldsymbol{\rho}$ or $\boldsymbol{\mu} = \nabla_\xi \boldsymbol{\rho}$, and with $m_n = 1$ (for $n = 0$) or $m_n = \boldsymbol{p}_{\mathrm{j}}^n$ for some $\mathrm{j} \in \{1, 2, 3\}$, we obtain

$$\frac{\mathrm{d}}{\mathrm{d}t}\|\boldsymbol{\rho} m_n\|_q \leq \frac{1}{\hbar}\|[V_{\boldsymbol{\rho}}, m_n]\boldsymbol{\rho}\|_q + \frac{1}{\hbar}\|[h^3\mathsf{X}_{\boldsymbol{\rho}}, m_n]\boldsymbol{\rho}\|_q, \tag{87}$$

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t}\|\nabla_x \boldsymbol{\rho} m_n\|_q &\leq \frac{1}{\hbar}\|[V_{\boldsymbol{\rho}}, m_n]\nabla_x \boldsymbol{\rho}\|_q + \frac{1}{\hbar}\|[E_{\boldsymbol{\rho}}, \boldsymbol{\rho}]m_n\|_q \\ &\quad + \frac{1}{\hbar}\|[h^3\mathsf{X}_{\boldsymbol{\rho}}, m_n]\nabla_x \boldsymbol{\rho}\|_q + \frac{1}{\hbar}\|[h^3\mathsf{X}_{\nabla_x\boldsymbol{\rho}}, \boldsymbol{\rho}]m_n\|_q, \end{aligned} \tag{88}$$

$$\begin{aligned} \frac{\mathrm{d}}{\mathrm{d}t}\|\nabla_\xi \boldsymbol{\rho} m_n\|_q &\leq \frac{1}{\hbar}\|[V_{\boldsymbol{\rho}}, m_n]\nabla_\xi \boldsymbol{\rho}\|_q + \|\nabla_x \boldsymbol{\rho}\, m_n\|_q \\ &\quad + \frac{1}{\hbar}\|[h^3\mathsf{X}_{\boldsymbol{\rho}}, m_n]\nabla_\xi \boldsymbol{\rho}\|_q + \frac{1}{\hbar}\|[h^3\mathsf{X}_{\nabla_\xi\boldsymbol{\rho}}, \boldsymbol{\rho}]m_n\|_q, \end{aligned} \tag{89}$$

where we have used the fact that $[H, m_n] = [V_{\boldsymbol{\rho}} - h^3\mathsf{X}_{\boldsymbol{\rho}}, m_n]$ since $[|\boldsymbol{p}|^2, m_n] = 0$. In the next sections, we will bound all the weighted Schatten norms of the commutators appearing on the right-hand sides of inequalities (87)–(89) in order to get a Grönwall-type inequality.

Proof of Lemma 6.6. First notice that

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

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

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\|\boldsymbol{\mu} m_n\|_{2p}^{2p} &= \frac{\mathrm{d}}{\mathrm{d}t}\operatorname{Tr}((m_n\boldsymbol{\mu}^2 m_n)^p) = p\operatorname{Tr}\Big(m_n\Big(\frac{\mathrm{d}}{\mathrm{d}t}(\boldsymbol{\mu}^2)\Big)m_n(m_n\boldsymbol{\mu}^2 m_n)^{p-1}\Big)\\ &= \frac{p}{i\hbar}\operatorname{Tr}\big(m_n([\mathsf{A},\boldsymbol{\mu}^2]+[\mathsf{B},\boldsymbol{\rho}]\boldsymbol{\mu}+\boldsymbol{\mu}[\mathsf{B},\boldsymbol{\rho}])m_n(m_n\boldsymbol{\mu}^2 m_n)^{p-1}\big)\\ &=: I_{\mathsf{A}} + I_{\mathsf{B}}. \end{aligned} \tag{90}$$

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

$$\begin{aligned} I_{\mathsf{A}} &= \frac{p}{i\hbar}\operatorname{Tr}\big(\mathsf{A}\boldsymbol{\mu}^2 m_n^2(\boldsymbol{\mu}^2 m_n^2)^{p-2}\boldsymbol{\mu}^2 m_n^2 - \boldsymbol{\mu}^2\mathsf{A}m_n^2(\boldsymbol{\mu}^2 m_n^2)^{p-2}\boldsymbol{\mu}^2 m_n^2\big)\\ &= \frac{p}{i\hbar}\operatorname{Tr}\big(m_n^2\mathsf{A}\boldsymbol{\mu}^2 m_n^2(\boldsymbol{\mu}^2 m_n^2)^{p-2}\boldsymbol{\mu}^2 - \mathsf{A}m_n^2(\boldsymbol{\mu}^2 m_n^2)^{p-2}\boldsymbol{\mu}^2 m_n^2\boldsymbol{\mu}^2\big)\\ &= \frac{p}{i\hbar}\operatorname{Tr}\big([m_n^2,\mathsf{A}](\boldsymbol{\mu}^2 m_n^2)^{p-1}\boldsymbol{\mu}^2\big). \end{aligned}$$

This can also be written as

$$\begin{aligned} I_{\mathsf{A}} &= \frac{p}{i\hbar}\operatorname{Tr}\big(\boldsymbol{\mu}([m_n,\mathsf{A}]m_n + m_n[m_n,\mathsf{A}])\boldsymbol{\mu}|m_n\boldsymbol{\mu}|^{2(p-1)}\big)\\ &= \frac{2p}{i\hbar}\operatorname{Im}\big(\operatorname{Tr}(\boldsymbol{\mu} m_n[m_n,\mathsf{A}]\boldsymbol{\mu}|m_n\boldsymbol{\mu}|^{2(p-1)})\big). \end{aligned}$$

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

$$\begin{aligned} |I_{\mathsf{A}}| &\leq \frac{2p}{\hbar}\|\boldsymbol{\mu} m_n\|_{2p}\|[m_n,\mathsf{A}]\boldsymbol{\mu}\|_{2p}\|m_n\boldsymbol{\mu}\|_{2p}^{2(p-1)}\\ &\leq \frac{q}{\hbar}\|\boldsymbol{\mu} m_n\|_q^{q-1}\|[\mathsf{A},m_n]\boldsymbol{\mu}\|_q, \end{aligned} \tag{91}$$

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

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

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

$$|I_{\mathsf{B}}| \leq \frac{q}{\hbar}\|m_n[\mathsf{B},\boldsymbol{\rho}]\|_q\|\boldsymbol{\mu} m_n\|_q^{q-1}. \tag{92}$$

We conclude the proof by combining inequalities (91) and (92) with formula (90) and using the fact that $\frac{\mathrm{d}}{\mathrm{d}t}\|\boldsymbol{\mu} m_n\|_q = \frac{1}{q}\|\boldsymbol{\mu} m_n\|_q^{1-q}\frac{\mathrm{d}}{\mathrm{d}t}\|\boldsymbol{\mu} m_n\|_q^q$. ∎

6.2. *Preliminary inequalities*

In order to simplify the computations, we will sometimes use weights of the form

$$m_n = 1 + |\boldsymbol{p}|^n \quad \text{and} \quad \tilde{m}_n = 1 + \sum_{\mathrm{j}=1}^{3}\boldsymbol{p}_{\mathrm{j}}^n.$$

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

Lemma 6.7. *Let $n \in \mathbb{N}$ be even. Then there exists $C > 0$ such that for any $p \in [1, \infty]$ and any operator $\boldsymbol{\rho}$,*

$$C^{-1}\|\boldsymbol{\rho}\tilde{m}_n\|_p \le \|\boldsymbol{\rho} m_n\|_p \le C\|\boldsymbol{\rho}\tilde{m}_n\|_p, \tag{93}$$

$$C^{-1}\|\boldsymbol{\rho}\boldsymbol{p}_{\mathrm{j}}^n\|_p \le \|\boldsymbol{\rho} m_n\|_p \le C\Big(\|\boldsymbol{\rho}\|_p + \sum_{\mathrm{j}=1}^{3}\|\boldsymbol{\rho}\boldsymbol{p}_{\mathrm{j}}^n\|_p\Big). \tag{94}$$

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

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

which proves the first inequality of (93). The second one follows by reversing the roles of $\tilde{m}_n$ and m_n, and the first inequality of (94) by replacing $\tilde{m}_n$ by $\boldsymbol{p}_{\mathrm{j}}^n$. The second inequality of (94) follows from the second inequality of (93) and the triangle inequality for Schatten norms. ∎

We will need the following *operator rearrangement inequality* similar to [49, (56)].

Lemma 6.8. *Let $p \ge 1$ and $(n, m) \in \mathbb{N}^2$. Then for any self-adjoint operators A and B,*

$$\|B^n A B^m\|_p \le 2\|A B^{n+m}\|_p. \tag{95}$$

Proof. Assume first that $A \ge 0$. Then by Hölder's inequality,

$$\|B^n A B^m\|_p \le \|B^n A^{\frac{n}{n+m}}\|_{\frac{n+m}{n}p}\|A^{\frac{m}{n+m}} B^m\|_{\frac{n+m}{m}p}. \tag{96}$$

Now observe that since by definition of the absolute value we have $|BA| = \big||B|A\big|$, and since the Schatten norm is invariant by taking the adjoint,

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

Now, by the Araki–Lieb–Thirring inequality,

$$\big\||B|^n A^{\frac{n}{n+m}}\big\|_{\frac{n+m}{n}p} \le \big\||B|^{n+m} A\big\|_p^{\frac{n}{n+m}} = \|A B^{n+m}\|_p^{\frac{n}{n+m}},$$

$$\big\||B|^m A^{\frac{m}{n+m}}\big\|_{\frac{n+m}{m}p} \le \big\||B|^{n+m} A\big\|_p^{\frac{m}{n+m}} = \|A B^{n+m}\|_p^{\frac{m}{n+m}}.$$

Combining these inequalities with (96) leads to

$$\|B^n A B^m\|_p \le \|A B^{n+m}\|_p. \tag{97}$$

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 (97) and the triangle inequality for Schatten norms, we get

$$\begin{aligned}\|B^n A B^m\|_p &\le \|A_+ B^{n+m}\|_p + \|A_- B^{n+m}\|_p \\ &\le \tfrac{1}{2}\Big(\big\||A|B^{n+m} + AB^{n+m}\big\|_p + \big\||A|B^{n+m} - AB^{n+m}\big\|_p\Big) \\ &\le \big\||A|B^{n+m}\big\|_p + \|AB^{n+m}\|_p\end{aligned}$$

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

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

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

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 rearrangement inequality (95). ∎

Lemma 6.10. *Let $(p_0, p_1) \in [2, \infty]^2$ and $(n_0, n_1) \in \mathbb{R}_+^2$. Then for any A self-adjoint and $\theta \in [0, 1]$,*

$$\|AB^{n_\theta}\|_{p_\theta} \leq \|AB^{n_0}\|_{p_0}^{1-\theta} \|AB^{n_1}\|_{p_1}^{\theta}, \tag{98}$$

where $\frac{1}{p_\theta} = \frac{1-\theta}{p_0} + \frac{\theta}{p_1}$ and $n_\theta = (1-\theta)n_0 + \theta n_1$.

Proof. Let S be the set of values of $\theta \in [0, 1]$ such that (98) holds. Then 0 and 1 are in S. Moreover, if θ_1 and θ_2 are in S, then for $\theta := (\theta_1 + \theta_2)/2$, since the Schatten norms are invariant by taking the adjoint and A and B are self-adjoint,

$$\|AB^{n_\theta}\|_{p_\theta} = \|B^{n_\theta} A\|_{p_\theta} = \|AB^{2n_\theta} A\|_{p_\theta/2}^{1/2}$$

Hence, as $2n_\theta = n_{\theta_1} + n_{\theta_2}$, $p_\theta \geq 2$ and $2/p_\theta = 1/n_{\theta_1} + 1/n_{\theta_2}$, by Hölder's inequality we get

$$\|AB^{2n_\theta} A\|_{p_\theta/2}^{1/2} \leq \|AB^{n_{\theta_1}}\|_{p_{\theta_1}}^{1/2} \|AB^{n_{\theta_2}}\|_{p_{\theta_2}}^{1/2},$$

where we have used again the invariance of Schatten norms by taking the adjoint. Hence $\theta \in S$, and so we deduce finally that S is a dense subset of [0, 1]. ∎

The next proposition allows us to control $\|\nabla\rho\|_{L^p}$ by $\|\nabla_x \boldsymbol{\rho}\, m_n\|_{\mathcal{L}^p}$ for some weight m_n.

Proposition 6.11. *Let $p \in [1, \infty]$ and $n > 3/p'$. Then there exists a constant $C > 0$ such that for any compact self-adjoint operator $\boldsymbol{\mu}$,*

$$\|\mathrm{diag}(\boldsymbol{\mu})\|_{L^p} \leq C \|\boldsymbol{\mu} m_n\|_{\mathcal{L}^p}$$

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

Remark 6.12. In particular, since for $k \in \mathbb{N}$, $\nabla^k \rho = \mathrm{diag}(\nabla_x^k \boldsymbol{\rho})$, the above estimate implies

$$\|\nabla^k \rho\|_{L^p} \leq C \|\nabla_x^k \boldsymbol{\rho} m_n\|_{\mathcal{L}^p}.$$

Proof of Proposition 6.11. Let $\rho_{\boldsymbol{\mu}}(x) := \operatorname{diag}(\boldsymbol{\mu})(x) = h^3\boldsymbol{\mu}(x,x)$. 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

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

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

$$\|\rho_{\boldsymbol{\mu}}\|_{L^p} \leq 2 \sup_{\substack{\varphi\geq 0\\ \|\varphi\|_{L^{p'}}\leq 1}}\left|\int_{\mathbb{R}^3}\rho_{\boldsymbol{\mu}}\varphi\right| = 2 \sup_{\substack{\varphi\geq 0\\ \|\varphi\|_{L^{p'}}\leq 1}} |h^3\operatorname{Tr}(\boldsymbol{\mu}\varphi)|. \tag{99}$$

Taking $m_n(y) := \sqrt{1+|y|^n}$ and $w(y) = m_n(y)^{-1}$, we see that $\boldsymbol{m} := m_n(\boldsymbol{p})$ 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

$$h^3\operatorname{Tr}(\boldsymbol{\mu}\varphi) = h^3\operatorname{Tr}(\boldsymbol{m}\boldsymbol{\mu}\boldsymbol{m}\boldsymbol{w}\varphi\boldsymbol{w}) \leq \|\boldsymbol{m}\boldsymbol{\mu}\boldsymbol{m}\|_{\mathfrak{L}^p}\|\boldsymbol{w}\varphi\boldsymbol{w}\|_{\mathfrak{L}^{p'}}. \tag{100}$$

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

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

where to get the last inequality we have used the Kato–Seiler–Simon inequality (21) since $2p' \geq 2$. Combining the above inequality with inequalities (99) and (100) yields

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

where the second inequality is a consequence of Lemma 6.8, and $C_{p,n} = 2\|w\|^2_{L^{2p'}}$ is finite because $n > 3/p'$ by assumption. ∎

6.3. *Commutators involving the direct term*

In the semiclassical case, instead of $\nabla E_{\boldsymbol{\rho}}\cdot\nabla_\xi f$ (see (82)), the time derivative of the gradient brings about the term $\frac{1}{i\hbar}[E_{\boldsymbol{\rho}},\boldsymbol{\rho}]$ (see (85)). Hence we will need to get semiclassical estimates on this quantity, which is the purpose of the following proposition.

Proposition 6.13 (Commutator estimates). *Let $a \in (0,1]$, $\mathfrak{b} = \frac{3}{a+1}$ and $(q,r) \in [2,\infty]^2$ be such that $1/r + 1/q = 1/2$. Then for any compact operator $\boldsymbol{\rho}_2$,*

$$\frac{1}{\hbar}\|[E_{\boldsymbol{\rho}},\boldsymbol{\rho}_2]\|_{\mathfrak{L}^q} \leq C\|\rho\|_{B^{1-3(1/r'-1/\mathfrak{b})}_{r,1}}\|\nabla_\xi\boldsymbol{\rho}_2\|_{\mathfrak{L}^q}. \tag{101}$$

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

$$\frac{1}{\hbar}\|[E_{\boldsymbol{\rho}},\boldsymbol{\rho}_2]\|_{\mathfrak{L}^2} \leq C\|\nabla\rho\|_{L^{\mathfrak{b}',1}}\|\nabla_\xi\boldsymbol{\rho}_2\|_{\mathfrak{L}^2} \tag{102}$$

for $a \in [1/2, 1]$*, and*

$$\frac{1}{\hbar}\|[E_{\boldsymbol{\rho}}, \boldsymbol{\rho}_2]\|_{\mathcal{L}^2} \leq C\|\rho\|_{L^{\frac{3}{1-a}},1}\|\nabla_\xi \boldsymbol{\rho}_2\|_{\mathcal{L}^2} \tag{103}$$

for $a \in (0, 1/2)$.

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 6.14. *Let* $(q,r) \in (2,\infty] \times (\mathfrak{b}',\infty)$ *be such that* $1/r + 1/q = 1/2$*. Then*

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

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

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

Proof of Proposition 6.13. First observe that the integral kernel of the operator $[E_{\boldsymbol{\rho}}, \boldsymbol{\rho}_2]$ can be written as

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

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 $\nabla_\xi \boldsymbol{\rho}_2$ is $\frac{x-y}{i\hbar}\boldsymbol{\rho}_2(x,y)$, we get

$$\begin{aligned}\frac{1}{\hbar}\|[E_{\boldsymbol{\rho}}, \boldsymbol{\rho}_2]\|_2 &= \left(\iint_{\mathbb{R}^6} \left|\frac{(E_{\boldsymbol{\rho}}(x) - E_{\boldsymbol{\rho}}(y)) \otimes (x-y)}{|x-y|^2} \cdot \nabla_\xi \boldsymbol{\rho}_2(x,y)\right|^2 \mathrm{d}x\,\mathrm{d}y\right)^{1/2} \\ &\leq \|\nabla E_{\boldsymbol{\rho}}\|_{L^\infty}\|\nabla_\xi \boldsymbol{\rho}_2\|_2.\end{aligned} \tag{104}$$

In particular, for $a \in [1/2, 1]$, since $\nabla E_{\boldsymbol{\rho}} = \nabla K * \nabla \rho$ with $\nabla K \in L^{\mathfrak{b},\infty}$, we deduce inequality (102) using the fact that the dual of $L^{\mathfrak{b}',1}$ is $L^{\mathfrak{b},\infty}$ (see e.g. [44])

If $a \in (0, 1/2)$, we use $\nabla E_{\boldsymbol{\rho}} = \nabla^2 K * \rho$ with $\nabla^2 K \in L^{\frac{3}{a+2},\infty}$. Thus (103) 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

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

which implies that denoting by e_ω the operator of multiplication by $e^{2i\pi\omega\cdot x}$, we have

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

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

$$\frac{1}{\hbar}\|[E_{\boldsymbol{\rho}}, \boldsymbol{\rho}_2]\|_\infty \leq \int_{[0,1]\times\mathbb{R}^3} |\widehat{\nabla E_{\boldsymbol{\rho}}}(z)|\, \|\nabla_\xi \boldsymbol{\rho}_2\|_\infty \,\mathrm{d}\theta\,\mathrm{d}z = \|\widehat{\nabla E_{\boldsymbol{\rho}}}\|_{L^1} \|\nabla_\xi \boldsymbol{\rho}_2\|_\infty. \tag{105}$$

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 $\boldsymbol{\mu} := \nabla_\xi \boldsymbol{\rho}_2$, we observe 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 $B^{3/2}_{2,1} \subset \mathcal{F}(L^1)$, inequalities (104) and (105) imply

$$\|\Lambda(E,\boldsymbol{\mu})\|_2 \leq C\|E\|_{B^1_{\infty,1}}\|\boldsymbol{\mu}\|_2, \quad \|\Lambda(E,\boldsymbol{\mu})\|_\infty \leq C\|E\|_{B^{1+3/2}_{2,1}}\|\boldsymbol{\mu}\|_\infty.$$

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 Besov spaces involved is given by $[B^1_{\infty,1}, B^{1+3/2}_{2,1}]_{2/r} = B^{1+3/r}_{r,1}$ (see for example [16, Theorem 6.4.5]), while the complex interpolation of Schatten spaces $\mathfrak{S}^q$ gives $[\mathfrak{S}^2,\mathfrak{S}^\infty]_{1-2/q} = \mathfrak{S}^q$ (see for example [75, Section 1.19.7]), so that by bilinear interpolation (see [16, Section 4.4]) we obtain

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

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

$$\|E_{\boldsymbol{\rho}}\|_{B^{1+3/r}_{r,1}} \leq C\|\rho\|_{B^{3/r+a-1}_{r,1}} = \|\rho\|_{B^{1-3(1/r'-1/\mathfrak{b})}_{r,1}}.$$

Taking $\boldsymbol{\mu} = \nabla_\xi \boldsymbol{\rho}_2$ yields the results. ■

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

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

To control the $\mathcal{L}^q$ norm of the first term of the right-hand side we use Proposition 6.13, which gives

$$\frac{1}{\hbar}\|[E_{\boldsymbol{\rho}}, \boldsymbol{\rho}\boldsymbol{p}_{\mathrm{j}}^{2n}]\|_{\mathcal{L}^q} \leq C\|\rho\|_{B^{1-3(1/r'-1/\mathfrak{b})}_{r,1}}\|\nabla_\xi(\boldsymbol{\rho}\boldsymbol{p}_{\mathrm{j}}^{2n})\|_{\mathcal{L}^q},$$

and we can also replace $\|\rho\|_{B^{1-3(1/r'-1/\mathfrak{b})}_{r,1}}$ by $\|\nabla\rho\|_{L^{\mathfrak{b}',1}}$ when $q = 2$.

To bound the second term, we will write the potential $K(x)$ as a sum of a singular part localized near $x = 0$ and a long-range part and use Propositions 6.15 and 6.17 below. More precisely, for some infinitely smooth and compactly supported function χ satisfying $\mathbb{1}_{|x|\leq 1} \leq \chi(x) \leq \mathbb{1}_{|x|\leq 2}$, we can write

$$K = K_0 + K_\infty \tag{106}$$

with

$$K_0 = \chi K \quad \text{and} \quad K_\infty = (1-\chi)K.$$

Now the first part of K satisfies $\nabla K_0 \in L^{\mathfrak{b}}$ for any $\mathfrak{b} < 3/2$, while $K_\infty \in L^\infty \cap C^\infty$. We start with the following proposition to control the singular part of the potential.

Proposition 6.15 (Weighted commutator estimate). *Let $E^0_{\boldsymbol{\rho}} = -\nabla K_0 * \rho$ with $K_0 = \chi K$ as described above and let $m_n := 1 + |\boldsymbol{p}|^n$. Take $(q, r, r_1) \in [3/2, \infty] \times [1, \infty]^2$ such that*

$$\frac{1}{r} + \frac{1}{r_1} = \frac{1}{q} + \frac{1}{3}. \tag{107}$$

Then for any $n_0 > 3/\mathfrak{b} - 1$, $k' > 3/r' - 2$ and $k > 3/r - 1$ there exists a constant $C > 0$ such that

$$\frac{1}{\hbar}\|[E^0_{\boldsymbol{\rho}}, \boldsymbol{p}_{\mathrm{j}}^{2n}]\boldsymbol{\mu}\|_{\mathfrak{L}^q} \leq C(\|\nabla_{x_{\mathrm{j}}}\boldsymbol{\rho}\, m_{n+n_0}\|_{\mathfrak{L}^{\mathfrak{b}'}}\|\boldsymbol{\mu} m_{2n-1}\|_{\mathfrak{L}^q} + \|\nabla_{x_{\mathrm{j}}}\boldsymbol{\rho}\, m_{2n+k'}\|_{\mathfrak{L}^r}\|\boldsymbol{\mu} m_{n+k}\|_{\mathfrak{L}^{r_1}}).$$

Replacing $E^0_{\boldsymbol{\rho}}$ by $V^0_{\boldsymbol{\rho}} = K_0 * \rho$ just amounts to replacing $\nabla_{x_{\mathrm{j}}}\boldsymbol{\rho}$ by $\boldsymbol{\rho}$, hence by the same proof,

$$\frac{1}{\hbar}\|[V^0_{\boldsymbol{\rho}}, \boldsymbol{p}_{\mathrm{j}}^{2n}]\boldsymbol{\mu}\|_{\mathfrak{L}^q} \leq C(\|\boldsymbol{\rho} m_{n+n_0}\|_{\mathfrak{L}^{\mathfrak{b}'}}\|\boldsymbol{\mu} m_{2n-1}\|_{\mathfrak{L}^q} + \|\boldsymbol{\rho} m_{2n+k'}\|_{\mathfrak{L}^r}\|\boldsymbol{\mu} m_{n+k}\|_{\mathfrak{L}^{r_1}}).$$

Proof of Proposition 6.15. To shorten notation, let $E := E^0_{\boldsymbol{\rho}}$. We notice that $[E, \boldsymbol{p}_{\mathrm{j}}] = E\boldsymbol{p}_{\mathrm{j}} - \boldsymbol{p}_{\mathrm{j}}E = i\hbar\partial_{\mathrm{j}}E$ 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

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

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

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

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

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

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 the 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 $g_\ell(x) = (\boldsymbol{p}_{\mathrm{j}}^\ell(\partial_{\mathrm{j}} E))(x)$, as usual also identified with a multiplication operator. This yields

$$\frac{1}{\hbar}\|[E, \boldsymbol{p}_{\mathrm{j}}^{2n}]\boldsymbol{\mu}\|_{\mathfrak{L}^q} \leq \sum_{\ell=0}^{2n-1} C_\ell \|g_\ell \boldsymbol{p}_{\mathrm{j}}^{2n-1-\ell}\boldsymbol{\mu}\|_{\mathfrak{L}^q},$$

where $C_\ell = \sum_{k=\ell}^{2n-1}\binom{k}{\ell}$. We will now distinguish two cases to bound the terms of the sum depending on the values of ℓ.

1. Case ℓ small. Take $\ell < n$. In this case, we use Hölder's inequality for Schatten norms and the fact that the norm of the operator of multiplication by a function is the L^∞ norm of this function to deduce that

$$\|g_\ell \boldsymbol{p}_{\mathrm{j}}^{2n-1-\ell}\boldsymbol{\mu}\|_{\mathfrak{L}^q} \leq \|g_\ell\|_{L^\infty}\|\boldsymbol{p}_{\mathrm{j}}^{2n-1-\ell}\boldsymbol{\mu}\|_{\mathfrak{L}^q} \leq \|g_\ell\|_{L^\infty}\|\boldsymbol{\mu} m_{2n-1}\|_{\mathfrak{L}^q},$$

where we have used inequality (94). Now, observe that

$$g_\ell = -\nabla K_0 * (\boldsymbol{p}_{\mathrm{j}}^\ell \partial_{\mathrm{j}}\rho) = -\nabla K_0 * \operatorname{diag}(\operatorname{ad}_{\boldsymbol{p}_{\mathrm{j}}}^\ell(\nabla_{x_{\mathrm{j}}}\boldsymbol{\rho})).$$

Therefore, since $\nabla K_0 \in L^{\mathfrak{b}}$ with $\mathfrak{b} < 3/2$, by Young's inequality

$$\|g_\ell\|_{L^\infty} \leq C_K \|\operatorname{diag}(\operatorname{ad}_{\boldsymbol{p}_{\mathrm{j}}}^\ell(\nabla_{x_{\mathrm{j}}}\boldsymbol{\rho}))\|_{L^{\mathfrak{b}'}},$$

where $C_K = \|\nabla K_0\|_{L^{\mathfrak{b}}}$. By Proposition 6.11 and Lemma 6.9, for any $n_0 > 3/\mathfrak{b} - 1 > 0$,

$$\|g_\ell\|_{L^\infty} \leq C_{K,n_0}\|\operatorname{ad}_{\boldsymbol{p}_{\mathrm{j}}}^\ell(\nabla_{x_{\mathrm{j}}}\boldsymbol{\rho}) m_{2+n_0}\|_{\mathfrak{L}^{\mathfrak{b}'}} \leq 2^{\ell+1} C_{K,n_0}\|\nabla_{x_{\mathrm{j}}}\boldsymbol{\rho}\, m_{n+n_0}\|_{\mathfrak{L}^{\mathfrak{b}'}}$$

where we have used the fact that $\ell \leq n-1$.

2. Case ℓ large. Take $\ell \in \mathbb{N} \cap [n, 2n-1]$ and define $1/\tilde{q} = 1/q + 1/3$. Then since $\tilde{q} \leq q$,

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

Since $1/r = 1/\tilde{q} - 1/r_1$, multiplying and dividing by $m_k := 1 + |\boldsymbol{p}|^k$ we deduce

$$\begin{aligned}\|g_\ell \boldsymbol{p}_{\mathrm{j}}^{2n-1-\ell}\boldsymbol{\mu}\|_{\mathfrak{L}^q} &\leq h^{-1}\|g_\ell m_k^{-1} m_k \boldsymbol{p}_{\mathrm{j}}^{2n-1-\ell}\boldsymbol{\mu}\|_{\mathfrak{L}^{\tilde{q}}} \\ &\leq C_m^{1/r} h^{-1}\|g_\ell\|_{L^r}\|\boldsymbol{\mu} m_{n+k-1}\|_{\mathfrak{L}^{r_1}},\end{aligned}$$

where $C_m = \int_{\mathbb{R}^3}\frac{\mathrm{d}x}{(1+|x|^k)^r}$ is finite because $k < 3/r$ and we have used the fact that $\ell \geq n$. Note that since $\ell \geq 1$,

$$g_\ell = -\partial_{\mathrm{j}}\nabla K_0 * \boldsymbol{p}_{\mathrm{j}}^\ell \rho = i\hbar(\partial_{\mathrm{j}}\nabla K_0) * \operatorname{diag}(\operatorname{ad}_{\boldsymbol{p}_{\mathrm{j}}}^{\ell-1}(\nabla_{x_{\mathrm{j}}}\boldsymbol{\rho})).$$

Hence, to control g_ℓ, we can use the fact that the convolution by $\partial_{\mathrm{j}}\nabla K_0$ is continuous from L^r to L^r by the Calderón–Zygmund Theorem (see e.g. [28, Theorem 5.1]) to obtain

$$\|g_\ell\|_{L^r} \leq C_K h \|\mathrm{diag}(\mathrm{ad}_{\boldsymbol{p}_{\mathrm{j}}}^{\ell-1}(\nabla_{x_{\mathrm{j}}}\boldsymbol{\rho}))\|_{L^r}.$$

By Proposition 6.11 and Lemma 6.9, this yields, for any $\varepsilon = k' + 2 - 3/r' > 0$,

$$h^{-1}\|g_\ell\|_{L^r} \leq C_{K,\varepsilon}\|\mathrm{ad}_{\boldsymbol{p}_{\mathrm{j}}}^{\ell-1}(\nabla_{x_{\mathrm{j}}}\boldsymbol{\rho}) m_{3/r'+\varepsilon}\|_{\mathcal{L}^r} \leq 2^\ell C_{K,k'}\|\nabla_{x_{\mathrm{j}}}\boldsymbol{\rho}\, m_{2n+k'}\|_{\mathcal{L}^r}. \qquad \blacksquare$$

Thanks to Lemma 6.10, we can modify Proposition 6.15 in a way depending only on the $\mathcal{L}^2$ and $\mathcal{L}^4$ norms.

Corollary 6.16. *Assume $n \geq 3$. Then there exist $\theta \in (0,1)$ and $C > 0$ such that*

$$\frac{C}{\hbar}\|[E^0_{\boldsymbol{\rho}}, \boldsymbol{p}_{\mathrm{j}}^{2n}]\boldsymbol{\mu}\|_{\mathcal{L}^2} \leq \|\nabla_{x_{\mathrm{j}}}\boldsymbol{\rho}\, m_{2n}\|_{\mathcal{L}^2}^{1-\theta}\|\nabla_{x_{\mathrm{j}}}\boldsymbol{\rho}\, m_{2n-2}\|_{\mathcal{L}^4}^{\theta}\|\boldsymbol{\mu} m_{2n}\|_{\mathcal{L}^2} + \|\nabla_{x_{\mathrm{j}}}\boldsymbol{\rho}\, m_{2n}\|_{\mathcal{L}^2}\|\boldsymbol{\mu} m_{2n}\|_{\mathcal{L}^2}^{1/3}\|\boldsymbol{\mu} m_{2n-2}\|_{\mathcal{L}^4}^{2/3}$$

and

$$\frac{C}{\hbar}\|[E^0_{\boldsymbol{\rho}}, \boldsymbol{p}_{\mathrm{j}}^{2n}]\boldsymbol{\mu}\|_{\mathcal{L}^4} \leq \|\nabla_{x_{\mathrm{j}}}\boldsymbol{\rho}\, m_{2n+2}\|_{\mathcal{L}^2}^{1-\theta}\|\nabla_{x_{\mathrm{j}}}\boldsymbol{\rho}\, m_{2n}\|_{\mathcal{L}^4}^{\theta}\|\boldsymbol{\mu} m_{2n}\|_{\mathcal{L}^4} + \|\nabla_{x_{\mathrm{j}}}\boldsymbol{\rho}\, m_{2n+2}\|_{\mathcal{L}^2}^{1/3}\|\nabla_{x_{\mathrm{j}}}\boldsymbol{\rho}\, m_{2n}\|_{\mathcal{L}^4}^{2/3}\|\boldsymbol{\mu} m_{2n}\|_{\mathcal{L}^4}.$$

Proof. In the case $q = 2$, use Proposition 6.15 with $r = 2$, $r_1 = 3$ to get, for any $n_0 > 3/\mathfrak{b} - 1$ and $k > 1/2$,

$$\frac{1}{\hbar}\|[E^0_{\boldsymbol{\rho}}, \boldsymbol{p}_{\mathrm{j}}^{2n}]\boldsymbol{\mu}\|_{\mathcal{L}^2} \leq C(\|\nabla_{x_{\mathrm{j}}}\boldsymbol{\rho}\, m_{n+n_0}\|_{\mathcal{L}^{\mathfrak{b}'}}\|\boldsymbol{\mu} m_{2n}\|_{\mathcal{L}^2} + \|\nabla_{x_{\mathrm{j}}}\boldsymbol{\rho}\, m_{2n}\|_{\mathcal{L}^2}\|\boldsymbol{\mu} m_{n+k}\|_{\mathcal{L}^3}).$$

Since $\nabla K_0 \in L^{\mathfrak{b}}$ for any $\mathfrak{b} < 3/2$, we can in particular take $\mathfrak{b} \in (4/3, 3/2)$ so that $\mathfrak{b}' \in (3,4)$ and we can apply Lemma 6.10 with $p_0 = 2$, $p_1 = 4$ and $p_\theta = b'$, leading to

$$\|\nabla_{x_{\mathrm{j}}}\boldsymbol{\rho}\, m_{n+n_0}\|_{\mathcal{L}^{\mathfrak{b}'}} \leq \|\nabla_{x_{\mathrm{j}}}\boldsymbol{\rho}\, m_{2n}\|_{\mathcal{L}^2}^{1-\theta}\|\nabla_{x_{\mathrm{j}}}\boldsymbol{\rho}\, m_{\tilde{n}}\|_{\mathcal{L}^4}^{\theta},$$

where $\theta = 4(1/b - 1/2) \in (2/3, 1)$ and $\tilde{n} \geq \frac{(2\theta-1)n+n_0}{\theta} \in (\frac{n+3n_0}{2}, n+n_0)$. On the other hand, taking $p_\theta = 3$ yields

$$\|\boldsymbol{\mu} m_{n+k}\|_{\mathcal{L}^3} \leq \|\boldsymbol{\mu} m_{2n}\|_{\mathcal{L}^2}^{1/3}\|\boldsymbol{\mu} m_{\tilde{n}}\|_{\mathcal{L}^4}^{2/3}$$

with $\tilde{n} \geq (n+3k)/2$. In particular, when $n \geq 3$, taking $\mathfrak{b}$ close to $3/2$, k close to $1/2$ and n_0 close to 1 allows one to take $\tilde{n} \leq 2n - 2$.

In the case $q = 4$, take $r = 3$ and $r_1 = 4$ in Proposition 6.15 to get, for any $n_0 > 3/\mathfrak{b} - 1$ and $k' > 0$,

$$\frac{1}{\hbar}\|[E^0_{\boldsymbol{\rho}}, \boldsymbol{p}_{\mathrm{j}}^{2n}]\boldsymbol{\mu}\|_{\mathcal{L}^4} \leq C(\|\nabla_{x_{\mathrm{j}}}\boldsymbol{\rho}\, m_{n+n_0}\|_{\mathcal{L}^{\mathfrak{b}'}}\|\boldsymbol{\mu} m_{2n}\|_{\mathcal{L}^4} + \|\nabla_{x_{\mathrm{j}}}\boldsymbol{\rho}\, m_{2n+k'}\|_{\mathcal{L}^3}\|\boldsymbol{\mu} m_{2n}\|_{\mathcal{L}^4}).$$

As previously, we interpolate the $\mathcal{L}^{\mathfrak{b}'}$ norm between the $\mathcal{L}^2$ and the $\mathcal{L}^4$ norm, leading to

$$\|\nabla_{x_{\mathrm{j}}}\boldsymbol{\rho}\, m_{n+n_0}\|_{\mathcal{L}^{\mathfrak{b}'}} \leq \|\nabla_{x_{\mathrm{j}}}\boldsymbol{\rho}\, m_{\tilde{n}}\|_{\mathcal{L}^2}^{1-\theta}\|\nabla_{x_{\mathrm{j}}}\boldsymbol{\rho}\, m_{2n}\|_{\mathcal{L}^4}^{\theta}$$

with again $\theta = 4(1/\mathfrak{b} - 1/2) \in (2/3, 1)$ but with $\tilde{n} \geq \frac{(1-2\theta)n+n_0}{\theta}$ possibly negative. On the other hand, taking $p_\theta = 3$ yields

$$\|\nabla_{x_j}\boldsymbol{\rho}\, m_{2n+k'}\|_{\mathfrak{L}^3} \leq \|\nabla_{x_j}\boldsymbol{\rho}\, m_{\tilde{n}}\|_{\mathfrak{L}^2}^{1/3} \|\nabla_{x_j}\boldsymbol{\rho}\, m_{2n}\|_{\mathfrak{L}^4}^{2/3}$$

with $\tilde{n} \geq 2n + 3k'$. In particular, taking b close to $3/2$, n_0 close to 1 and k' sufficiently small allows one to take $\tilde{n} \leq 2n + 2$. ■

Now we treat the long range part K_∞ of the potential.

Proposition 6.17. *Let $E^\infty_{\boldsymbol{\rho}} = -\nabla K_\infty * \rho$ and $V^\infty_{\boldsymbol{\rho}} = K_\infty * \rho$ with $\rho = \mathrm{diag}(\boldsymbol{\rho})$ and $n \geq 1$ be an integer. Then there exists a constant $C > 0$ independent of $\hbar$ such that for any $q \in [1, \infty]$ and any positive compact operators $\boldsymbol{\rho}$ and $\boldsymbol{\mu}$,*

$$\frac{1}{\hbar}\|[E^\infty_{\boldsymbol{\rho}}, \boldsymbol{p}_j^{2n}]\boldsymbol{\mu}\|_{\mathfrak{L}^q} \leq C(\|\boldsymbol{\rho} m_{2n}\|_{\mathfrak{L}^2} + \hbar\|\nabla_{x_j}\boldsymbol{\rho}\, m_{2n}\|_{\mathfrak{L}^2})\|\boldsymbol{\mu} m_{2n}\|_{\mathfrak{L}^q},$$
$$\frac{1}{\hbar}\|[V^\infty_{\boldsymbol{\rho}}, \boldsymbol{p}_j^{2n}]\boldsymbol{\mu}\|_{\mathfrak{L}^q} \leq C(\|\rho\|_{L^1} + \hbar\|\boldsymbol{\rho} m_{2n}\|_{\mathfrak{L}^2})\|\boldsymbol{\mu} m_{2n}\|_{\mathfrak{L}^q}.$$

Proof. As in the proof of Proposition 6.15, and with the same notations, we have

$$\frac{1}{\hbar}\|[E^\infty_{\boldsymbol{\rho}}, \boldsymbol{p}_j^{2n}]\boldsymbol{\mu}\|_{\mathfrak{L}^q} \leq \sum_{\ell=0}^{2n-1} C_\ell \|g_\ell \boldsymbol{p}_j^{2n-1-\ell}\boldsymbol{\mu}\|_{\mathfrak{L}^q},$$

where $C_\ell = \sum_{k=\ell}^{2n-1}\binom{k}{\ell}$. We use Hölder's inequality for Schatten norms and the fact that the norm of the operator of multiplication by a function is the L^∞ norm of this function to deduce that

$$\|g_\ell \boldsymbol{p}_j^{2n-1-\ell}\boldsymbol{\mu}\|_{\mathfrak{L}^q} \leq \|g_\ell\|_{L^\infty}\|\boldsymbol{p}_j^{2n-1-\ell}\boldsymbol{\mu}\|_{\mathfrak{L}^q} \leq \|g_\ell\|_{L^\infty}\|\boldsymbol{\mu} m_{2n}\|_{\mathfrak{L}^q},$$

where we have used inequality (94). Now, observe that

$$g_\ell = -\partial_j \nabla K_\infty * (\boldsymbol{p}_j^\ell \rho) = -\partial_j \nabla K_\infty * \mathrm{diag}(\mathrm{ad}^\ell_{\boldsymbol{p}_j}(\boldsymbol{\rho})).$$

Therefore, since $\partial_j \nabla K_\infty \in L^2$, by Young's inequality, which is just the Cauchy–Schwarz inequality in this case,

$$\|g_\ell\|_{L^\infty} \leq C_K \|\mathrm{diag}(\mathrm{ad}^\ell_{\boldsymbol{p}_j}(\boldsymbol{\rho}))\|_{L^2},$$

where $C_K = \|\partial_j \nabla K_\infty\|_{L^2}$. By Proposition 6.11, we get

$$\|g_\ell\|_{L^\infty} \leq C\|\mathrm{ad}^\ell_{\boldsymbol{p}_j}(\boldsymbol{\rho}) m_2\|_{\mathfrak{L}^2}.$$

When $\ell = 0$, since $2n \geq 2$, this implies

$$\|g_\ell\|_{L^\infty} \leq C\|\boldsymbol{\rho} m_{2n}\|_{\mathfrak{L}^2}.$$

When $\ell > 0$, we use the fact that $\mathrm{ad}_{\boldsymbol{p}_j}(\boldsymbol{\rho}) = -i\hbar\nabla_{x_j}\boldsymbol{\rho}$, $\ell \leq 2n - 1$ and Lemma 6.9 to get

$$\|g_\ell\|_{L^\infty} \leq C\hbar\|\mathrm{ad}^{\ell-1}_{\boldsymbol{p}_j}(\nabla_{x_j}\boldsymbol{\rho})m_2\|_{\mathfrak{L}^2} \leq 2^\ell C_{K,n_0}\hbar\|\nabla_{x_j}\boldsymbol{\rho}\, m_{2n}\|_{\mathfrak{L}^2}.$$

When $E^\infty_{\boldsymbol{\rho}}$ is replaced by $V^\infty_{\boldsymbol{\rho}}$, one obtains the same estimates with $\ell > 0$ and $\nabla_{x_j}\boldsymbol{\rho}$ replaced by $\boldsymbol{\rho}$. The only remaining point is the case $\ell = 0$, that is, defining $g_\ell = -\partial_j K_\infty * (\boldsymbol{p}_j^\ell \rho)$, it remains to notice that since $\partial_j K_\infty \in L^\infty$,

$$\|g_0\|_{L^\infty} = \|\partial_j K_\infty * \rho\|_{L^\infty} \leq C_K \|\rho\|_{L^1}$$

with $C_K = \|\nabla K_\infty\|_{L^\infty}$. ■

6.4. *Preliminary properties of the exchange operator*

6.4.1. Preliminary identities. Let $\mathsf{X} = \mathsf{X}_{\boldsymbol{\rho}}$ be the operator with 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 6.18. *Let $a \in (0, 1]$. Then the following identities hold:*

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

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

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 $\varphi \in C^\infty_c$, integrate by parts and use the fact that $\nabla_x K(x - y) = -\nabla_y K(x - y)$ to get

$$\begin{aligned}[\nabla, \mathsf{X}_{\boldsymbol{\rho}}]\varphi(x) &= \nabla \int_{\mathbb{R}^3} \frac{\boldsymbol{\rho}(x, y)}{|x - y|^a}\varphi(y)\,\mathrm{d}y - \int_{\mathbb{R}^3} \frac{\boldsymbol{\rho}(x, y)}{|x - y|^a}\nabla\varphi(y)\,\mathrm{d}y \\ &= \int_{\mathbb{R}^3} (\nabla_x + \nabla_y)\left(\frac{\boldsymbol{\rho}(x, y)}{|x - y|^a}\right)\varphi(y)\,\mathrm{d}y = \int_{\mathbb{R}^3} \frac{(\nabla_x + \nabla_y)(\boldsymbol{\rho}(x, y))}{|x - y|^a}\varphi(y)\,\mathrm{d}y,\end{aligned}$$

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

Lemma 6.19. *Let $\eta = 1$, $\boldsymbol{p}_j$ or x_j. Then*

$$\eta^n \mathsf{X}_{\boldsymbol{\rho}} = \sum_{k=0}^n \binom{n}{k} \mathsf{X}_{\mathrm{ad}^k_\eta(\boldsymbol{\rho})}\eta^{n-k}, \tag{108}$$

$$[\eta^n, \mathsf{X}_{\boldsymbol{\rho}}] = \sum_{k=1}^n \binom{n}{k} \mathsf{X}_{\mathrm{ad}^k_\eta(\boldsymbol{\rho})}\eta^{n-k}. \tag{109}$$

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

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

Hence we deduce the result by taking $B = \mathsf{X}_{\boldsymbol{\rho}}$ and using Lemma 6.18. ■

6.4.2. Preliminary inequalities. We know from [49, (39a)] that if $a \in [0, 3/2)$ and $q = 2$, then

$$\|\mathsf{X}_{\boldsymbol{\rho}}\|_q \le C h^{-a} \|\boldsymbol{\rho} |\boldsymbol{p}|^a\|_2. \tag{110}$$

Since Schatten norms of smaller order control 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 another operator $\boldsymbol{\mu}$ instead of $\boldsymbol{\rho}$.

Lemma 6.20. *Let $\boldsymbol{\mu}$ and $\tilde{\boldsymbol{\mu}}$ be compact operators. Then for any $q \in [2, \infty]$ and any $\theta \in \{0, 1\}$,*

$$\|\mathsf{X}_{\tilde{\boldsymbol{\mu}}} \boldsymbol{\mu}\|_q \le C_a h^{-a} \|\tilde{\boldsymbol{\mu}} |\boldsymbol{p}|^{a(1-\theta)}\|_2 \|\boldsymbol{\mu}^* |\boldsymbol{p}|^{\theta a}\|_\infty, \tag{111}$$

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

Proof. Let $\boldsymbol{\mu}_2$ be a compact but possibly non-self-adjoint operator. Then

$$\begin{aligned} \|\mathsf{X}_{\boldsymbol{\mu}_2}\|_2^2 = \mathrm{Tr}(\mathsf{X}_{\boldsymbol{\mu}_2}^* \mathsf{X}_{\boldsymbol{\mu}_2}) &= \iint_{\mathbb{R}^6} \frac{\boldsymbol{\mu}_2^*(x,y)\boldsymbol{\mu}_2(y,x)}{|x-y|^{2a}} \,\mathrm{d}x\,\mathrm{d}y \\ &= \iint_{\mathbb{R}^6} \frac{|\boldsymbol{\mu}_2(x,y)|^2}{|x-y|^{2a}} \,\mathrm{d}x\,\mathrm{d}y = \iint_{\mathbb{R}^6} \frac{|\boldsymbol{\mu}_2(x,y+x)|^2}{|y|^{2a}} \,\mathrm{d}x\,\mathrm{d}y, \end{aligned}$$

so that by the Hardy–Rellich inequality,

$$\begin{aligned} \|\mathsf{X}_{\boldsymbol{\mu}_2}\|_2^2 &\le \mathscr{C}_a \iint_{\mathbb{R}^6} |\Delta_y^{a/2} \boldsymbol{\mu}_2(x, y+x)|^2 \,\mathrm{d}x\,\mathrm{d}y = \mathscr{C}_a \iint_{\mathbb{R}^6} |\Delta_y^{a/2} \boldsymbol{\mu}_2(x,y)|^2 \,\mathrm{d}x\,\mathrm{d}y \\ &\le C_a h^{-2a} \iint_{\mathbb{R}^6} |(\boldsymbol{\mu}_2 |\boldsymbol{p}|^a)(x,y)|^2 \,\mathrm{d}x\,\mathrm{d}y, \end{aligned}$$

where $\mathscr{C}_a$ is the constant appearing in the Hardy–Rellich inequality and $C_a = (2\pi)^a \mathscr{C}_a$. From this we deduce the generalization of (110) for possibly non-self-adjoint operators:

$$\|\mathsf{X}_{\boldsymbol{\mu}_2}\|_2 \le C_a h^{-a} \|\boldsymbol{\mu}_2 |\boldsymbol{p}|^a\|_2. \tag{112}$$

By Hölder's inequality, taking $\boldsymbol{\mu}_2 = \tilde{\boldsymbol{\mu}}$, this implies (111) when $\theta = 0$. Now, noticing that we have the following integration by parts like formula:

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

and using the cyclicity of the trace, Hölder's inequality and inequality (112) with $\boldsymbol{\mu}_2 = \mathsf{X}_{\tilde{\boldsymbol{\mu}}}\boldsymbol{\mu}\boldsymbol{\mu}^*$, we get

$$\begin{aligned}\|\mathsf{X}_{\tilde{\boldsymbol{\mu}}}\boldsymbol{\mu}\|_2^2 &= \operatorname{Tr}(\mathsf{X}_{\tilde{\boldsymbol{\mu}}^*}\mathsf{X}_{\tilde{\boldsymbol{\mu}}}\boldsymbol{\mu}\boldsymbol{\mu}^*) = \operatorname{Tr}(\tilde{\boldsymbol{\mu}}^*\mathsf{X}_{(\mathsf{X}_{\tilde{\boldsymbol{\mu}}}\boldsymbol{\mu}\boldsymbol{\mu}^*)}) \\ &\leq \|\tilde{\boldsymbol{\mu}}\|_2\|\mathsf{X}_{(\mathsf{X}_{\tilde{\boldsymbol{\mu}}}\boldsymbol{\mu}\boldsymbol{\mu}^*)}\|_2 \leq C_a h^{-a}\|\tilde{\boldsymbol{\mu}}\|_2\|\mathsf{X}_{\tilde{\boldsymbol{\mu}}}\boldsymbol{\mu}\boldsymbol{\mu}^*|\boldsymbol{p}|^a\|_2.\end{aligned}$$

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 $q \geq 2$, $\|\mathsf{X}_{\tilde{\boldsymbol{\mu}}}\boldsymbol{\mu}\|_q \leq \|\mathsf{X}_{\tilde{\boldsymbol{\mu}}}\boldsymbol{\mu}\|_2$. ∎

The following lemma will allow us to replace the Hilbert–Schmidt norm on the right-hand side of (110) by another Schatten norm with higher index at the expense of using a less sharp power on $|\boldsymbol{p}|$.

Lemma 6.21. *Let $\boldsymbol{\mu}$ be a compact operator. Then for any $\alpha > a$ and any $q \in [2, \infty]$,*

$$\|\mathsf{X}_{\boldsymbol{\mu}}\|_q \leq C h^{-\alpha}\|\boldsymbol{\mu}(1 + |\boldsymbol{p}|^\alpha)\|_q \tag{113}$$

for a constant C depending only on a and α.

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

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

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 as

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

with $g(x) = |x|^{a-3}$ and $m_\alpha = 1 + |\boldsymbol{p}|^\alpha$. Now taking $1 \leq 3/\alpha < p_0' < 3/a < p_1' \leq \infty$ such that $1/p_0' + 1/p_1' = a/3$, 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 $p \geq 1$ satisfying $p' > 3/\alpha$. Then, by Hölder's inequality for Schatten norms, Lemma 6.8 and the Kato–Seiler–Simon inequality (21), we have

$$\begin{aligned}&h^3|\operatorname{Tr}(m_\alpha^{1/2}\boldsymbol{\mu}m_\alpha^{1/2}m_\alpha^{-1/2}\varphi\tilde{g}(\boldsymbol{p})\phi m_\alpha^{-1/2})| \\ &\qquad\leq \|m_\alpha^{1/2}\boldsymbol{\mu}m_\alpha^{1/2}\|_\infty\|m_\alpha^{-1/2}\varphi^{1/p'}\|_{\mathfrak{L}^{2p'}}\|\varphi^{\frac{1}{p}}\tilde{g}(\boldsymbol{p})^{1/2}\|_{\mathfrak{L}^{2p}}\|\tilde{g}(\boldsymbol{p})^{1/2}\phi^{\frac{1}{p}}\|_{\mathfrak{L}^{2p}} \\ &\qquad\quad\cdot\|\phi^{1/p'}m_\alpha^{-1/2}\|_{\mathfrak{L}^{2p'}} \\ &\qquad\leq C_p^{1/p'}\|\boldsymbol{\mu}m_\alpha\|_\infty\|\varphi\|_{L^2}\|\tilde{g}\|_{L^p}\|\phi\|_{L^2},\end{aligned}$$

where we use the notation $z^b = |z|^{b-1}z$ and $C_p = \int_{\mathbb{R}^3}\frac{\mathrm{d}y}{(1+|y|^\alpha)^{p'}}$. This constant is finite since $\alpha p' > 3$. This proves inequality (113) when $q = \infty$. When $q = 2$, the inequality follows from (112). The other cases follow by complex interpolation. ∎

6.5. Commutators involving the exchange term

Proposition 6.22. *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 $n \geq 2a - 1$,*

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

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

Proof. By (109), and the triangle inequality, we have

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

Now, Lemma 6.20 gives the bound

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

Using the fact that $\mathrm{ad}_{\boldsymbol{p}_{\mathrm{j}}}(\boldsymbol{\rho}) = -i\hbar\nabla_{x_{\mathrm{j}}}\boldsymbol{\rho}$ and expanding the $k-1$ commutators in $\mathrm{ad}^{k-1}_{\boldsymbol{p}_{\mathrm{j}}}$ by Lemma 6.9, we get

$$\|\mathrm{ad}^k_{\boldsymbol{p}_{\mathrm{j}}}(\boldsymbol{\rho}) |\boldsymbol{p}|^{a(1-\theta)}\|_2 \leq 2^k \hbar \|\nabla_{x_{\mathrm{j}}}\boldsymbol{\rho} |\boldsymbol{p}|^{a(1-\theta)+k-1}\|_2.$$

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

$$\frac{1}{\hbar}\|[\mathsf{X}_{\boldsymbol{\rho}}, \boldsymbol{p}_{\mathrm{j}}^n]\boldsymbol{\mu}\|_q \leq C h^{-a} \sum_{k=1}^{n} \binom{n}{k} 2^k \|\nabla_{x_{\mathrm{j}}}\boldsymbol{\rho}\, m_n\|_2 \|\boldsymbol{\mu} m_n\|_\infty.$$

We conclude by using the fact that $\|\boldsymbol{\mu} m_n\|_\infty \leq \|\boldsymbol{\mu} m_n\|_q$ and the definition (20) of the $\mathcal{L}^2$ norm. ∎

Proposition 6.23. *Let $a \in [0, 1]$, $\mathfrak{b} = \frac{3}{a+1}$ and $n \in \mathbb{N}$ satisfy $n \geq 2a$. Then for any $\alpha \in (a, n-a]$ and any $q \in [2, \infty]$,*

$$\frac{1}{\hbar}\|[h^3 \mathsf{X}_{\boldsymbol{\mu}}, \boldsymbol{\rho}]\boldsymbol{p}_{\mathrm{j}}^n\|_{\mathcal{L}^q} \leq 3^n C h^{3(1/q+1/2-1/\mathfrak{b})} \|\boldsymbol{\rho} m_n\|_{\mathcal{L}^\infty} \|\boldsymbol{\mu} m_n\|_{\mathcal{L}^2}, \tag{114}$$

$$\frac{1}{\hbar}\|[h^3 \mathsf{X}_{\boldsymbol{\mu}}, \boldsymbol{\rho}]\boldsymbol{p}_{\mathrm{j}}^n\|_{\mathcal{L}^q} \leq 3^n C \|\boldsymbol{\rho} m_n\|_{\mathcal{L}^\infty} (h^{3/\beta'} \|\boldsymbol{\mu} m_n\|_{\mathcal{L}^q} + h^{3/2-a} \|\nabla_{x_{\mathrm{j}}}\boldsymbol{\mu} m_n\|_{\mathcal{L}^2}), \tag{115}$$

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

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

Proof of Proposition 6.23. Since the exchange term is vanishing when $\hbar \to 0$, we can estimate the two parts of the commutator separately by writing

$$\|[\mathsf{X}_{\boldsymbol{\mu}}, \boldsymbol{\rho}]\boldsymbol{p}_{\mathrm{j}}^n\|_q = \|\boldsymbol{p}_{\mathrm{j}}^n[\mathsf{X}_{\boldsymbol{\mu}}, \boldsymbol{\rho}]\|_q \leq \|\boldsymbol{p}_{\mathrm{j}}^n\boldsymbol{\rho}\mathsf{X}_{\boldsymbol{\mu}}\|_q + \|\boldsymbol{p}_{\mathrm{j}}^n\mathsf{X}_{\boldsymbol{\mu}}\boldsymbol{\rho}\|_q.$$

The first term in the right-hand side can be bounded using Hölder's inequality for Schatten norms and Lemma 6.20 with $\theta = 0$, leading to

$$\|\boldsymbol{p}_{\mathrm{j}}^n\boldsymbol{\rho}\mathsf{X}_{\boldsymbol{\mu}}\|_q \leq Ch^{-a}\|\boldsymbol{p}_{\mathrm{j}}^n\boldsymbol{\rho}\|_\infty\|\boldsymbol{\mu}|\boldsymbol{p}|^a\|_2 \leq Ch^{-a}\|\boldsymbol{\rho}m_n\|_\infty\|\boldsymbol{\mu}m_n\|_2. \tag{116}$$

We can also use Lemma 6.21 with $\alpha \in (a, n]$ to get

$$\|\boldsymbol{p}_{\mathrm{j}}^n\boldsymbol{\rho}\mathsf{X}_{\boldsymbol{\mu}}\|_q \leq Ch^{-\alpha}\|\boldsymbol{p}_{\mathrm{j}}^n\boldsymbol{\rho}\|_\infty\|\boldsymbol{\mu}(1 + |\boldsymbol{p}|^\alpha)\|_q \leq Ch^{-\alpha}\|\boldsymbol{\rho}m_n\|_\infty\|\boldsymbol{\mu}m_n\|_q. \tag{117}$$

To treat the second term, we want to put the first weight m_n either on $\boldsymbol{\mu}$ or on $\boldsymbol{\rho}$. To obtain this effect, we use (108) to get

$$\|\boldsymbol{p}_{\mathrm{j}}^n\mathsf{X}_{\boldsymbol{\mu}}\boldsymbol{\rho}\|_q \leq \sum_{k=0}^n \binom{n}{k}\|\mathsf{X}_{\mathrm{ad}_{\boldsymbol{p}_{\mathrm{j}}}^k(\boldsymbol{\mu})}\boldsymbol{p}_{\mathrm{j}}^{n-k}\boldsymbol{\rho}\|_q. \tag{118}$$

Now we use Lemma 6.20 and then expand the commutators by Lemma 6.9 to get, for any $\theta \in \{0, 1\}$,

$$\begin{aligned}\|\mathsf{X}_{\mathrm{ad}_{\boldsymbol{p}_{\mathrm{j}}}^k(\boldsymbol{\mu})}\boldsymbol{p}_{\mathrm{j}}^{n-k}\boldsymbol{\rho}\|_q &\leq Ch^{-a}\|\mathrm{ad}_{\boldsymbol{p}_{\mathrm{j}}}^k(\boldsymbol{\mu})|\boldsymbol{p}|^{a(1-\theta)}\|_2\|\boldsymbol{\rho}\boldsymbol{p}_{\mathrm{j}}^{n-k}|\boldsymbol{p}|^{\theta a}\|_\infty \\ &\leq 2^kCh^{-a}\|\boldsymbol{\mu}(1 + |\boldsymbol{p}|^{k+a(1-\theta)})\|_2\|\boldsymbol{\rho}(1 + |\boldsymbol{p}|^{n-k+\theta a})\|_\infty,\end{aligned}$$

and similarly to the proof of Proposition 6.22, 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 (118), we obtain

$$\|\boldsymbol{p}_{\mathrm{j}}^n\mathsf{X}_{\boldsymbol{\mu}}\boldsymbol{\rho}\|_q \leq 3^nCh^{-a}\|\boldsymbol{\rho}m_n\|_\infty\|\boldsymbol{\mu}m_n\|_2. \tag{119}$$

Combining inequalities (116) and (119) and using the definition (20) of $\mathcal{L}^q$ norms yields (114).

To get (115), we start from inequality (118). If $k > a$, so that in particular $k \geq 1$, we use again Lemmas 6.20 and 6.9 but we use first the fact that $\mathrm{ad}_{\boldsymbol{p}_j}(\boldsymbol{\mu}) = -i\hbar\nabla_{x_{\mathrm{j}}}\boldsymbol{\mu}$ to get an additional $\hbar$. This yields

$$\|\mathsf{X}_{\mathrm{ad}_{\boldsymbol{p}_{\mathrm{j}}}^k(\boldsymbol{\mu})}\boldsymbol{p}_{\mathrm{j}}^{n-k}\boldsymbol{\rho}\|_q \leq 2^kCh^{1-a}\|\nabla_{x_{\mathrm{j}}}\boldsymbol{\mu}(1 + |\boldsymbol{p}|^{k-1})\|_2\|\boldsymbol{\rho}(1 + |\boldsymbol{p}|^{n-k+a})\|_\infty.$$

If $k \leq a$, we use Lemma 6.21 with $\alpha \in (a, n - a]$ to get

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

Therefore, inequality (118) implies

$$\|\boldsymbol{p}_{\mathrm{j}}^n\mathsf{X}_{\boldsymbol{\mu}}\boldsymbol{\rho}\|_q \leq 3^nC\|\boldsymbol{\rho}m_n\|_\infty(h^{-\alpha}\|\boldsymbol{\mu}m_n\|_q + h^{1-a}\|\nabla_{x_{\mathrm{j}}}\boldsymbol{\mu}m_n\|_2), \tag{120}$$

and together with inequality (116) and the definition of the $\mathcal{L}^q$ norm, this implies (115).

∎

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 (87)–(89) and find a Grönwall-type inequality on $\|\boldsymbol{\rho}\|_{\mathcal{W}^{1,q}(m_{2n})}$, where we renamed n as $2n$ as we need the number of moments to be even. In particular, we will see that to close the Grönwall argument for $q = 2$, we need to estimate $\|\boldsymbol{\rho}\|_{\mathcal{W}^{1,q}(m_{2n})}$ for $q \in \{2, 4\}$. We will therefore proceed by interpolation and define

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

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

We now look at equation (87). Splitting the interaction K as in (106), by Propositions 6.17 and 6.15 we find that, for $1/r + 1/r_1 = 1/q + 1/3$,

$$\begin{aligned}\frac{1}{\hbar}\|[V_{\boldsymbol{\rho}}, m_{2n}]\boldsymbol{\rho}\|_{\mathcal{L}^q} &\leq C(\|\boldsymbol{\rho} m_{n+n_0}\|_{\mathcal{L}^{\mathfrak{b}'}}\|\boldsymbol{\rho} m_{2n-1}\|_{\mathcal{L}^q} + \|\boldsymbol{\rho} m_{2n+k'}\|_{\mathcal{L}^r}\|\boldsymbol{\rho} m_{n+k}\|_{\mathcal{L}^{r_1}}) \\ &\quad + C(\|\rho\|_{L^1} + \hbar\|\boldsymbol{\rho} m_{2n}\|_{\mathcal{L}^2})\|\boldsymbol{\rho} m_{2n}\|_{\mathcal{L}^q}\end{aligned}$$

with

$$n_0 > 3/\mathfrak{b} - 1, \quad k' > 3/r' - 2, \quad k > 3/r - 1.$$

The contribution given by the exchange term on the right-hand side of (87) can be bounded by Proposition 6.22 with $\boldsymbol{\mu} = \boldsymbol{\rho}$. Therefore, we obtain the following bounds on the right-hand side of (87):

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\|\boldsymbol{\rho} m_{2n}\|_{\mathcal{L}^q} \leq C(&\|\boldsymbol{\rho} m_{n+n_0}\|_{\mathcal{L}^{\mathfrak{b}'}}\|\boldsymbol{\rho} m_{2n-1}\|_{\mathcal{L}^q} + \|\boldsymbol{\rho} m_{2n+k'}\|_{\mathcal{L}^r}\|\boldsymbol{\rho} m_{n+k}\|_{\mathcal{L}^{r_1}} \\ &+ \|\rho\|_{L^1}\|\boldsymbol{\rho} m_{2n}\|_{\mathcal{L}^q} + \hbar\|\boldsymbol{\rho} m_{2n}\|_{\mathcal{L}^2}\|\boldsymbol{\rho} m_{2n}\|_{\mathcal{L}^q} \\ &+ h^{3/2-a}\|\nabla_x\boldsymbol{\rho}\, m_{2n}\|_{\mathcal{L}^2}\|\boldsymbol{\rho} m_{2n}\|_{\mathcal{L}^q}).\end{aligned}$$

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

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\|\boldsymbol{\rho} m_{2n}\|_{\mathcal{L}^\infty} \leq C(&\|\boldsymbol{\rho} m_{n+n_0}\|_{\mathcal{L}^{\mathfrak{b}'}}\|\boldsymbol{\rho} m_{2n-1}\|_{\mathcal{L}^\infty} + \|\boldsymbol{\rho} m_{2n+k'}\|_{\mathcal{L}^r}\|\boldsymbol{\rho} m_{n+k}\|_{\mathcal{L}^{r_1}} \\ &+ \|\rho\|_{L^1}\|\boldsymbol{\rho} m_{2n}\|_{\mathcal{L}^\infty} + \hbar\|\boldsymbol{\rho} m_{2n}\|_{\mathcal{L}^2}\|\boldsymbol{\rho} m_{2n}\|_{\mathcal{L}^\infty} \\ &+ h^{3/2-a}\|\nabla_x\boldsymbol{\rho}\, m_{2n}\|_{\mathcal{L}^2}\|\boldsymbol{\rho} m_{2n}\|_{\mathcal{L}^\infty}).\end{aligned}$$

Note that in order to close the Grönwall inequality we will need bounds on $\nabla_x\boldsymbol{\rho}$ and $\nabla_\xi\boldsymbol{\rho}$. To this end, we look at equations (88) and (89). We start bounding the right-hand side of (88). By Propositions 6.15 and 6.17 we obtain

$$\begin{aligned}&\frac{1}{\hbar}\|[V_{\boldsymbol{\rho}}, m_{2n}]\nabla_x\boldsymbol{\rho}\|_{\mathcal{L}^q} \\ &\quad\leq C(\|\boldsymbol{\rho} m_{n+n_0}\|_{\mathcal{L}^{\mathfrak{b}'}}\|\nabla_x\boldsymbol{\rho}\, m_{2n-1}\|_{\mathcal{L}^q} + \|\boldsymbol{\rho} m_{2n+k'}\|_{\mathcal{L}^r}\|\nabla_x\boldsymbol{\rho}\, m_{n+k}\|_{\mathcal{L}^{r_1}} \\ &\qquad + \|\rho\|_{L^1}\|\nabla_x\boldsymbol{\rho}\, m_{2n}\|_{\mathcal{L}^q} + \hbar\|\boldsymbol{\rho} m_{2n}\|_{\mathcal{L}^2}\|\nabla_x\boldsymbol{\rho}\, m_{2n}\|_{\mathcal{L}^q})\end{aligned} \tag{121}$$

with the usual constraints on r, r_1, n_0, k, k'.

By writing $[E_{\boldsymbol{\rho}}, \boldsymbol{\rho}]m_{2n} = [E_{\boldsymbol{\rho}}, \boldsymbol{\rho} m_{2n}] + \boldsymbol{\rho}[E_{\boldsymbol{\rho}}, m_{2n}]$, applying Proposition 6.13 with $\boldsymbol{\rho}_2 = \boldsymbol{\rho} m_{2n}$, and Propositions 6.15 and 6.17 with $\boldsymbol{\mu} = \boldsymbol{\rho}$, we get

$$\begin{aligned}\frac{1}{\hbar}\|[E_{\boldsymbol{\rho}}, \boldsymbol{\rho}]m_{2n}\|_{\mathcal{L}^q} \leq C(&\|\rho\|_{L^r}^{1-s}\|\rho\|_{W^{1,r}}^{s}\|\nabla_\xi \boldsymbol{\rho}\, m_{2n}\|_{\mathcal{L}^q} \\ &+ \|\nabla_x \boldsymbol{\rho}\, m_{n+n_0}\|_{\mathcal{L}^{\mathfrak{b}'}}\|\boldsymbol{\rho} m_{2n-1}\|_{\mathcal{L}^q} + \|\nabla_x \boldsymbol{\rho}\, m_{2n+k'}\|_{\mathcal{L}^r}\|\boldsymbol{\rho} m_{n+k}\|_{\mathcal{L}^{r_1}} \\ &+ \|\boldsymbol{\rho} m_{2n}\|_{\mathcal{L}^2}\|\boldsymbol{\rho} m_{2n}\|_{\mathcal{L}^q} + \hbar\|\nabla_x \boldsymbol{\rho}\, m_{2n}\|_{\mathcal{L}^2}\|\boldsymbol{\rho} m_{2n}\|_{\mathcal{L}^q})\end{aligned} \tag{122}$$

for $q > 2$ and $s = 1 - 3(1/r' - 1/\mathfrak{b}')$, where we have used the interpolation of Besov spaces stated in Corollary 6.14.

For $q = 2$, we have

$$\begin{aligned}\frac{1}{\hbar}\|[E_{\boldsymbol{\rho}}, \boldsymbol{\rho}]m_{2n}\|_{\mathcal{L}^2} \leq C(&\|\nabla\rho\|_{L^{\mathfrak{b}',1}}\|\nabla_\xi \boldsymbol{\rho}\, m_{2n}\|_{\mathcal{L}^2} \\ &+ \|\nabla_x \boldsymbol{\rho}\, m_{2n}\|_{\mathcal{L}^2}^{1-\theta}\|\nabla_x \boldsymbol{\rho}\, m_{2n-2}\|_{\mathcal{L}^4}^{\theta}\|\boldsymbol{\rho} m_{2n}\|_{\mathcal{L}^2} \\ &+ \|\nabla_x \boldsymbol{\rho}\, m_{2n}\|_{\mathcal{L}^2}\|\boldsymbol{\rho} m_{2n}\|_{\mathcal{L}^2}^{1/3}\|\boldsymbol{\rho} m_{2n-2}\|_{\mathcal{L}^4}^{2/3} \\ &+ \|\boldsymbol{\rho} m_{2n}\|_{\mathcal{L}^2}^2 + \hbar\|\nabla_x \boldsymbol{\rho}\, m_{2n}\|_{\mathcal{L}^2}\|\boldsymbol{\rho} m_{2n}\|_{\mathcal{L}^2})\end{aligned} \tag{123}$$

for $a \in [1/2, 1]$, and

$$\begin{aligned}\frac{1}{\hbar}\|[E_{\boldsymbol{\rho}}, \boldsymbol{\rho}]m_{2n}\|_{\mathcal{L}^2} \leq C(&\|\rho\|_{L^{\frac{3}{1-a},1}}\|\nabla_\xi \boldsymbol{\rho}\, m_{2n}\|_{\mathcal{L}^2} \\ &+ \|\nabla_x \boldsymbol{\rho}\, m_{2n}\|_{\mathcal{L}^2}^{1-\theta}\|\nabla_x \boldsymbol{\rho}\, m_{2n-2}\|_{\mathcal{L}^4}^{\theta}\|\boldsymbol{\rho} m_{2n}\|_{\mathcal{L}^2} \\ &+ \|\nabla_x \boldsymbol{\rho}\, m_{2n}\|_{\mathcal{L}^2}\|\boldsymbol{\rho} m_{2n}\|_{\mathcal{L}^2}^{1/3}\|\boldsymbol{\rho} m_{2n-2}\|_{\mathcal{L}^4}^{2/3} \\ &+ \|\boldsymbol{\rho} m_{2n}\|_{\mathcal{L}^2}^2 + \hbar\|\nabla_x \boldsymbol{\rho}\, m_{2n}\|_{\mathcal{L}^2}\|\boldsymbol{\rho} m_{2n}\|_{\mathcal{L}^2})\end{aligned} \tag{124}$$

for $a \in (0, 1/2)$.

The contributions of the exchange term can be bounded using Propositions 6.22 and 6.23. Combining them with (121) and (122) leads to, for $q > 2$,

$$\begin{aligned}&\frac{\mathrm{d}}{\mathrm{d}t}\|\nabla_x \boldsymbol{\rho}\, m_{2n}\|_{\mathcal{L}^q} \\ &\quad\leq C(\|\boldsymbol{\rho} m_{n+n_0}\|_{\mathcal{L}^{\mathfrak{b}'}}\|\nabla_x \boldsymbol{\rho}\, m_{2n-1}\|_{\mathcal{L}^q} + \|\boldsymbol{\rho} m_{2n+k'}\|_{\mathcal{L}^r}\|\nabla_x \boldsymbol{\rho}\, m_{n+k}\|_{\mathcal{L}^{r_1}} \\ &\qquad+ \|\rho\|_{L^1}\|\nabla_x \boldsymbol{\rho}\, m_{2n}\|_{\mathcal{L}^q} + \hbar\|\boldsymbol{\rho} m_{2n}\|_{\mathcal{L}^2}\|\nabla_x \boldsymbol{\rho}\, m_{2n}\|_{\mathcal{L}^q}) \\ &\qquad+ C(\|\rho\|_{L^r}^{1-s}\|\rho\|_{W^{1,r}}^{s}\|\nabla_\xi \boldsymbol{\rho}\, m_{2n}\|_{\mathcal{L}^q} + \|\nabla_x \boldsymbol{\rho}\, m_{n+n_0}\|_{\mathcal{L}^{\mathfrak{b}'}}\|\boldsymbol{\rho} m_{2n-1}\|_{\mathcal{L}^q} \\ &\qquad+ \|\nabla_x \boldsymbol{\rho}\, m_{2n+k'}\|_{\mathcal{L}^r}\|\boldsymbol{\rho} m_{n+k}\|_{\mathcal{L}^{r_1}} + \|\boldsymbol{\rho} m_{2n}\|_{\mathcal{L}^2}\|\boldsymbol{\rho} m_{2n}\|_{\mathcal{L}^q} \\ &\qquad+ \hbar\|\nabla_x \boldsymbol{\rho}\, m_{2n}\|_{\mathcal{L}^2}\|\boldsymbol{\rho} m_{2n}\|_{\mathcal{L}^q}) \\ &\qquad+ C h^{3/2-a}\|\nabla_x \boldsymbol{\rho}\, m_{2n}\|_{\mathcal{L}^2}\|\nabla_x \boldsymbol{\rho}\, m_{2n}\|_{\mathcal{L}^q} \\ &\qquad+ C h^{3(1/q+1/2-1/\mathfrak{b})}\|\boldsymbol{\rho} m_{2n}\|_{\mathcal{L}^\infty}\|\nabla_x \boldsymbol{\rho}\, m_{2n}\|_{\mathcal{L}^2}.\end{aligned}$$

To bound the right-hand side of (89), we use Proposition 6.15 for the contribution due to the direct term and Propositions 6.22 and 6.23 to estimate the contributions of the exchange term. Hence,

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\|\nabla_\xi \boldsymbol{\rho}\, m_{2n}\|_{\mathcal{L}^q} \le C(&\|\boldsymbol{\rho} m_{n+n_0}\|_{\mathcal{L}^{\mathfrak{b}'}}\|\nabla_\xi \boldsymbol{\rho}\, m_{2n-1}\|_{\mathcal{L}^q} + \|\boldsymbol{\rho} m_{2n+k'}\|_{\mathcal{L}^r}\|\nabla_\xi \boldsymbol{\rho}\, m_{n+k}\|_{\mathcal{L}^{r_1}}\\ &+ \|\rho\|_{L^1}\|\nabla_\xi \boldsymbol{\rho}\, m_{2n}\|_{\mathcal{L}^q} + \hbar\|\boldsymbol{\rho} m_{2n}\|_{\mathcal{L}^2}\|\nabla_\xi \boldsymbol{\rho}\, m_{2n}\|_{\mathcal{L}^q})\\ &+ \|\nabla_x \boldsymbol{\rho}\, m_{2n}\|_{\mathcal{L}^q}\\ &+ C h^{3/2-a}\|\nabla_x \boldsymbol{\rho}\, m_{2n}\|_{\mathcal{L}^2}\|\nabla_\xi \boldsymbol{\rho}\, m_{2n}\|_{\mathcal{L}^q}\\ &+ C h^{3(1/q+1/2-1/\mathfrak{b})}\|\boldsymbol{\rho} m_{2n}\|_{\mathcal{L}^\infty}\|\nabla_\xi \boldsymbol{\rho}\, m_{2n}\|_{\mathcal{L}^2}.\end{aligned}$$

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 $q = 4$ using Corollary 6.16 and proceed by interpolation.

To establish a Grönwall-type inequality for $a \ge 1/2$, we observe that the sum $M_2(t) + M_4(t) + M_\infty(t)$ satisfies

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}(M_2(t) + M_4(t) + M_\infty(t)) \le C(&M_2(t) + M_4(t) + M_\infty(t))\\ &+ C(1 + h^{3/2-a} + h^{3/\mathfrak{b}'} + h^{3(3/4-1/\mathfrak{b})})\\ &\times (M_2(t) + M_4(t) + M_\infty(t))^2, \qquad (125)\end{aligned}$$

where we have used an interpolation inequality with $\theta \in (0,1)$ and Young's inequality for products to bound the $\mathcal{L}^r, \mathcal{L}^{r'}, L^{\mathfrak{b}'}$ norms with $r, r', \mathfrak{b}' \in [2,4]$. Furthermore, we have used the following simple inequality: for an operator $\boldsymbol{\mu}$, $k \in (0,2n)$ and $q \ge 2$,

$$\|\boldsymbol{\mu} m_{2n-k}\|_{\mathcal{L}^q} \le \|\boldsymbol{\mu} m_{2n}\|_{\mathcal{L}^q}\|m_k^{-1}\|_{\mathcal{L}^\infty}.$$

We observe that (125) is a Grönwall-type inequality of the same form as (83). Thus there exists a time $T > 0$, depending only in the initial data, such that $M_2(t) + M_4(t) + M_\infty(t)$ is bounded for all $t \in [0,T]$.

For $a < 1/2$, we consider the quantity $M_2(t) + M_4(t)$ and use the fact that

$$\|\boldsymbol{\rho} m_{2n}\|_{\mathcal{L}^\infty} \le C h^{-3/q}\|\boldsymbol{\rho} m_{2n}\|_{\mathcal{L}^q}.$$

Hence

$$\begin{aligned}&\frac{\mathrm{d}}{\mathrm{d}t}(M_2(t) + M_4(t))\\ &\qquad \le C(M_2(t) + M_4(t)) + C(1 + h^{3/2-a} + h^{3(1/\mathfrak{b}'-1/2)})(M_2(t) + M_4(t))^2.\end{aligned}$$

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 $\boldsymbol{\rho} \in L^\infty((0,T), \mathcal{W}^{1,2}(m_{2n}) \cap \mathcal{W}^{1,4}(m_{2n}) \cap \mathcal{L}^\infty(m_{2n}))$. Moreover, $\rho \in L^\infty((0,T), H^1 \cap W^{1,4} \cap L^1 \cap L^\infty)$ thanks to Proposition 6.11 and the bounds on $M_2(t)$, $M_4(t)$ and $M_\infty(t)$. ∎

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 $\boldsymbol{\rho}$:

$$\begin{aligned} i\hbar\partial_t \nabla_x^2 \boldsymbol{\rho} &= [H, \nabla_x^2 \boldsymbol{\rho}] - 2[E_{\boldsymbol{\rho}}, \nabla_x \boldsymbol{\rho}] - [\nabla_x E_{\boldsymbol{\rho}}, \boldsymbol{\rho}] - 2[h^3 \mathsf{X}_{\nabla_x \boldsymbol{\rho}}, \nabla_x \boldsymbol{\rho}] - [h^3 \mathsf{X}_{\nabla_x^2 \boldsymbol{\rho}}, \boldsymbol{\rho}], \\ i\hbar\partial_t \nabla_\xi^2 \boldsymbol{\rho} &= [H, \nabla_\xi^2 \boldsymbol{\rho}] - i\hbar \nabla_\xi \nabla_x \boldsymbol{\rho} - 2[h^3 \mathsf{X}_{\nabla_\xi \boldsymbol{\rho}}, \nabla_\xi \boldsymbol{\rho}] - [h^3 \mathsf{X}_{\nabla_\xi^2 \boldsymbol{\rho}}, \boldsymbol{\rho}], \\ i\hbar\partial_t \nabla_\xi \nabla_x \boldsymbol{\rho} &= [H, \nabla_\xi \nabla_x \boldsymbol{\rho}] - i\hbar \nabla_x^2 \boldsymbol{\rho} - [E_{\boldsymbol{\rho}}, \nabla_\xi \boldsymbol{\rho}] - [h^3 \mathsf{X}_{\nabla_\xi \nabla_x \boldsymbol{\rho}}, \boldsymbol{\rho}] - [h^3 \mathsf{X}_{\nabla_x \boldsymbol{\rho}}, \nabla_\xi \boldsymbol{\rho}], \end{aligned} \tag{126}$$

that are of the form

$$i\hbar\partial_t \boldsymbol{\mu} = [\mathsf{A}, \boldsymbol{\mu}] + [\mathsf{B}, \nabla_x \boldsymbol{\rho}] + [\mathsf{C}, \boldsymbol{\rho}], \tag{127}$$

with A, B and C being self-adjoint operators. The proof of Lemma 6.6 proves also the following statement.

Lemma 6.24 (Lemma 6.6 bis). *Let $\boldsymbol{\rho}, \mathsf{A}, \mathsf{B}, \mathsf{C}$ be self-adjoint operators and $\boldsymbol{\mu} = \boldsymbol{\mu}(t)$ be a family of self-adjoint operators satisfying* (127). *Then, formally, for any even integer $q \geq 2$ we have*

$$\frac{\mathrm{d}}{\mathrm{d}t} \|\boldsymbol{\mu} m_{2n}\|_q \leq \frac{1}{\hbar} \|[\mathsf{A}, m_{2n}]\boldsymbol{\mu}\|_q + \frac{1}{\hbar} \|[\mathsf{B}, \nabla_x \boldsymbol{\rho}] m_{2n}\|_q + \frac{1}{\hbar} \|[\mathsf{C}, \boldsymbol{\rho}] m_{2n}\|_q.$$

We consider the identities (126) and bound them by Lemma 6.24. This yields

$$\begin{aligned} \hbar \frac{\mathrm{d}}{\mathrm{d}t} \|\nabla_x^2 \boldsymbol{\rho}\, m_{2n}\|_q &\leq C \|[V_{\boldsymbol{\rho}}, m_{2n}] \nabla_x^2 \boldsymbol{\rho}\|_q + C \|[E_{\boldsymbol{\rho}}, \nabla_x \boldsymbol{\rho}] m_{2n}\|_q \\ &\quad + C \|[\nabla_x E_{\boldsymbol{\rho}}, \boldsymbol{\rho}] m_{2n}\|_q + C \|[h^3 \mathsf{X}_{\boldsymbol{\rho}}, m_{2n}] \nabla_x^2 \boldsymbol{\rho}\|_q \\ &\quad + C \|[h^3 \mathsf{X}_{\nabla_x \boldsymbol{\rho}}, \nabla_x \boldsymbol{\rho}] m_{2n}\|_q + C \|[h^3 \mathsf{X}_{\nabla_x^2 \boldsymbol{\rho}}, \boldsymbol{\rho}] m_{2n}\|_q, \end{aligned} \tag{128}$$

$$\begin{aligned} \hbar \frac{\mathrm{d}}{\mathrm{d}t} \|\nabla_\xi^2 \boldsymbol{\rho}\, m_{2n}\|_q &\leq C \|[V_{\boldsymbol{\rho}}, m_{2n}] \nabla_\xi^2 \boldsymbol{\rho}\|_q + C \|\nabla_\xi \nabla_x \boldsymbol{\rho}\, m_{2n}\|_q \\ &\quad + C \|[h^3 \mathsf{X}_{\boldsymbol{\rho}}, m_{2n}] \nabla_\xi^2 \boldsymbol{\rho}\|_q + C \|[h^3 \mathsf{X}_{\nabla_\xi \boldsymbol{\rho}}, \nabla_\xi \boldsymbol{\rho}] m_{2n}\|_q \\ &\quad + C \|[h^3 \mathsf{X}_{\nabla_\xi^2 \boldsymbol{\rho}}, \boldsymbol{\rho}] m_{2n}\|_q, \end{aligned} \tag{129}$$

$$\begin{aligned} \hbar \frac{\mathrm{d}}{\mathrm{d}t} \|\nabla_\xi \nabla_x \boldsymbol{\rho}\, m_{2n}\|_q &\leq C \|[V_{\boldsymbol{\rho}}, m_{2n}] \nabla_\xi \nabla_x \boldsymbol{\rho}\|_q + C \|[E_{\boldsymbol{\rho}}, \nabla_\xi \boldsymbol{\rho}] m_{2n}\|_q \\ &\quad + C \|\nabla_x^2 \boldsymbol{\rho} m_{2n}\|_q + C \|[h^3 \mathsf{X}_{\boldsymbol{\rho}}, m_{2n}] \nabla_\xi \nabla_x \boldsymbol{\rho}\|_q \\ &\quad + C \|[h^3 \mathsf{X}_{\nabla_x \boldsymbol{\rho}}, \nabla_\xi \boldsymbol{\rho}] m_{2n}\|_q + C \|[h^3 \mathsf{X}_{\nabla_\xi \nabla_x \boldsymbol{\rho}}, \boldsymbol{\rho}] m_{2n}\|_q. \end{aligned} \tag{130}$$

We now estimate the right-hand side of (128). The first three contributions are related to the direct term in the Hartree equation, whereas in the others the exchange operator appears. By Propositions 6.15 and 6.17 we have

$$\begin{aligned} \frac{1}{\hbar} \|[V_{\boldsymbol{\rho}}, m_{2n}] \nabla_x^2 \boldsymbol{\rho}\|_{\mathcal{L}^q} &\leq C \|\boldsymbol{\rho} m_{n+n_0}\|_{\mathcal{L}^{\mathfrak{b}'}} \|\nabla_x^2 \boldsymbol{\rho}\, m_{2n-1}\|_{\mathcal{L}^q} \\ &\quad + C \|\boldsymbol{\rho} m_{2n+k'}\|_{\mathcal{L}^r} \|\nabla_x^2 \boldsymbol{\rho}\, m_{n+k}\|_{\mathcal{L}^{r_1}} + C \|\rho\|_{L^1} \|\nabla_x^2 \boldsymbol{\rho}\, m_{2n}\|_{\mathcal{L}^q} \\ &\quad + C\hbar \|\boldsymbol{\rho} m_{2n}\|_{\mathcal{L}^2} \|\nabla_x^2 \boldsymbol{\rho}\, m_{2n}\|_{\mathcal{L}^q}. \end{aligned} \tag{131}$$

As for the second term on the right-hand side of (128), we rewrite it as follows:

$$\frac{1}{\hbar}\|[E_{\boldsymbol{\rho}}, \nabla_x \boldsymbol{\rho}] m_{2n}\|_{\mathcal{L}^q} = \frac{1}{\hbar}\|[E_{\boldsymbol{\rho}}, \nabla_x \boldsymbol{\rho}\, m_{2n}]\|_{\mathcal{L}^q} + \frac{1}{\hbar}\|[E_{\boldsymbol{\rho}}, m_{2n}]\nabla_x \boldsymbol{\rho}\|_{\mathcal{L}^q}.$$

By Proposition 6.13 and Corollary 6.14, we get

$$\frac{1}{\hbar}\|[E_{\boldsymbol{\rho}}, \nabla_x \boldsymbol{\rho}\, m_{2n}]\|_{\mathcal{L}^q} \leq C\|\rho\|_{L^r}^{1-s}\|\rho\|_{W^{1,r}}^{s}\|\nabla_\xi \nabla_x \boldsymbol{\rho}\, m_{2n}\|_{\mathcal{L}^q}, \tag{132}$$

for $1/r + 1/q = 1/2$ and $s = 1 - 3(1/r' - 1/\mathfrak{b})$. By Propositions 6.15 and 6.17 we have

$$\begin{aligned}\frac{1}{\hbar}\|[E_{\boldsymbol{\rho}}, m_{2n}]\nabla_x \boldsymbol{\rho}\|_{\mathcal{L}^q} \leq C\|\nabla_x \boldsymbol{\rho}\, m_{n+n_0}\|_{\mathcal{L}^{\mathfrak{b}'}}\|\nabla_x \boldsymbol{\rho}\, m_{2n-1}\|_{\mathcal{L}^q}& \\ + \|\nabla_x \boldsymbol{\rho}\, m_{2n+k'}\|_{\mathcal{L}^r}\|\nabla_x \boldsymbol{\rho}\, m_{n+k}\|_{\mathcal{L}^{r_1}} + \|\boldsymbol{\rho} m_{2n}\|_{\mathcal{L}^2}\|\nabla_x \boldsymbol{\rho}\, m_{2n}\|_{\mathcal{L}^q}& \\ + \hbar\|\nabla_x \boldsymbol{\rho}\, m_{2n}\|_{\mathcal{L}^2}\|\nabla_x \boldsymbol{\rho}\, m_{2n}\|_{\mathcal{L}^q}.&\end{aligned}$$

This, together with (132), controls the second term on the right-hand side of (128). The third term can be dealt with analogously to the second by using the fact that $\nabla_x E_{\boldsymbol{\rho}} = E_{\nabla_x \boldsymbol{\rho}}$ and Proposition 6.15. This gives

$$\begin{aligned}\frac{1}{\hbar}\|[\nabla_x E_{\boldsymbol{\rho}}, \boldsymbol{\rho}] m_{2n}\|_{\mathcal{L}^q} \leq C\|\rho\|_{L^r}^{1-s}\|\rho\|_{W^{1,r}}^{s}\|\nabla_\xi \nabla_x \boldsymbol{\rho}\, m_{2n}\|_{\mathcal{L}^q}& \\ + \|\nabla_x^2 \boldsymbol{\rho}\, m_{n+n_0}\|_{\mathcal{L}^{\mathfrak{b}'}}\|\boldsymbol{\rho} m_{2n-1}\|_{\mathcal{L}^q} + \|\nabla_x^2 \boldsymbol{\rho}\, m_{2n+k'}\|_{\mathcal{L}^r}\|\boldsymbol{\rho} m_{n+k}\|_{\mathcal{L}^{r_1}}& \\ + \|\nabla_x \boldsymbol{\rho}\, m_{2n}\|_{\mathcal{L}^2}\|\boldsymbol{\rho} m_{2n}\|_{\mathcal{L}^q} + \hbar\|\nabla_x^2 \boldsymbol{\rho}\, m_{2n}\|_{\mathcal{L}^2}\|\boldsymbol{\rho} m_{2n}\|_{\mathcal{L}^q}.&\end{aligned}$$

We now turn to terms to which the exchange term contributes. By Proposition 6.22 we obtain

$$\frac{1}{\hbar}\|[h^3 \mathsf{X}_{\boldsymbol{\rho}}, m_{2n}]\nabla_x^2 \boldsymbol{\rho}\|_{\mathcal{L}^q} \leq C\hbar^{3/2-a}\|\nabla_x \boldsymbol{\rho}\, m_{2n}\|_{\mathcal{L}^2}\|\nabla_x^2 \boldsymbol{\rho}\, m_{2n}\|_{\mathcal{L}^q}. \tag{133}$$

By Proposition 6.23 we get the bound

$$\frac{1}{\hbar}\|[h^3 \mathsf{X}_{\nabla_x \boldsymbol{\rho}}, \nabla_x \boldsymbol{\rho}] m_{2n}\|_{\mathcal{L}^q} \leq C\hbar^{3(1/q+1/2-1/\mathfrak{b})}\|\nabla_x \boldsymbol{\rho}\, m_{2n}\|_{\mathcal{L}^2}\|\nabla_x \boldsymbol{\rho}\, m_{2n}\|_{\mathcal{L}^\infty}. \tag{134}$$

Finally, by noticing that $\nabla_x \mathsf{X}_{\nabla_x \boldsymbol{\rho}} = \mathsf{X}_{\nabla_x^2 \boldsymbol{\rho}}$, we apply Proposition 6.23 to the last term on the right-hand side in (128):

$$\frac{1}{\hbar}\|[h^3 \mathsf{X}_{\nabla_x^2 \boldsymbol{\rho}}, \boldsymbol{\rho}] m_{2n}\|_{\mathcal{L}^q} \leq C\hbar^{3(1/q+1/2-1/\mathfrak{b})}\|\boldsymbol{\rho} m_{2n}\|_{\mathcal{L}^\infty}\|\nabla_x^2 \boldsymbol{\rho}\, m_{2n}\|_{\mathcal{L}^2}. \tag{135}$$

Therefore, using Proposition 6.1 and estimates (131)–(135) we obtain a bound on the time derivative of $\|\nabla_x^2 \boldsymbol{\rho}\, m_{2n}\|_{\mathcal{L}^q}$.

We now look at the right-hand side of (129). By using Propositions 6.1, 6.15, 6.17, 6.22, 6.23, and by Proposition 6.23 with $\nabla_\xi \mathsf{X}_{\nabla_\xi \boldsymbol{\rho}} = \mathsf{X}_{\nabla_\xi^2 \boldsymbol{\rho}}$, we obtain a bound on the time derivative of $\|\nabla_\xi^2 \boldsymbol{\rho}\, m_{2n}\|_{\mathcal{L}^q}$.

As for the mixed term (130), its right-hand side can be bounded as follows. By Propositions 6.15 and 6.17 we get

$$\frac{1}{\hbar}\|[V_{\boldsymbol{\rho}}, m_{2n}]\nabla_\xi\nabla_x\boldsymbol{\rho}\|_{\mathcal{L}^q} \leq C\|\boldsymbol{\rho}m_{n+n_0}\|_{\mathcal{L}^{\mathfrak{b}'}}\|\nabla_\xi\nabla_x\boldsymbol{\rho}\, m_{2n-1}\|_{\mathcal{L}^q} + \|\boldsymbol{\rho}m_{2n+k'}\|_{\mathcal{L}^r}\|\nabla_\xi\nabla_x\boldsymbol{\rho}\, m_{n+k}\|_{\mathcal{L}^{r_1}} + (\|\rho\|_{L^1} + \hbar\|\boldsymbol{\rho}m_{2n}\|_{\mathcal{L}^2})\|\nabla_\xi\nabla_x\boldsymbol{\rho}\, m_{2n}\|_{\mathcal{L}^q}. \tag{136}$$

As for the second term on the right-hand side of (130), we rewrite it as

$$\frac{1}{\hbar}\|[E_{\boldsymbol{\rho}}, \nabla_\xi\boldsymbol{\rho}]m_{2n}\|_{\mathcal{L}^q} = \frac{1}{\hbar}\|[E_{\boldsymbol{\rho}}, \nabla_\xi\boldsymbol{\rho}\, m_{2n}]\|_{\mathcal{L}^q} + \frac{1}{\hbar}\|[E_{\boldsymbol{\rho}}, m_{2n}]\nabla_\xi\boldsymbol{\rho}\|_{\mathcal{L}^q}.$$

and use again Proposition 6.13 and Corollary 6.14 for the first term on the right-hand side and Propositions 6.15 and 6.17 for the second term. We now turn to the terms to which the contribution of the exchange term appears. By Proposition 6.22 we obtain

$$\frac{1}{\hbar}\|[\mathsf{X}_{\boldsymbol{\rho}}, m_{2n}]\nabla_\xi\nabla_x\boldsymbol{\rho}\|_{\mathcal{L}^q} \leq C\hbar^{3/2-a}\|\nabla_x\boldsymbol{\rho}\, m_{2n}\|_{\mathcal{L}^2}\|\nabla_\xi\nabla_x\boldsymbol{\rho}\, m_{2n}\|_{\mathcal{L}^q}. \tag{137}$$

By Proposition 6.23 we get the bounds

$$\frac{1}{\hbar}\|[\mathsf{X}_{\nabla_x\boldsymbol{\rho}}, \nabla_\xi\boldsymbol{\rho}]m_{2n}\|_{\mathcal{L}^q} \leq C\hbar^{3(1/q+1/2-1/\mathfrak{b})}\|\nabla_\xi\boldsymbol{\rho}\, m_{2n}\|_{\mathcal{L}^\infty}\|\nabla_x\boldsymbol{\rho}\, m_{2n}\|_{\mathcal{L}^2}, \tag{138}$$

$$\frac{1}{\hbar}\|[\mathsf{X}_{\nabla_\xi\nabla_x\boldsymbol{\rho}}, \nabla_x\boldsymbol{\rho}]m_{2n}\|_{\mathcal{L}^q} \leq C\hbar^{3(1/q+1/2-1/\mathfrak{b})}\|\nabla_x\boldsymbol{\rho}\, m_{2n}\|_{\mathcal{L}^\infty}\|\nabla_\xi\nabla_x\boldsymbol{\rho}\, m_{2n}\|_{\mathcal{L}^2}. \tag{139}$$

Therefore, using Proposition 6.1 and estimates (136)–(139) yields

$$\frac{\mathrm{d}}{\mathrm{d}t}\|\nabla_\xi\nabla_x\boldsymbol{\rho}\, m_{2n}\|_{\mathcal{L}^q} \leq C(\|\nabla_\xi\nabla_x\boldsymbol{\rho}\, m_{2n}\|_{\mathcal{L}^{r_1}} + \|\nabla_\xi^2\boldsymbol{\rho}\, m_{2n}\|_{\mathcal{L}^q} + \hbar^{3/2-a}\|\nabla_\xi\nabla_x\boldsymbol{\rho}\, m_{2n}\|_{\mathcal{L}^q}) + C\hbar^{3(1/q+1/2-1/\mathfrak{b})}(\|\nabla_\xi\boldsymbol{\rho}\, m_{2n}\|_{\mathcal{L}^\infty} + \|\nabla_\xi\nabla_x\boldsymbol{\rho}\, m_{2n}\|_{\mathcal{L}^2})$$

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

$$N_{x,q}(t) := \|\nabla_x^2\boldsymbol{\rho}\, m_{2n}\|_{\mathcal{L}^q}, \quad N_{v,q}(t) := \|\nabla_\xi^2\boldsymbol{\rho}\, m_{2n}\|_{\mathcal{L}^q}, \quad N_{xv,q}(t) := \|\nabla_\xi\nabla_x\boldsymbol{\rho}\, m_{2n}\|_{\mathcal{L}^q}$$

and denote by $N_{2n,q}(t)$ the quantity

$$N_{2n,q}(t) = N_{x,q}(t) + N_{v,q}(t) + N_{xv,q}(t).$$

Then we proceed as for the first-order gradients. Using Proposition 6.1, we obtain a bound on the time derivative of $N_{2n,2}(t) + N_{2n-2,4}$.

For $a \in [1/2, 1]$, we consider the quantity

$$F_{2n,\infty}(t) := N_{2n,2}(t) + N_{2n-2,4} + \|\boldsymbol{\rho}m_{2n}\|_{\dot{\mathcal{W}}^{1,\infty}}$$

and look for a Grönwall-type inequality. From (88) and (89) with $q = \infty$, we obtain an upper bound on the time derivative of $F_{2n,\infty}(t)$, and using (105) and Proposition 6.11 and standard interpolation allows us to conclude by Grönwall's lemma.

For $a \in (0, 1/2)$, since $\boldsymbol{\rho} \in \mathcal{W}^{1,4}(m_{2n-2})$ by Proposition 6.1 and

$$\|\nabla_x \boldsymbol{\rho}\, m_{2n-2}\|_{\mathcal{L}^\infty} \leq C h^{-3/4} \|\nabla_x \boldsymbol{\rho}\, m_{2n-2}\|_{\mathcal{L}^4},$$
$$\|\nabla_\xi \boldsymbol{\rho}\, m_{2n-2}\|_{\mathcal{L}^\infty} \leq C h^{-3/4} \|\nabla_\xi \boldsymbol{\rho}\, m_{2n-2}\|_{\mathcal{L}^4},$$

we get an estimate on the time derivative of $N_{2n,2}(t) + N_{2n-2,4}(t)$. By Grönwall's inequality we conclude that $\boldsymbol{\rho} \in \mathcal{W}^{2,2}(m_{2n}) \cap \mathcal{W}^{2,4}(m_{2n-2})$ for $a \in (0, 1/2)$. ■

Proof of Proposition 6.4. We observe that analogously to (87)–(89), the following bounds hold:

$$\hbar \frac{\mathrm{d}}{\mathrm{d}t} \|\sqrt{\boldsymbol{\rho}}\, m_{2n}\|_q \leq \|[V_{\boldsymbol{\rho}}, m_{2n}]\sqrt{\boldsymbol{\rho}}\|_q + \|[h^3 X_{\boldsymbol{\rho}}, m_{2n}]\sqrt{\boldsymbol{\rho}}\|_q,$$

$$\begin{aligned}\hbar \frac{\mathrm{d}}{\mathrm{d}t} \|\nabla_x \sqrt{\boldsymbol{\rho}}\, m_{2n}\|_q &\leq \|[V_{\boldsymbol{\rho}}, m_{2n}]\nabla_x \sqrt{\boldsymbol{\rho}}\|_q + \|[E_{\boldsymbol{\rho}}, \sqrt{\boldsymbol{\rho}}] m_{2n}\|_q \\ &\quad + \|[h^3 X_{\boldsymbol{\rho}}, m_{2n}]\nabla_x \sqrt{\boldsymbol{\rho}}\|_q + \|[h^3 X_{\nabla_x \boldsymbol{\rho}}, \sqrt{\boldsymbol{\rho}}] m_{2n}\|_q, \end{aligned} \tag{140}$$

$$\begin{aligned}\hbar \frac{\mathrm{d}}{\mathrm{d}t} \|\nabla_\xi \sqrt{\boldsymbol{\rho}}\, m_{2n}\|_q &\leq \|[V_{\boldsymbol{\rho}}, m_{2n}]\nabla_\xi \sqrt{\boldsymbol{\rho}}\|_q + \|\nabla_x \sqrt{\boldsymbol{\rho}}\, m_{2n}\|_q \\ &\quad + \|[h^3 \mathsf{X}_{\boldsymbol{\rho}}, m_{2n}]\nabla_\xi \sqrt{\boldsymbol{\rho}}\|_q + \|[h^3 \mathsf{X}_{\nabla_\xi \boldsymbol{\rho}}, \sqrt{\boldsymbol{\rho}}] m_{2n}\|_q. \end{aligned} \tag{141}$$

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

$$\widetilde{M}_q(t) = \|\sqrt{\boldsymbol{\rho}}\|_{\mathcal{L}^2(m_{2n})} + \|\sqrt{\boldsymbol{\rho}}\|_{\mathcal{L}^q(m_{2n})}$$

for $q \in [2, \infty]$ and notice that, because of Propositions 6.15, 6.17 and 6.22,

$$\frac{\mathrm{d}}{\mathrm{d}t} \widetilde{M}_q(t) \leq C M_r(t) \widetilde{M}_{r_1}(t) + C M_2(t) \widetilde{M}_q(t),$$

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

We now define the quantity

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

for $q \in [2, \infty]$ and using (140) and (141) we compute

$$\frac{\mathrm{d}}{\mathrm{d}t}(\widetilde{N}_2(t) + \widetilde{N}_q(t)). \tag{142}$$

The contributions due to the direct term in (142) can be estimated in terms of M_r and $\widetilde{N}_r$ by Proposition 6.15, in terms of $M_r^{1+\theta}$ (for $\theta \in (0, 1)$) and $\widetilde{N}_q$ by Proposition 6.13, together with $\widetilde{N}_r$ by Proposition 6.15. The contributions due to the exchange term in (142) can be estimated in terms of M_2 and $\widetilde{N}_q$ by Proposition 6.22, and in terms of $\widetilde{M}_q$, $\widetilde{N}_q$ and N_2 by Proposition 6.23. Hence, in the same spirit of the proofs of Propositions 6.1 and 6.2, using these propositions and Grönwall's lemma we obtain the boundedness of $\widetilde{N}_q$ for $q \in [2, \infty]$. ■

Part III
Mean-field limit

7. Scaling

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

$$\omega := \lambda \boldsymbol{\rho} \quad \text{with} \quad \lambda = N h^3 \tag{143}$$

so that $\mathrm{Tr}(\omega) = N$ and $0 \leq \omega \leq \lambda \mathcal{C}_\infty \leq 1$. Notice 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 $0 \leq \omega \leq 1$. With these definitions, we obtain the following behavior for the Schatten norms for $p \in [1, \infty]$:

$$\|\omega\|_p = \mathcal{C}_p N h^{3/p'}, \quad \|v\|_p = \mathcal{C}_{p/2}^{1/2} N^{1/2} h^{3(1/2-1/p)},$$

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, one can prove that $0 \leq 1 - u \leq \omega$, hence $1 - u$ is of the same order of magnitude as ω. Since $\nabla_\eta u = -\nabla_\eta (1-u)$, this explains why we can expect the gradients of u to be of the same order as $\nabla_\eta \omega$, as indicated more precisely in the following lemma.

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

$$C \|\nabla_\eta u\, m\|_p \leq \|\nabla_\eta \omega\, m\|_p + \|\omega \nabla_\eta m\|_p,$$

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

$$C \|\nabla_\xi u\, m\|_p \leq \mathcal{D}_p N h^{3/p'},$$

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

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

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

Expanding the gradient with the product rule for commutators gives

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

which leads to

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

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 conclusion follows by combining the last two 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.

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 setting

$$\mathrm{d}\Gamma_{\sigma,\sigma'}(O) = \int_{\mathbb{R}^6} O(x, y) a^*_{x,\sigma} a_{y,\sigma'}\, \mathrm{d}x\, \mathrm{d}y, \tag{144a}$$

$$\mathrm{d}\Gamma^+_{\sigma,\sigma'}(O) = \int_{\mathbb{R}^6} O(x, y) a^*_{x,\sigma} a^*_{y,\sigma'}\, \mathrm{d}x\, \mathrm{d}y, \tag{144b}$$

$$\mathrm{d}\Gamma^-_{\sigma,\sigma'}(O) = \int_{\mathbb{R}^6} O(x, y) a_{x,\sigma} a_{y,\sigma'}\, \mathrm{d}x\, \mathrm{d}y, \tag{144c}$$

where the operators are expressed in terms of operator-valued distributions (44). When $\sigma = \sigma'$, we write $\mathrm{d}\Gamma^\circ_\sigma := \mathrm{d}\Gamma^\circ_{\sigma,\sigma}$ where $\circ$ denotes either $+$, $-$, or null. Moreover,

$$\mathrm{d}\Gamma_{\sigma,\sigma'}(O)^* = \mathrm{d}\Gamma_{\sigma',\sigma}(O^*) \quad \text{and} \quad \mathrm{d}\Gamma^+_{\sigma,\sigma'}(O)^* = \mathrm{d}\Gamma^-_{\sigma',\sigma}(O^*). \tag{145}$$

We begin by extending [11, Lemma 4.2] to the case of Schatten class operators between different Hilbert spaces. See [76, 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*

$$\|\mathrm{d}\Gamma_\sigma(O)\Psi\|_{\mathscr{G}} \leq \|O\|_p \|\mathcal{N}^{1/p'}\Psi\|_{\mathscr{G}} \tag{146}$$

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

$$\|\mathrm{d}\Gamma^-_{\sigma,\sigma'}(O)\Psi\|_{\mathscr{G}} \leq \|O\|_p \|\mathcal{N}^{1/p'}\Psi\|_{\mathscr{G}}, \tag{147a}$$

$$\|\mathrm{d}\Gamma^+_{\sigma,\sigma'}(O)\Psi\|_{\mathscr{G}} \leq \|O\|_p \|(\mathcal{N}+2)^{1/p'}\Psi\|_{\mathscr{G}} \tag{147b}$$

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

Proof. The $p = \infty$ case of (146) and the $p = 2$ cases of (147a) and (147b) are proved in [11, Lemma 4.2].

For any compact operator 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 $\mu_j \geq 0$ are the singular values of O (see e.g. [76, Theorem 7.6]). Thus, using $a^\sharp$ to denote either a or a^*, we have

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

where $\tilde{\phi}_j$ is either ϕ_j or $\bar{\phi}_j$. Since $\|a^\sharp_\sigma(\varphi)\|_\infty \leq \|\varphi\|_{L^2} = 1$, we obtain

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

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

As an immediate application, we can bound the expectation values of the operators (144) 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*

$$\langle \Psi \,|\, \mathrm{d}\Gamma_\sigma(O)\Psi \rangle_{\mathcal{G}} \leq \|O\|_p \langle \Psi \,|\, \mathcal{N}^{1/p'} \Psi \rangle_{\mathcal{G}} \tag{148}$$

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

$$\langle \Psi \,|\, \mathrm{d}\Gamma^+_{\sigma,\sigma'}(O)\Psi \rangle_{\mathcal{G}} \leq 2^{\frac{1}{2p'}} \|O\|_p \langle \Psi \,|\, (\mathcal{N} + 1)^{1/p'} \Psi \rangle_{\mathcal{G}}, \tag{149a}$$

$$\langle \Psi \,|\, \mathrm{d}\Gamma^-_{\sigma,\sigma'}(O)\Psi \rangle_{\mathcal{G}} \leq 2^{\frac{1}{2p'}} \|O\|_p \langle \Psi \,|\, (\mathcal{N} + 1)^{1/p'} \Psi \rangle_{\mathcal{G}} \tag{149b}$$

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

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

$$\begin{aligned} \langle \Psi \,|\, \mathrm{d}\Gamma(O)\Psi \rangle_{\mathcal{G}} &= \langle (\mathcal{N} + \epsilon)^{\frac{1}{2p'}} \Psi \,|\, (\mathcal{N} + \epsilon)^{-\frac{1}{2p'}} \mathrm{d}\Gamma(O)\Psi \rangle_{\mathcal{G}} \\ &= \langle (\mathcal{N} + \epsilon)^{\frac{1}{2p'}} \Psi \,|\, \mathrm{d}\Gamma(O)(\mathcal{N} + \epsilon)^{-\frac{1}{2p'}} \Psi \rangle_{\mathcal{G}}. \end{aligned}$$

Applying the Cauchy–Schwarz inequality and Lemma 8.1 yields

$$\begin{aligned} \langle \Psi \,|\, \mathrm{d}\Gamma(O)\Psi \rangle_{\mathcal{G}} &\leq \|O\|_p \|(\mathcal{N} + \epsilon)^{\frac{1}{2p'}} \Psi\|_{\mathcal{G}} \|\mathcal{N}^{1/p'} (\mathcal{N} + \epsilon)^{-\frac{1}{2p'}} \Psi\|_{\mathcal{G}} \\ &\leq \|O\|_p \|(\mathcal{N} + \epsilon)^{\frac{1}{2p'}} \Psi\|_{\mathcal{G}} \|\mathcal{N}^{\frac{1}{2p'}} \Psi\|_{\mathcal{G}}. \end{aligned}$$

Then inequality (148) 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

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

from which we deduce (149a). Inequality (149b) follows immediately from (145). ∎

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

$$\Psi_{\text{fluc}} = \mathsf{R}_{\boldsymbol{\rho}}^* \Phi_t = \mathsf{R}_{\boldsymbol{\rho}}^* e^{-i(t/\hbar)\mathsf{L}_N} \mathsf{R}_{\boldsymbol{\rho}_0} \Psi^{\text{in}} \tag{150}$$

and consider its mean number of particles

$$\langle \Psi_{\text{fluc}} \mid \mathcal{N} \Psi_{\text{fluc}} \rangle_{\mathcal{G}} = \|\mathcal{N}^{1/2} \Psi_{\text{fluc}}\|_{\mathcal{G}}^2.$$

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

$$\|\Psi_{\text{fluc}}\|_{\mathcal{G}_k} := \|(\mathcal{N} + 1)^k \Psi_{\text{fluc}}\|_{\mathcal{G}} \tag{151}$$

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 the quantity (151) 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 Theorem 4.1. Then, for any $p \in [1, \infty]$,*

$$\|\boldsymbol{\rho}_{N:1} - \boldsymbol{\rho}\|_{\mathfrak{L}^p} \le \frac{C_p}{\min(N^{1/2}, Nh^{3/p'})} \|\Psi\|_{\mathcal{G}_{\frac{1}{2p}}}^2,$$

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

Proof. Following [11, proof of Theorem 2.1], we have

$$\begin{aligned} Nh^3 \boldsymbol{\rho}_{N:1}(x,y) - \omega(x,y) &= \langle \Psi_N \mid a_{y,l}^* a_{x,l} \Psi_N \rangle_{\mathcal{G}} = \langle \Psi \mid \mathsf{R}_{\boldsymbol{\rho}}^* a_{y,l}^* a_{x,l} \mathsf{R}_{\boldsymbol{\rho}} \Psi \rangle_{\mathcal{G}} \\ &= \big\langle \Psi \bigm| \big(a_l^*(u_y) a_l(u_x) - a_l^*(u_y) a_r^*(\overline{v}_x) \\ &\qquad - a_r(\overline{v}_y) a_l(u_x) - a_r^*(\overline{v}_x) a_r(\overline{v}_y) \big) \Psi \big\rangle_{\mathcal{G}}. \end{aligned}$$

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

$$\begin{aligned} (\boldsymbol{\rho}_{N:1} - \boldsymbol{\rho})(x,y) = \frac{1}{Nh^3} \langle \Psi \mid (a_l^*(u_y) a_l(u_x) - a_l^*(u_y) a_r^*(\overline{v}_x) \\ - a_r(\overline{v}_y) a_l(u_x) - a_r^*(\overline{v}_x) a_r(\overline{v}_y)) \Psi \rangle_{\mathcal{G}}. \end{aligned} \tag{152}$$

In particular, pairing the operator (152) with an observable O yields

$$\begin{aligned} &\operatorname{Tr}(O(\boldsymbol{\rho}_{N:1} - \boldsymbol{\rho})) \\ &\quad = \frac{1}{Nh^3} \big\langle \Psi \bigm| \big(\mathrm{d}\Gamma_l(uOu) - \mathrm{d}\Gamma_r(\overline{v}\overline{O}^* v) - \mathrm{d}\Gamma_{l,r}^+(vOu) - \mathrm{d}\Gamma_{r,l}^-(vOu) \big) \Psi \big\rangle_{\mathcal{G}}. \end{aligned}$$

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

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

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

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

$$\begin{aligned} |\langle \Psi \,|\, (\mathrm{d}\Gamma^+_{l,r}(vOu) + \mathrm{d}\Gamma^-_{r,l}(vOu))\Psi \rangle_{\mathcal{G}}| &= 2 |\langle \Psi \,|\, \mathrm{d}\Gamma^-_{r,l}(vOu)\Psi \rangle_{\mathcal{G}}| \\ &\leq 2^{5/4} \|v\|_r \|O\|_{p'} \langle \Psi \,|\, (\mathcal{N}+1)^{1/2} \Psi \rangle_{\mathcal{G}}. \end{aligned}$$

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

$$\begin{aligned} &|\langle \Psi \,|\, (\mathrm{d}\Gamma^+_{l,r}(vOu) + \mathrm{d}\Gamma^-_{r,l}(vOu))\Psi \rangle_{\mathcal{G}}| \\ &\qquad \leq 2^{5/4} \|O\|_{p'} \mathcal{C}^{1/2}_{r/2} N^{1/2} h^{3/p'} \langle \Psi \,|\, (\mathcal{N}+1)^{1/2} \Psi \rangle_{\mathcal{G}}. \end{aligned}$$

So, we have the estimate

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

which yields the desired result. ■

To better understand what it means to have a small number of particles after having performed the Bogolyubov transformation, it is useful to see how the latter acts on the number operator. From the definition (72), we obtain the following formula for $\sigma \in \{r, l\}$:

$$\mathsf{R}_{\boldsymbol{\rho}} \mathcal{N}_\sigma \mathsf{R}^*_{\boldsymbol{\rho}} = \mathsf{A}_\sigma + \mathsf{C} + \mathsf{C}^*, \tag{153}$$

where

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

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

$$\mathsf{R}^*_{\boldsymbol{\rho}} \mathcal{N}_\sigma \mathsf{R}_{\boldsymbol{\rho}} = \mathsf{A}_\sigma - \mathsf{C} - \mathsf{C}^*. \tag{154}$$

From these 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 Bogolyubov transform of the vacuum in $\mathcal{G}$ commutes with the number of particles operator.

Lemma 9.2. *Let* $\boldsymbol{\nu}_{\boldsymbol{\rho}} := \mathsf{I}^{-1}_{\mathcal{G}}(\mathsf{R}_{\boldsymbol{\rho}}\Omega)$. *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 $\Phi_\rho := \mathsf{R}_\rho \Omega = \mathsf{I}_{\mathscr{G}} \boldsymbol{\nu}_\rho$. Then $\mathcal{N}_l \Phi_\rho = \mathsf{I}_{\mathscr{G}}(\mathcal{N} \boldsymbol{\nu}_\rho)$ and $\mathcal{N}_r \Phi_\rho = \mathsf{I}_{\mathscr{G}}(\boldsymbol{\nu}_\rho \mathcal{N})$, so

$$\mathsf{I}_{\mathscr{G}}^{-1}[\mathcal{N}, \boldsymbol{\nu}_\rho] = (\mathcal{N}_l - \mathcal{N}_r)\Phi_\rho = (\mathcal{N}_l - \mathcal{N}_r)\mathsf{R}_\rho \Omega.$$

Now we use (154), yielding

$$(\mathcal{N}_l - \mathcal{N}_r)\mathsf{R}_\rho \Omega = \mathsf{R}_\rho (\mathsf{A}_l - \mathsf{A}_r)\Omega = \mathsf{R}_\rho (\mathcal{N}_l - \mathcal{N}_r)\Omega = 0,$$

which proves the result. ■

Since the number operator on the double Fock space $\mathscr{G}$ is given by $\mathcal{N} = \mathcal{N}_l + \mathcal{N}_r$, equations (153) and (154) imply

$$\mathsf{R}_\rho \mathcal{N} \mathsf{R}_\rho^* = \mathsf{A} + 2\mathsf{C} + 2\mathsf{C}^*, \tag{155}$$

$$\mathsf{R}_\rho^* \mathcal{N} \mathsf{R}_\rho = \mathsf{A} - 2\mathsf{C} - 2\mathsf{C}^*, \tag{156}$$

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 9.3. *Let $k \in \mathbb{N}$. Then for any $\Psi \in \mathscr{G}_k$,*

$$\|\mathcal{N}^k \mathsf{R}_\rho^* \Psi\|_{\mathscr{G}} \le 3^k \|(\mathcal{N} + 2N + 2k)^k \Psi\|_{\mathscr{G}},$$
$$\|\mathcal{N}^k \mathsf{R}_\rho \Psi\|_{\mathscr{G}} \le 3^k \|(\mathcal{N} + 2N + 2k)^k \Psi\|_{\mathscr{G}}.$$

Remark 9.4. With a similar proof, one obtains

$$\|\mathsf{R}_\rho^* \Psi\|_{\mathscr{G}_{1/2}} \le 3^{1/2} \|(\mathcal{N} + 2N)^{1/2} \Psi\|_{\mathscr{G}}$$

and so by interpolation, for any $s \in [0, 1/2]$,

$$\|\mathsf{R}_\rho^* \Psi\|_{\mathscr{G}_s} \le 3^s \|(\mathcal{N} + 2N)^s \Psi\|_{\mathscr{G}}. \tag{157}$$

Proof of Lemma 9.3. Since $\mathsf{R}_\rho^* \mathcal{N} \mathsf{R}_\rho$ and $\mathsf{R}_\rho \mathcal{N} \mathsf{R}_\rho^*$ are positive operators, by adding (155) and (156) 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 $\Psi \in \mathscr{G}_1$,

$$\|\mathsf{A}^{1/2} \Psi\|_{\mathscr{G}} \le \|(\mathcal{N} + 2N)^{1/2} \Psi\|_{\mathscr{G}}.$$

Since A commutes with $\mathcal{N} + 2N$, we deduce that

$$\|\mathsf{A}\Psi\|_{\mathscr{G}} \le \|(\mathcal{N} + 2N)\Psi\|_{\mathscr{G}}.$$

On the other hand, by (147a) and (147b) and the fact that $\|u\|_\infty \le 1$ and $\|v\|_2 = N^{1/2}$, we have

$$\|\mathsf{C}^* \Psi\|_{\mathscr{G}} \le \|uv\|_2 \|(\mathcal{N} + 2)^{1/2} \Psi\|_{\mathscr{G}} \le \tfrac{1}{2} \|(\mathcal{N} + N + 2)\Psi\|_{\mathscr{G}},$$

and similarly $\|\mathsf{C}\Psi\|_{\mathscr{G}} \leq \frac{1}{2}\|(\mathcal{N} + N)\Psi\|_{\mathscr{G}}$. 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

$$\begin{aligned}\|(\mathcal{N} + c_j)^j \mathsf{R}_{\boldsymbol{\rho}} \mathcal{N} \mathsf{R}_{\boldsymbol{\rho}}^* \Psi\|_{\mathscr{G}} &\leq \|\mathsf{A}(\mathcal{N} + c_j)^j \Psi\|_{\mathscr{G}} + 2\|\mathsf{C}(\mathcal{N} + c_j - 2)^j \Psi\|_{\mathscr{G}} \\ &\quad + 2\|\mathsf{C}^*(\mathcal{N} + c_j + 2)^j \Psi\|_{\mathscr{G}} \\ &\leq 3\|(\mathcal{N} + c_{j+1})^{j+1} \Psi\|_{\mathscr{G}}.\end{aligned}$$

By induction, this implies that for any $(j, k) \in \mathbb{N}^2$,

$$\|(\mathcal{N} + c_j)^j (\mathsf{R}_{\boldsymbol{\rho}} \mathcal{N} \mathsf{R}_{\boldsymbol{\rho}}^*)^k \Psi\|_{\mathscr{G}} \leq 3^k \|(\mathcal{N} + c_{j+k})^{j+k} \Psi\|_{\mathscr{G}}.$$

Taking $j = 0$ and using the fact that $\mathsf{R}_{\boldsymbol{\rho}}$ is unitary and therefore $(\mathsf{R}_{\boldsymbol{\rho}} \mathcal{N} \mathsf{R}_{\boldsymbol{\rho}}^*)^k = \mathsf{R}_{\boldsymbol{\rho}} \mathcal{N}^k \mathsf{R}_{\boldsymbol{\rho}}^*$, we get

$$\|\mathcal{N}^k \mathsf{R}_{\boldsymbol{\rho}}^* \Psi\|_{\mathscr{G}} = \|(\mathsf{R}_{\boldsymbol{\rho}} \mathcal{N} \mathsf{R}_{\boldsymbol{\rho}}^*)^k \Psi\|_{\mathscr{G}} \leq 3^k \|(\mathcal{N} + c_k)^k \Psi\|_{\mathscr{G}}.$$

The case of $\mathcal{N}^k \mathsf{R}_{\boldsymbol{\rho}}$ can be handled in the same way. ∎

10. The fluctuation dynamics

With the scaling provided in (143), we have $\rho(x) = N^{-1}\omega(x, x)$. Let us define, as in [11], $X_\omega(x, y) := N^{-1} K(x - y)\omega(x, y)$. This gives $X_\omega = h^3 \mathsf{X}_{\boldsymbol{\rho}}$. Thus, the Hartree–Fock equation (5) can be rewritten as

$$i\hbar\partial_t \omega = [H_\omega, \omega] \quad \text{with} \quad H_\omega = -\frac{\hbar^2}{2}\Delta + K * \rho - X_\omega. \tag{158}$$

By [11, Proposition 3.1], we know that the dynamics of Ψ_{fluc} satisfies

$$i\hbar\partial_t \mathsf{U}_{t,s} = \mathsf{G}_t \mathsf{U}_{t,s} \quad \text{with} \quad \mathsf{U}_{s,s} = 1 \;\text{ for all } s \in \mathbb{R}$$

and the generator G_t is given by

$$\mathsf{G} = \mathrm{d}\Gamma_l(H_\omega) - \mathrm{d}\Gamma_r(\overline{H}_\omega) + \mathsf{D} + \mathsf{Q} + \mathsf{Q}^* + \tilde{\mathsf{Q}} + \tilde{\mathsf{Q}}^*, \tag{159}$$

where

$$\begin{aligned}\mathsf{D} = \frac{1}{2N}\int_{\mathbb{R}^6} K(x - y)\big(&a_l^*(u_x)a_l^*(u_y)a_l(u_y)a_l(u_x) - a_r^*(\overline{u}_x)a_r^*(\overline{u}_y)a_r(\overline{u}_y)a_r(\overline{u}_x) \\ &+ 2a_l^*(u_x)a_r^*(v_x)a_r(v_y)a_l(u_y) - 2a_l^*(u_x)a_r^*(\overline{v}_y)a_r(\overline{v}_y)a_l(u_x) \\ &+ 2a_r^*(\overline{u}_x)a_l^*(v_y)a_l(v_y)a_r(\overline{u}_x) - 2a_r^*(\overline{u}_x)a_l^*(v_x)a_l(v_y)a_r(\overline{u}_y) \\ &+ a_r^*(\overline{v}_y)a_r^*(\overline{v}_x)a_r(\overline{v}_x)a_r(\overline{v}_y) - a_l^*(v_y)a_l^*(v_x)a_l(v_x)a_l(v_y)\big)\,\mathrm{d}x\,\mathrm{d}y\end{aligned}$$

$$\begin{aligned}\mathsf{Q}^* = \frac{1}{N}\int_{\mathbb{R}^6} K(x - y)\big(&a_l^*(u_x)a_l^*(u_y)a_r^*(\overline{v}_x)a_l(u_y) - a_r^*(\overline{u}_x)a_l^*(v_y)a_l^*(v_x)a_l(v_y) \\ &+ a_r^*(\overline{u}_x)a_r^*(\overline{u}_y)a_l^*(v_x)a_r(\overline{u}_y) - a_l^*(u_x)a_r^*(\overline{v}_y)a_r^*(\overline{v}_x)a_r(\overline{v}_y)\big)\,\mathrm{d}x\,\mathrm{d}y\end{aligned}$$

$$\begin{aligned}\tilde{\mathsf{Q}}^* = \frac{1}{2N}\int_{\mathbb{R}^6} K(x - y)\big(&a_l^*(u_x)a_l^*(u_y)a_r^*(\overline{v}_y)a_r^*(\overline{v}_x) \\ &- a_r^*(\overline{u}_x)a_r^*(\overline{u}_y)a_l^*(v_y)a_l^*(v_x)\big)\,\mathrm{d}x\,\mathrm{d}y\end{aligned}$$

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 the mean number of particles for the fluctuation dynamics.

We fix $p \in [1,2]$ with

$$p < \mathfrak{b} = \frac{3}{a+1} \tag{160}$$

and take $1 \leq q_0 < q_1 \leq \infty$ such that

$$\frac{1}{2}\left(\frac{1}{q_1} + \frac{1}{q_0}\right) = \frac{1}{p} - \frac{1}{\mathfrak{b}}. \tag{161}$$

We choose $T > 0$ so that the following two quantities are uniformly bounded on $[0,T]$:

$$\tilde{\mathfrak{D}}_{q_0,q_1} := \|\nabla_\xi \sqrt{\rho}\, m\|^{1/2}_{\mathcal{L}^{q_0}} \|\nabla_\xi \sqrt{\rho}\, m\|^{1/2}_{\mathcal{L}^{q_1}}, \tag{162a}$$

$$\mathfrak{D}_{q_0,q_1} := (\mathfrak{D}_{q_0}\mathfrak{D}_{q_1})^{1/2}, \tag{162b}$$

with $\mathfrak{D}_q$ 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 $t \in [0,T]$,*

$$\|\mathsf{U}_{t,0}\Psi\|_{\mathcal{G}_{k_0}} \leq C_M e^{C_M \lambda_\alpha t}\left(\|\Psi\|_{\mathcal{G}_{k_0+3k/2}} + \frac{h^{(\alpha-1)k}}{N^{k/2-k_0}} t\|\Psi\|_{\mathcal{G}_{3k/2}}\right),$$

where $\alpha := 3/p - 3/2$, $C_M = C^{k+k_0}(1 + N^{-1/2}h^{-1})$ for some constant $C > 0$, and

$$\lambda_\alpha = C_{p,a,q_0}|\kappa| h^{-\alpha}(1 + N^{1/2}h^{3/2}) \sup_{[0,T]}\left(\|\rho(t)\|_{L^{p_a}}, \mathfrak{D}_{q_0,q_1}(t), \tilde{\mathfrak{D}}_{q_0,q_1}(t)\right) \tag{163}$$

with $p_a = \frac{3}{3-2a}$.

Remark 10.2. With the cut-off given in Remark 4.3, one obtains

$$\|\mathsf{U}_{t,0}\Psi\|_{\mathcal{G}_{k_0}} \leq C_M e^{C_M \lambda_R t}\left(\|\Psi\|_{\mathcal{G}_{k_0+3k/2}} + \frac{R^{3\alpha k} t}{N^{k/2-k_0} h^k}\|\Psi\|_{\mathcal{G}_{3k/2}}\right)$$

with

$$\lambda_R = C_{p,a,q_0}|\kappa| R^{-3\alpha}(1 + N^{1/2}h^{3/2}) \sup_{[0,T]}\left(\|\rho(t)\|_{L^{p_a}}, \mathfrak{D}_{q_0,q_1}(t), \tilde{\mathfrak{D}}_{q_0,q_1}(t)\right).$$

To prove Proposition 10.1, we will first obtain uniform (in $\hbar$) estimates for the generator (159). 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 10.3 ([49, Proposition 4.6]). *Let* $a \in (-1, 3/2)$, $p \in [1, \mathfrak{b})$, *and* q_0, q_1 *satisfy* (161). *Then, for* $n > a+1$, *there exists a constant* $C > 0$ *such that*

$$\|[K_x, \boldsymbol{\rho}]\|_p \leq C h^{1-3/\mathfrak{b}} \|\nabla_\xi \boldsymbol{\rho} m\|_{q_0}^{1/2} \|\nabla_\xi \boldsymbol{\rho}\, m\|_{q_1}^{1/2}.$$

Here, K_x *denotes the multiplication operator by* $K_x(y) := K(x-y)$.

Then we have the following result.

Lemma 10.4. *Let* $a \in (-1, 3/2)$ *and* $p \in [1, 2]$ *satisfy* $p < \mathfrak{b}$. *Then, for any* $(\Psi_1, \Psi_2) \in \mathcal{G}^2$,

$$\frac{1}{\hbar} \langle \Psi_1 \,|\, \tilde{\mathsf{Q}}^* \Psi_2 \rangle_{\mathcal{G}} \leq |\kappa| (\tilde{C}_1 h^{3(1/2-1/p)} + \tilde{C}_2 N^{1/2} h^{3/p'}) \|\Psi_1\|_{\mathcal{G}_{1/2}} \|\Psi_2\|_{\mathcal{G}_{1/p'}}, \tag{164}$$

where $\tilde{C}_1 = C \tilde{\mathcal{D}}_{q_0,q_1}$ *and* $\tilde{C}_2 = C(N h^3 \mathscr{C}_\infty)^{1/2} \mathcal{D}_{q_0,q_1}$ *for some constant* $C > 0$ *depending only on* a, p *and* q_0.

Proof. Recall the definition of $\tilde{\mathsf{Q}}^*$ given in (159). By the anti-commutation relations (40), 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 notations defined in (144) and the notation $K_x(y) = K(x-y)$, we set $\mathrm{d}\Gamma_{l,r}^+(u K_x v) := \int_{\mathbb{R}^3} K(x-y) a_l^*(u_y) a_r^*(\overline{v}_y) \,\mathrm{d}y$. Therefore, we can rewrite $\tilde{\mathsf{Q}}^*$ as

$$\tilde{\mathsf{Q}}^* = \frac{1}{2N} \int_{\mathbb{R}^3} [\mathrm{d}\Gamma_{l,r}^+(u K_x v) \mathrm{d}\Gamma_{l,r}^+(u \delta_x v) - \mathrm{d}\Gamma_{l,r}^+(v \delta_x u) \mathrm{d}\Gamma_{l,r}^+(u K_x v)] \,\mathrm{d}x. \tag{165}$$

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 (165) to handle the $\hbar^{-1}$ on the left-hand side of (164). We begin by using the fact that u commutes with v to deduce the identity

$$u K_x v = v K_x u + u[K_x, v] - v[K_x, u] =: v K_x u + c_x \tag{166}$$

for any $x \in \mathbb{R}^3$. Moreover, the symmetry of K allows us to write

$$\int_{\mathbb{R}^3} \mathrm{d}\Gamma_{l,r}^+(v K_x u) \mathrm{d}\Gamma_{l,r}^+(u \delta_x v) \,\mathrm{d}x = \int_{\mathbb{R}^3} \mathrm{d}\Gamma_{l,r}^+(v \delta_x u) \mathrm{d}\Gamma_{l,r}^+(u K_x v) \,\mathrm{d}x. \tag{167}$$

By (166)–(167), we make the commutator structure appear more explicitly:

$$\begin{aligned}(165) &= \frac{1}{2N} \int_{\mathbb{R}^3} [\mathrm{d}\Gamma_{l,r}^+(v K_x u + c_x) \mathrm{d}\Gamma_{l,r}^+(u \delta_x v) - \mathrm{d}\Gamma_{l,r}^+(v \delta_x u) \mathrm{d}\Gamma_{l,r}^+(u K_x v - c_x)] \,\mathrm{d}x \\ &= \frac{1}{2N} \int_{\mathbb{R}^3} [\mathrm{d}\Gamma_{l,r}^+(c_x) \mathrm{d}\Gamma_{l,r}^+(u \delta_x v) + \mathrm{d}\Gamma_{l,r}^+(v \delta_x u) \mathrm{d}\Gamma_{l,r}^+(c_x)] \,\mathrm{d}x.\end{aligned}$$

Again, using the fact that the creation operators anti-commute, we obtain

$$\tilde{\mathsf{Q}}^* = \frac{1}{2N}\int_{\mathbb{R}^3}\big(a_l^*(u_x)a_r^*(\overline{v}_x) + a_l^*(v_x)a_r^*(\overline{u}_x)\big)\mathrm{d}\Gamma_{l,r}^+(u[K_x,v] - v[K_x,u])\,\mathrm{d}x.$$

Expanding the product in the integrand 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,

$$\begin{aligned}\langle\Psi_1 \mid \tilde{J}_1\Psi_2\rangle_{\mathscr{G}} &= \int_{\mathbb{R}^3}\langle a_l(u_x)\Psi_1 \mid a_r^*(\overline{v}_x)\mathrm{d}\Gamma_{l,r}^+(u[K_x,v])\Psi_2\rangle_{\mathscr{G}}\,\mathrm{d}x\\ &\le \left(\int_{\mathbb{R}^3}\|a_l(u_x)\Psi_1\|_{\mathscr{G}}^2\,\mathrm{d}x\right)^{1/2}\left(\int_{\mathbb{R}^3}\|a_r^*(\overline{v}_x)\mathrm{d}\Gamma_{l,r}^+(u[K_x,v])\Psi_2\|_{\mathscr{G}}^2\,\mathrm{d}x\right)^{1/2}.\end{aligned}$$

The first factor can be written as

$$\int_{\mathbb{R}^3}\|a_l(u_x)\Psi_1\|_{\mathscr{G}}^2\,\mathrm{d}x = \left\langle\Psi_1 \,\middle|\, \int_{\mathbb{R}^3}a_l^*(u_x)a_l(u_x)\,\mathrm{d}x\,\Psi_1\right\rangle_{\mathscr{G}} = \langle\Psi_1 \mid \mathrm{d}\Gamma_l(1-\omega)\Psi_1\rangle_{\mathscr{G}},$$

which is smaller than $\langle\Psi_1 \mid \mathcal{N}_l\Psi_1\rangle_{\mathscr{G}}$. To estimate the second factor, we use the fact that

$$\|a_r^*(\overline{v}_x)\|_\infty^2 = \|v_x\|_{L^2}^2 = N\rho(x)$$

together with Lemma 8.1 and the fact that $\|u\|_\infty \le 1$ to get

$$\|a_r^*(\overline{v}_x)\mathrm{d}\Gamma_{l,r}^+(u[K_x,v])\Psi_2\|_{\mathscr{G}} \le (N\rho(x))^{1/2}\|[K_x,v]\|_p\|(\mathcal{N}+2)^{1/p'}\Psi_2\|_{\mathscr{G}}.$$

Combining the above inequalities leads to

$$\langle\Psi_1 \mid \tilde{J}_1\Psi_2\rangle_{\mathscr{G}} \le N^{1/2}\left(\int_{\mathbb{R}^3}\|[K_x,v]\|_p^2\rho(x)\,\mathrm{d}x\right)^{1/2}\langle\Psi_1 \mid \mathcal{N}\Psi_1\rangle_{\mathscr{G}}^{1/2}\|(\mathcal{N}+2)^{1/p'}\Psi_2\|_{\mathscr{G}}.$$

Applying Lemma 10.3, since $p < \mathfrak{b}$, and the scaling relation (161), we get

$$\|[K_x,v]\|_p \le C|\kappa|N^{1/2}h^{1+3(1/2-1/p)}\tilde{\mathcal{D}}_{q_0,q_1}. \tag{168}$$

Therefore, we finally obtain the inequality

$$\frac{1}{N\hbar}\langle\Psi_1 \mid \tilde{J}_1\Psi_2\rangle_{\mathscr{G}} \le C'|\kappa|\tilde{\mathcal{D}}_{q_0,q_1}h^{3(1/2-1/p)}\|\Psi_1\|_{\mathscr{G}_{1/2}}\|\Psi_2\|_{\mathscr{G}_{1/p'}}.$$

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 that in this case, we apply Lemma 7.1 and the fact that $\|v\|_\infty = \mathcal{C}_\infty^{1/2}(Nh^3)^{1/2}$ to get

$$\|v[K_x,u]\|_p \le C|\kappa|N^{3/2}h^{1+3(3/2-1/p)}\mathcal{C}_\infty^{1/2}\mathcal{D}_{q_0,q_1}. \tag{169}$$

So, we have obtained the claimed bound for $\tilde{\mathsf{Q}}^*$. ∎

Remark 10.5. In the case of the cut-off potential described in Remark 4.3, we can take $q_0 = q_1 = \infty$ and $p = 2$ in the above inequality, with an extra factor $R^{3(1/2-1/\mathfrak{b})}$, leading to

$$\frac{1}{\hbar}\langle \Psi_1 \,|\, \tilde{\mathsf{Q}}^* \Psi_2 \rangle_{\mathscr{G}} \leq |\kappa| R^{3(1/2-1/\mathfrak{b})} (\tilde{C}_1 + \tilde{C}_2 N^{1/2} h^{3/2}) \|\Psi_1\|_{\mathscr{G}_{1/2}} \|\Psi_2\|_{\mathscr{G}_{1/2}}. \tag{170}$$

More precisely, (170) is a direct consequence of the estimate

$$\frac{1}{\hbar}\|[K_{R,x}, \boldsymbol{\rho}]\|_{\mathscr{L}^2} \leq C|\kappa| R^{3(1/2-1/\mathfrak{b})} \|\nabla_\xi \boldsymbol{\rho}\, m\|_{\mathscr{L}^\infty},$$

which follows directly from [49, proof of Proposition 4.6].

10.1.2. Bounds for Q^*. We label the terms of Q^* given in (159) by

$$\mathsf{Q}^* = I_1 + I_2 + I_3 + I_4. \tag{171}$$

Using the fact that the creation operators anti-commute, we get

$$\begin{aligned} I_1 &= -\frac{1}{N}\int_{\mathbb{R}^6} K(x-y) a_l^*(u_x) a_r^*(\overline{v}_x) a_l^*(u_y) a_l(u_y) \,\mathrm{d}x\,\mathrm{d}y, \\ I_2 &= -\frac{1}{N}\int_{\mathbb{R}^6} K(x-y) a_l^*(v_x) a_r^*(\overline{u}_x) a_l^*(v_y) a_l(v_y) \,\mathrm{d}x\,\mathrm{d}y. \end{aligned}$$

I_3 and I_4 have similar forms with the "l" and "r" labels interchanged and (u, v) replaced by $(\overline{u}, \overline{v})$. To reveal hidden commutator structures, which are necessary when estimating Q^* uniformly in $\hbar$, we need to further decompose equation (171).

Let us start with the following decomposition lemma.

Lemma 10.6. *Let* Q^* *be as in* (171)*. Then*

$$I_1 + I_2 = J_1 + J_2 + J_{12} + I_{12},$$

where

$$\begin{aligned} J_1 &= \frac{1}{N}\int_{\mathbb{R}^3} a_r^*(u_x) a_l^*(\overline{v}_x) \mathrm{d}\Gamma_l(u[u, K_x]) \,\mathrm{d}x, \\ J_2 &= \frac{1}{N}\int_{\mathbb{R}^3} a_l^*(v_x) a_r^*(\overline{u}_x) \mathrm{d}\Gamma_l(v[v, K_x]) \,\mathrm{d}x, \\ J_{12} &= \frac{1}{N}\int_{\mathbb{R}^3} \mathrm{d}\Gamma_{l,r}^+([u, K_x]v + [K_x, v]u) a_l^*(\omega_x) a_{x,l} \,\mathrm{d}x, \\ I_{12} &= -\frac{1}{N}\int_{\mathbb{R}^3} a_l^*(u_x) a_r^*(\overline{v}_x) \mathrm{d}\Gamma_l(K_x) \,\mathrm{d}x. \end{aligned}$$

We have the same splitting for $I_3 + I_4$*, interchanging "l" with "r" and replacing* (u, v) *by* $(\overline{u}, \overline{v})$*. Hence,*

$$\mathsf{Q}^* = (J_1 + J_2 + J_3 + J_4 + J_{12} + J_{34}) + (I_{12} + I_{34}) =: \tilde{\mathsf{P}}^* + \mathsf{P}^*. \tag{172}$$

Proof. To simplify our computations, we use the Fefferman–de la Llave formula (see [31, 41]) in its smooth version. For the potential K it reads

$$K(x-y) = \kappa_a \int_0^\infty \int_{\mathbb{R}^3} s^{\frac{a+1}{2}} \varphi_{s,z}(x)\varphi_{s,z}(y)\, \mathrm{d}z\, \mathrm{d}s$$

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 as

$$I_1 = -\frac{\kappa_a}{N}\int_0^\infty \int_{\mathbb{R}^3} s^{\frac{a+1}{2}} \mathrm{d}\Gamma^+_{l,r}(u\varphi_{s,z}v)\mathrm{d}\Gamma_l(u\varphi_{s,z}u)\, \mathrm{d}z\, \mathrm{d}s,$$
$$I_2 = -\frac{\kappa_a}{N}\int_0^\infty \int_{\mathbb{R}^3} s^{\frac{a+1}{2}} \mathrm{d}\Gamma^+_{l,r}(v\varphi_{s,z}u)\mathrm{d}\Gamma_l(v\varphi_{s,z}v)\, \mathrm{d}z\, \mathrm{d}s,$$

where $\varphi_{s,z}$ is seen as a multiplication operator. Since $u^2 = 1-\omega$, we have the identity

$$\begin{aligned}\mathrm{d}\Gamma^+_{l,r}(u\varphi v)\mathrm{d}\Gamma_l(u\varphi u) &= \mathrm{d}\Gamma^+_{l,r}(u\varphi v)\mathrm{d}\Gamma_l(u[\varphi,u]) + \mathrm{d}\Gamma^+_{l,r}([u,\varphi]v)\mathrm{d}\Gamma_l((1-\omega)\varphi)\\ &\quad + \mathrm{d}\Gamma^+_{l,r}(\varphi uv)\mathrm{d}\Gamma_l((1-\omega)\varphi)\end{aligned}$$

where we have used the notation $\varphi = \varphi_{s,z}$. Similarly, since $v^2 = \omega$, we have

$$\begin{aligned}\mathrm{d}\Gamma^+_{l,r}(v\varphi u)\mathrm{d}\Gamma_l(v\varphi v) &= \mathrm{d}\Gamma^+_{l,r}(v\varphi u)\mathrm{d}\Gamma_l(v[\varphi,v]) + \mathrm{d}\Gamma^+_{l,r}([v,\varphi]u)\mathrm{d}\Gamma_l(\omega\varphi)\\ &\quad + \mathrm{d}\Gamma^+_{l,r}(\varphi uv)\mathrm{d}\Gamma_l(\omega\varphi).\end{aligned}$$

Combining the two identities yields

$$\begin{aligned}&\mathrm{d}\Gamma^+_{l,r}(u\varphi v)\mathrm{d}\Gamma_l(u\varphi u) + \mathrm{d}\Gamma^+_{l,r}(v\varphi u)\mathrm{d}\Gamma_l(v\varphi v)\\ &\quad = \mathrm{d}\Gamma^+_{l,r}(u\varphi v)\mathrm{d}\Gamma_l(u[\varphi,u]) + \mathrm{d}\Gamma^+_{l,r}(v\varphi u)\mathrm{d}\Gamma_l(v[\varphi,v])\\ &\qquad + \mathrm{d}\Gamma^+_{l,r}([\varphi,u]v + [v,\varphi]u)\mathrm{d}\Gamma_l(\omega\varphi) + \mathrm{d}\Gamma^+_{l,r}(u\varphi v)\mathrm{d}\Gamma_l(\varphi).\end{aligned} \tag{173}$$

Thus, using identity (173), we can write $I_1 + I_2 = J_1 + J_2 + J_{12} + I_{12}$ with

$$J_1 := \frac{\kappa_a}{N}\int_0^\infty \int_{\mathbb{R}^3} s^{\frac{a+1}{2}} \mathrm{d}\Gamma^+_{l,r}(u\varphi v)\mathrm{d}\Gamma_l(u[u,\varphi])\, \mathrm{d}z\, \mathrm{d}s,$$
$$J_2 := \frac{\kappa_a}{N}\int_0^\infty \int_{\mathbb{R}^3} s^{\frac{a+1}{2}} \mathrm{d}\Gamma^+_{l,r}(v\varphi u)\mathrm{d}\Gamma_l(v[v,\varphi])\, \mathrm{d}z\, \mathrm{d}s,$$
$$J_{12} := \frac{\kappa_a}{N}\int_0^\infty \int_{\mathbb{R}^3} s^{\frac{a+1}{2}} \mathrm{d}\Gamma^+_{l,r}([u,\varphi]v + [\varphi,v]u)\mathrm{d}\Gamma_l(\omega\varphi)\, \mathrm{d}z\, \mathrm{d}s,$$
$$I_{12} := -\frac{\kappa_a}{N}\int_0^\infty \int_{\mathbb{R}^3} s^{\frac{a+1}{2}} \mathrm{d}\Gamma^+_{l,r}(u\varphi v)\mathrm{d}\Gamma_l(\varphi)\, \mathrm{d}z\, \mathrm{d}s.$$

Reversing the Fefferman–de la Llave expansion gives us

$$\begin{aligned}J_1 &= \frac{\kappa_a}{N}\int_{\mathbb{R}^3}\int_0^\infty \int_{\mathbb{R}^3} s^{\frac{a+1}{2}} a^*_l(u_x)a^*_r(\overline{v}_x)\varphi(x)\mathrm{d}\Gamma_l(u[u,\varphi])\, \mathrm{d}z\, \mathrm{d}s\, \mathrm{d}x\\ &= \frac{1}{N}\int_{\mathbb{R}^3} a^*_l(u_x)a^*_r(\overline{v}_x)\mathrm{d}\Gamma_l(u[u,K_x])\, \mathrm{d}x.\end{aligned}$$

The same is true for J_2. Lastly, we have

$$\begin{aligned} J_{12} &= \frac{\kappa_a}{N}\int_0^\infty \int_{\mathbb{R}^3} s^{\frac{a+1}{2}} \mathrm{d}\Gamma^+_{l,r}([u,\varphi]v + [\varphi, v]u) a_l^*(\omega_x)\varphi(x) a_{x,l}\,\mathrm{d}z\,\mathrm{d}s \\ &= \frac{1}{N}\int_{\mathbb{R}^3} \mathrm{d}\Gamma^+_{l,r}([u, K_x]v + [K_x, v]u) a_l^*(\omega_x) a_{x,l}\,\mathrm{d}x. \end{aligned}$$

This completes the proof of the lemma. ∎

Let us first estimate the J terms, which can be treated in a similar manner to the $\tilde{\mathsf{Q}}^*$ case. One obtains the following bounds.

Lemma 10.7. *Assuming the same hypotheses as in Lemma 10.4. Then, for any* (Ψ_1, Ψ_2) *in* $\mathscr{G}^2$,

$$\frac{1}{\hbar}\langle \Psi_1 \,|\, J_1 \Psi_2\rangle_{\mathscr{G}} \leq C_1 |\kappa| N^{1/2} h^{3/p'} \|\Psi_1\|_{\mathscr{G}_{1/2}} \|\Psi_2\|_{\mathscr{G}_{1/p'}}, \tag{174a}$$

$$\frac{1}{\hbar}\langle \Psi_1 \,|\, J_2 \Psi_2\rangle_{\mathscr{G}} \leq C_2 |\kappa| N^{1/2} h^{3/p'} \|\Psi_1\|_{\mathscr{G}_{1/2}} \|\Psi_2\|_{\mathscr{G}_{1/p'}}, \tag{174b}$$

$$\frac{1}{\hbar}\langle \Psi_1 \,|\, J_{12} \Psi_2\rangle_{\mathscr{G}} \leq C_{12} |\kappa| N^{1/2} h^{3/p'} \|\Psi_1\|_{\mathscr{G}_{1/2}} \|\Psi_2\|_{\mathscr{G}_{1/p'}}, \tag{174c}$$

where $C_1 = C\mathcal{D}_{q_0,q_1}$, $C_2 = C\mathscr{C}_\infty^{1/2}\tilde{\mathcal{D}}_{q_0,q_1}$ *and* $C_{12} = C\mathscr{C}_2((Nh^3\mathscr{C}_\infty)^{1/2}\mathcal{D}_{q_0,q_1} + \tilde{\mathcal{D}}_{q_0,q_1})$ *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 10.3 and the fact that $\|u\|_\infty \leq 1$ gives

$$\|u[K_x, u]\|_p \leq C|\kappa| N h^{1+3/p'} \mathcal{D}_{q_0,q_1}.$$

Then, following the proof of Lemma 10.4, this yields inequality (174a). Similarly, by Lemma 10.3 and the fact that $\|v\|_\infty = (\mathscr{C}_\infty N h^3)^{1/2}$, we have

$$\|v[K_x, v]\|_p \leq C|\kappa| N h^{1+3/p'} \mathscr{C}_\infty^{1/2} \tilde{\mathcal{D}}_{q_0,q_1},$$

from which we arrive at (174b). Finally, by direct estimation, we see that

$$\langle \Psi_1 \,|\, J_{12}\Psi_2\rangle_{\mathscr{G}} \leq \frac{1}{N}\left(\int_{\mathbb{R}^3} \|a_l(\omega_x) \mathrm{d}\Gamma^+_{r,l}(v[K_x, u] - u[K_x, v])\Psi\|^2_{\mathscr{G}}\,\mathrm{d}x\right)^{1/2} \|\mathcal{N}_l^{1/2}\Psi\|_{\mathscr{G}}.$$

Then (174c) follows from Lemmas 8.1 and 10.3. ∎

Lastly, let us estimate $\mathsf{P}^* = I_{12} + I_{34}$.

Lemma 10.8. *Let* $p_a = \frac{3}{3-2a}$. *Then there exists* $C > 0$, *depending only on* a, *such that for any* $(\Psi_1, \Psi_2) \in \mathscr{G}^2$,

$$\frac{1}{\hbar}|\langle \Psi_1 \,|\, \mathsf{P}^* \Psi_2\rangle_{\mathscr{G}}| \leq \frac{C|\kappa|}{N^{1/2} h} \|\rho\|^{1/2}_{L^{p_a}} \langle \Psi_1 \,|\, \mathcal{N}\Psi_1\rangle^{1/2}_{\mathscr{G}} \langle \Psi_2 \,|\, \mathcal{N}\Psi_2\rangle^{1/2}_{\mathscr{G}}.$$

Proof. Let $(\Psi_1, \Psi_2) \in \mathscr{G}^2$. By the Cauchy–Schwarz inequality and the boundedness of a^*, we have

$$|\langle \Psi_1 \mid I_{12}\Psi_2\rangle_{\mathscr{G}}| \leq \frac{1}{N}\left(\int_{\mathbb{R}^3} \|a_l(u_x)\Psi_1\|_{\mathscr{G}}^2\,\mathrm{d}x\right)^{1/2}\left(\int_{\mathbb{R}^6} \|a_r^*(\overline{v}_x)\mathrm{d}\Gamma_l(K_x)\Psi_2\|_{\mathscr{G}}^2\,\mathrm{d}x\right)^{1/2}$$
$$\leq \frac{1}{N^{1/2}}\langle \Psi_1 \mid \mathcal{N}_l\Psi_1\rangle_{\mathscr{G}}^{1/2}\left(\int_{\mathbb{R}^3} \rho(x)\|\mathrm{d}\Gamma_l(K_x)\Psi_2\|_{\mathscr{G}}^2\,\mathrm{d}x\right)^{1/2}.$$

where we use $\|v_x\|_{L^2}^2 = N\rho(x)$. Moreover, since

$$(\mathrm{d}\Gamma_l(K_x)\Psi)^{(n,m)}(\underline{x}_n, \underline{y}_m) = \kappa\sum_{j=1}^{n}\frac{\Psi^{(n,m)}(\underline{x}_n, \underline{y}_m)}{|x-x_j|^a},$$

where $\underline{x}_n = (x_1, \ldots, x_n)$, $\underline{y}_m = (y_1, \ldots, y_m)$, it follows that

$$\|(\mathrm{d}\Gamma_l(K_x)\Psi)^{(n,m)}\|_{L^2(\mathbb{R}^{3(n+m)})}^2 \leq |\kappa|^2 n^2 \int_{\mathbb{R}^3}\frac{g(y)}{|x-y|^{2a}}\,\mathrm{d}y,$$

where we have defined $g(x) = \|\Psi^{(n,m)}(x, \underline{x}_{n-1}, \underline{y}_m)\|_{L^2(\mathrm{d}\underline{x}_{n-1}\,\mathrm{d}\underline{y}_m)}^2$. Finally, it follows from the Hardy–Littlewood–Sobolev inequality that

$$\int_{\mathbb{R}^3}\rho(x)\|(\mathrm{d}\Gamma_l(K_x)\Psi)^{(n,m)}\|_{L^2(\mathbb{R}^{3(n+m)})}^2\,\mathrm{d}x \leq |\kappa|^2 n^2\int_{\mathbb{R}^6}\frac{\rho(x)g(y)}{|x-y|^{2a}}\,\mathrm{d}x\,\mathrm{d}y$$
$$\leq C_{p_a,a}|\kappa|^2 n^2\|\rho\|_{L^{p_a}}\|g\|_{L^1},$$

where $\|g\|_{L^1} = \|\Psi^{(n,m)}\|_{L^2}^2$. This yields the desired estimate. The proof for the estimate on I_{34} is the same. ■

10.2. *Proof of Proposition 10.1*

To control the growth of the fluctuation dynamics in the $\mathscr{G}_k$ norms, the strategy consists in splitting the generator G, defined in (159), into two parts and then solving the problem perturbatively. More precisely, we define the splitting $\mathsf{G} = \tilde{\mathsf{G}} + \mathsf{B}$ with

$$\tilde{\mathsf{G}} = \mathrm{d}\Gamma_l(H_\omega) - \mathrm{d}\Gamma_r(\overline{H}_\omega) + \mathsf{D} + \tilde{\mathsf{Q}} + \tilde{\mathsf{Q}}^* + \tilde{\mathsf{P}} + \tilde{\mathsf{P}}^*, \tag{175a}$$
$$\mathsf{B} = \mathsf{P} + \mathsf{P}^*, \tag{175b}$$

where P and $\tilde{\mathsf{P}}$ are defined by (172). The idea is to view G as a small perturbation of $\tilde{\mathsf{G}}$. This is justifiable since, when $N^{1/2}h$ is large, the effect of the operator B is small in the following sense.

Lemma 10.9. *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*

$$\frac{1}{\hbar}\|\mathsf{B}\|_{\mathscr{G}_{j+3/2}\to\mathscr{G}_j} \leq C\frac{2^j|\kappa|}{N^{1/2}h}\|\rho\|_{L^{p_a}}^{1/2}. \tag{176}$$

Proof. This follows from Lemma 10.8. Notice that $(\mathcal{N}+1)^k \mathsf{P}^* = \mathsf{P}^*(\mathcal{N}+3)^k$. Then, by Lemma 10.8,

$$\begin{aligned} \|\mathsf{P}^*\Psi\|_{\mathscr{G}_j} &= \sup_{\|\Psi_1\|_{\mathscr{G}}\leq 1} \langle (\mathcal{N}+1)^{-1/2}\Psi_1 \,|\, \mathsf{P}^*(\mathcal{N}+3)^{j+1/2}\Psi\rangle_{\mathscr{G}} \\ &\leq \frac{C_a|\kappa|}{N^{1/2}}\|\rho\|_{L^{pa}}^{1/2}\|(\mathcal{N}+3)^{j+1/2}\mathcal{N}\Psi\|_{\mathscr{G}} \leq C_a\frac{2^j|\kappa|}{N^{1/2}}\|\rho\|_{L^{pa}}^{1/2}\|\Psi\|_{\mathscr{G}_{j+3/2}}. \end{aligned}$$

The estimate for P also follows immediately from Lemma 10.8:

$$\begin{aligned} \|\mathsf{P}\Psi\|_{\mathscr{G}_k} &= \sup_{\|\Psi_1\|_{\mathscr{G}}\leq 1} \langle \mathsf{P}^*(\mathcal{N}+1)^{-1}\Psi_1 \,|\, (\mathcal{N}-1)^{j+1}\Psi\rangle_{\mathscr{G}} \\ &\leq \frac{C_a|\kappa|}{N^{1/2}}\|\rho\|_{L^{pa}}^{1/2}\|(\mathcal{N}-1)^{j+1}\mathcal{N}^{1/2}\Psi\|_{\mathscr{G}} \leq \frac{C_a|\kappa|}{N^{1/2}}\|\rho\|_{L^{pa}}^{1/2}\|\Psi\|_{\mathscr{G}_{j+3/2}}. \end{aligned}$$

This completes the argument. ∎

In light of the above lemma, we define the auxiliary dynamics $\tilde{\mathsf{U}}_{t,s}$ to be the unitary dynamics generated by (175a), that is, for any $(t,s)\in\mathbb{R}^2$, $\tilde{\mathsf{U}}_{t,s}$ satisfies the differential equation

$$i\hbar\partial_t\tilde{\mathsf{U}}_{t,s}\Psi = \tilde{\mathsf{G}}_t\tilde{\mathsf{U}}_{t,s}\Psi \quad \text{with} \quad \tilde{\mathsf{U}}_{s,s}\Psi = \Psi \tag{177}$$

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 $\mathscr{G}_k$ norm under regularity assumptions on the solution of the Hartree equation.

Proposition 10.10. *Let $a\in(-1,3/2)$ and $p\in[1,2]$ satisfy $p<\mathfrak{b}=\frac{3}{a+1}$, and suppose $\Psi_t=\tilde{\mathsf{U}}_{t,s}\Psi$ is a solution to (177). Then, for any k such that $2k\in\mathbb{N}$, the inequality*

$$\frac{\mathrm{d}}{\mathrm{d}t}\|\Psi_t\|_{\mathscr{G}_k} \leq C_k|\kappa|(\tilde{\mathcal{D}}_{q_0,q_1}h^{3(1/2-1/p)} + C_{\boldsymbol{\rho}}N^{1/2}h^{3/p'})\|\Psi_t\|_{\mathscr{G}_{k+(1/2-1/p)}}$$

holds for some constants C_k of the form $C_k = C_{p,a,q_0}C^k$ and

$$C_{\boldsymbol{\rho}} = (1+\mathscr{C}_\infty^{1/2})(\mathcal{D}_{q_0,q_1}+\tilde{\mathcal{D}}_{q_0,q_1}),$$

where $\mathcal{D}_{q_0,q_1}$ and $\tilde{\mathcal{D}}_{q_0,q_1}$ are defined by (162a) and (162b).

Remark 10.11. Since $Nh^3\mathscr{C}_\infty\leq 1$, from Grönwall's inequality we deduce that

$$\|\tilde{\mathsf{U}}_{t,s}\|_{\mathscr{G}_k\to\mathscr{G}_k} \leq e^{C_{t,s}}, \tag{178}$$

where

$$C_{t,s} = C_k|\kappa|h^{-\alpha}(1+N^{1/2}h^{3/2})\int_s^t [\mathcal{D}_{q_0,q_1}(\tau)+\tilde{\mathcal{D}}_{q_0,q_1}(\tau)]\,\mathrm{d}\tau$$

with $\alpha := 3/p - 3/2 \geq 0$, which is 0 if and only if $p=2$, and $N^{1/2}h^{3/2}$ is bounded above uniformly in N and $\hbar$ by assumption (36).

Proof of Proposition 10.10. Let $k \in \mathbb{N}$. Since $\tilde{\mathsf{G}} = \tilde{\mathsf{G}}^*$, we get

$$\begin{aligned} i\hbar \frac{\mathrm{d}}{\mathrm{d}t} \|\Psi_t\|^2_{\mathcal{G}_{k/2}} &= \langle \Psi_t \,|\, [(\mathcal{N}+1)^k, \tilde{\mathsf{G}}]\Psi_t\rangle_{\mathcal{G}} \\ &= \sum_{j=1}^{k} \langle \Psi_t \,|\, (\mathcal{N}+1)^{j-1}[\mathcal{N}, \tilde{\mathsf{G}}](\mathcal{N}+1)^{k-j}\Psi_t\rangle_{\mathcal{G}}. \end{aligned}$$

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

$$[\mathcal{N}, \tilde{\mathsf{G}}] = [\mathcal{N}, \tilde{\mathsf{Q}}^* + \tilde{\mathsf{Q}} + \tilde{\mathsf{P}}^* + \tilde{\mathsf{P}}] = 4(\tilde{\mathsf{Q}}^* - \tilde{\mathsf{Q}}) + \tilde{\mathsf{P}}^* - \tilde{\mathsf{P}},$$

which leads to

$$\frac{\mathrm{d}}{\mathrm{d}t} \|\Psi_t\|^2_{\mathcal{G}_{k/2}} = \frac{2}{\hbar} \operatorname{Im}\Big(\sum_{j=1}^{k} \langle \Psi_t \,|\, (\mathcal{N}+1)^{j-1}(4\tilde{\mathsf{Q}}^* + \tilde{\mathsf{P}}^*)(\mathcal{N}+1)^{k-j}\Psi_t\rangle_{\mathcal{G}}\Big). \tag{179}$$

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

$$\begin{aligned} (\mathcal{N}+1)^{j-1}\tilde{\mathsf{Q}}^*(\mathcal{N}+1)^{k-j} &= (\mathcal{N}+1)^{\frac{k-1}{2}}\tilde{\mathsf{Q}}^*(\mathcal{N}+5)^{j-\frac{k+1}{2}}(\mathcal{N}+1)^{k-j}, \\ (\mathcal{N}+1)^{j-1}\tilde{\mathsf{Q}}^*(\mathcal{N}+1)^{k-j} &= (\mathcal{N}+1)^{\frac{k-1}{2}}\tilde{\mathsf{Q}}^*(\mathcal{N}+2)^{j-\frac{k+1}{2}}(\mathcal{N}+1)^{k-j}, \end{aligned}$$

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 Lemmas 10.4 and 10.7 to each term of the right-hand side of (179) and the fact that $Nh^3\mathcal{C}_\infty \le 1$ and $\mathcal{C}_2 \le \mathcal{C}_\infty^{1/2}$, we obtain

$$\begin{aligned} &\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\|\Psi_t\|^2_{\mathcal{G}_{k/2}} \\ &\quad \le C^k|\kappa|C_{p,a,q_0}(\tilde{\mathcal{D}}_{q_0,q_1}h^{3(1/2-1/p)} + C_{\boldsymbol{\rho}}N^{1/2}h^{3/p'})\|\Psi_t\|_{\mathcal{G}_{k/2}}\|\Psi_t\|_{\mathcal{G}_{k/2+(1/2-1/p)}}, \end{aligned}$$

which leads to the desired result. ∎

Moreover, by Proposition 9.3 and by weighted interpolation, we deduce that for any $t > 0$, $\mathsf{R}_{\boldsymbol{\rho}_t}$ is a bounded mapping from $\mathcal{G}_k$ to $\mathcal{G}_k$. More precisely, for any $k \in [0, 1/2]$, we have a bound of the form (157), 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 $k \in [0, 1/2]$,

$$\|\mathsf{U}_{t,s}\Psi\|_{\mathcal{G}_k} \le 3\|\Psi\|_{\mathcal{G}_k} + 5N^k\|\Psi\|_{\mathcal{G}}. \tag{180}$$

Combining the three inequalities (178), (176), (180), and using the Duhamel formula, we obtain the main result of this section.

Proof of Proposition 10.1. Let $\mathsf{B}_h := \frac{1}{i\hbar}\mathsf{B}$. Then the Duhamel formula can be written as

$$\mathsf{U}_{t,0} = \tilde{\mathsf{U}}_{t,0} + (\mathsf{U} \star \mathsf{B}_h\tilde{\mathsf{U}})_{t,0},$$

where we use the notation $\star$ for the time convolution of operators,

$$(\mathsf{U} \star \mathsf{V})_{t,s} := \int_s^t \mathsf{U}_{t,s'}\mathsf{V}_{s',s}\,\mathrm{d}s',$$

We now define the iterated time convolution $\mathsf{U}^{(\star k)}$ by $\mathsf{U}^{(\star 1)} = \mathsf{U}$ for $k = 1$ and by $\mathsf{U}^{(\star k)} = \mathsf{U} \star \mathsf{U}^{(\star(k-1))}$ for $k \geq 2$. With these notations, one can write the following iterated Duhamel formula:

$$\mathsf{U}_{t,0} = \sum_{j=0}^{k-1} (\tilde{\mathsf{U}} \star (\mathsf{B}_h\tilde{\mathsf{U}})^{(\star j)})_{t,0} + (\mathsf{U} \star (\mathsf{B}_h\tilde{\mathsf{U}})^{(\star k)})_{t,0} \tag{181}$$

and from (180), we deduce

$$\|\mathsf{U}_{t,0}\Psi\|_{\mathscr{G}_{k_0}} \leq \sum_{j=0}^{k-1} \|(\tilde{\mathsf{U}} \star (\mathsf{B}_h\tilde{\mathsf{U}})^{(\star j)})_{t,0}\Psi\|_{\mathscr{G}_{k_0}}$$
$$+ \int_0^t \left(3\|(\mathsf{B}_h\tilde{\mathsf{U}})^{(\star k)}_{s,0}\Psi\|_{\mathscr{G}_{k_0}} + 5N^{k_0}\|(\mathsf{B}_h\tilde{\mathsf{U}})^{(\star k)}_{s,0}\Psi\|_{\mathscr{G}}\right)\mathrm{d}s.$$

Since we know from Part II that $C_T := \sup_{[0,T]}(\|\rho\|_{L^{p_a}}, \mathscr{D}_{q_0,q_1}, \tilde{\mathscr{D}}_{q_0,q_1})$ is bounded, we deduce that

$$C_{t,s} \leq C_T C^{k_0} C_{p,a,q_0}|\kappa|h^{-\alpha}(1 + N^{1/2}h^{3/2})(t-s) =: \lambda_\alpha C^{k_0}(t-s).$$

From (176) and (178) we obtain, for any $0 \leq s \leq t \leq T$,

$$\|(\mathsf{B}_h\tilde{\mathsf{U}})_{t,s}\|_{\mathscr{G}_{k_0+3/2}\to\mathscr{G}_{k_0}} \leq \frac{2^{k_0}C\lambda_0}{M}e^{\lambda_\alpha C^k(t-s)},$$

where $M = N^{1/2}h$, which leads to

$$\|(\mathsf{B}_h\tilde{\mathsf{U}})^{(\star j)}_{t,s}\|_{\mathscr{G}_{k_0+3j/2}\to\mathscr{G}_{k_0}} \leq \frac{(C\lambda_0)^j 2^{(k_0+j)(j+1)}}{M^j(j-1)!}(t-s)^{j-1}e^{\lambda_\alpha C^k(t-s)}.$$

Hence, for U, we obtain

$$\|\mathsf{U}_{t,0}\Psi\|_{\mathscr{G}_{k_0}} \leq \sum_{j=0}^{k-1} \frac{(C\lambda_0)^j 2^{(k_0+j)(j+1)}}{M^j j!}t^j e^{\lambda_\alpha C^k t}\|\Psi\|_{\mathscr{G}_{k_0+3j/2}}$$
$$+ \frac{(2^k C\lambda_0)^k}{M^k k!\lambda_\alpha}t^k e^{\lambda_\alpha C^k t}(2^{k_0(k+1)}\|\Psi\|_{\mathscr{G}_{k_0+3k/2}} + N^{k_0}\|\Psi\|_{\mathscr{G}_{3k/2}})$$
$$\leq C_M e^{C_M\lambda_\alpha t}\|\Psi\|_{\mathscr{G}_{k_0+3k/2}} + \frac{(2^k C)^k\lambda_0^{k-1}}{k!}t^k e^{\lambda_\alpha C^k t}\frac{N^{k_0}h^{3\alpha}}{M^k}\|\Psi\|_{\mathscr{G}_{3k/2}}$$

where $C_M = C^{k+k_0}(1+1/M)$. Observing that $\lambda_0 = h^\alpha \lambda_\alpha$, this implies

$$\|\mathsf{U}_{t,0}\Psi\|_{\mathcal{G}_{k_0}} \leq C_M e^{C_M \lambda_\alpha t}\|\Psi\|_{\mathcal{G}_{k_0+3k/2}} + \frac{2^k C}{k}\frac{(2^k C)^{k-1}\lambda_\alpha^{k-1}}{(k-1)!} t^{k-1} e^{\lambda_\alpha C^k t}\frac{N^{k_0} h^{\alpha k} t}{M^k}\|\Psi\|_{\mathcal{G}_{3k/2}}$$

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 the result a bit and write

$$\begin{aligned}\|\mathsf{U}_{t,0}\Psi\|_{\mathcal{G}_{k_0}} &\leq C_M e^{C_M\lambda_\alpha t}\|\Psi\|_{\mathcal{G}_{k_0+3k/2}} + C^k e^{\lambda_\alpha C^k t}\frac{N^{k_0}h^{\alpha k} t}{M^k}\|\Psi\|_{\mathcal{G}_{3k/2}} \\ &\leq C_M e^{C_M \lambda_\alpha t}\left(\|\Psi\|_{\mathcal{G}_{k_0+3k/2}} + \frac{h^{(\alpha-1)k}}{N^{k/2-k_0}} t\|\Psi\|_{\mathcal{G}_{3k/2}}\right). \qquad \blacksquare\end{aligned}$$

11. Proofs of Theorems 4.1 and 3.4

We can now prove our general theorem.

Proof of Theorem 4.1. 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 $\alpha > a - 1/2$ are equivalent to $p_\alpha \in [5/6, 2]$ and $p_\alpha < \mathfrak{b}$, and imply that (80) is a nonempty condition. Therefore, p_α satisfies the assumption (160). Now we define

$$q_1 := q \quad \text{and} \quad \frac{1}{q_0} := 2\left(\frac{1}{p_\alpha} - \frac{1}{\mathfrak{b}}\right) - \frac{1}{q_1}, \tag{182}$$

so that (161) holds with $p = p_\alpha$. Assumption (80) can be written as

$$\frac{1}{q_1} \in \left[2\left(\frac{1}{p_\alpha} - \frac{1}{\mathfrak{b}}\right) - \frac{1}{2}, \frac{1}{p_\alpha} - \frac{1}{\mathfrak{b}}\right]. \tag{183}$$

Now (182) and (183) together imply that $2 \leq q_0 < q_1 \leq \infty$.

Next, we have to check that we have a uniform (in h) bound for the quantity

$$\sup_{[0,T]}\left(\|\rho(t)\|_{L^{p_\alpha}}, \mathcal{D}_{q_0,q_1}(t), \tilde{\mathcal{D}}_{q_0,q_1}(t)\right)$$

appearing in the growth rate λ_α defined in (163). 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 $\|\rho(t)\|_{L^{p_\alpha}}$ is bounded uniformly in h and in $t \in [0,T]$ for some $T = T_{\rho^{\text{in}}}$ depending on the initial condition of the Hartree–Fock equation (5). Then, by Proposition 6.4 we deduce that $\sqrt{\rho} \in \mathcal{W}^{1,q}(m_n)$ for any $q \in [2, q_1)$, and so

$$\tilde{\mathcal{D}}_{q_0,q_1} = \|\nabla_\xi\sqrt{\boldsymbol{\rho}}\, m_n\|_{\mathcal{L}^{q_0}}^{1/2}\|\nabla_\xi\sqrt{\boldsymbol{\rho}}\, m_n\|_{\mathcal{L}^{q_1}}^{1/2}$$

is uniformly bounded on $[0, T]$. Moreover, by Lemma 6.5, we obtain

$$\mathcal{D}_{q,q_0} = \|\nabla_\xi \boldsymbol{\rho}\, m_n\|_{\mathcal{L}^{q_0}}^{1/2} \|\nabla_\xi \boldsymbol{\rho}\, m_n\|_{\mathcal{L}^{q_1}}^{1/2} \leq \tilde{\mathcal{D}}_{q_0,q_1},$$

so $\mathcal{D}_{q,q_0}$ is also uniformly bounded on $[0, T]$. Therefore, by Proposition 10.1,

$$\|\mathsf{U}_{t,0}\Psi\|_{\mathcal{G}_{\frac{1}{2p}}}^2 \leq C_M^2 e^{C_M \lambda t/h^\alpha} \left(\|\Psi\|_{\mathcal{G}_{3k/2+\frac{1}{2p}}}^2 + \frac{h^{2k(\alpha-1)}}{N^{k-1/p}} t^2 \|\Psi\|_{\mathcal{G}_{3k/2}}^2 \right) \tag{184}$$

with λ uniformly bounded in $t \in [0, T]$ and in the Planck constant h. Then, by Proposition 9.1,

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

We conclude the proof by combining (184) 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 3.4. To this end, we come back to the setting of density operators over the Fock space by means of the following lemma.

Lemma 11.1. *Let* $\boldsymbol{\rho}_{N,\boldsymbol{\rho}} := |\mathsf{I}_{\mathcal{G}}^{-1}(\mathsf{R}_{\boldsymbol{\rho}}\Omega)|^2$ *as defined in* (77). *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*

$$\boldsymbol{\rho}_N = |\mathsf{I}_{\mathcal{G}}^{-1}(\mathsf{R}_{\boldsymbol{\rho}}\Psi)|^2 \tag{185}$$

and

$$\|\mathcal{N}^s\Psi\|_{\mathcal{G}}^2 \leq C_s \|(\mathcal{N} + 2N)^s(\boldsymbol{\rho}_N - \boldsymbol{\rho}_{N,\boldsymbol{\rho}})\|_{\mathcal{L}^1(\mathcal{F})} \tag{186}$$

with $C_s = 12^s(s+1)^s$.

Proof. Let $\Phi_{\boldsymbol{\rho}} = \mathsf{R}_{\boldsymbol{\rho}}\Omega = \mathsf{I}_{\mathcal{G}}(\boldsymbol{\upsilon}_{N,\boldsymbol{\rho}})$. Then $|\boldsymbol{\upsilon}_{N,\boldsymbol{\rho}}| = \sqrt{\boldsymbol{\rho}_{N,\boldsymbol{\rho}}}$, and by the polar decomposition of $\boldsymbol{\upsilon}_{N,\boldsymbol{\rho}}$, there exists a unique operator $U_{N,\boldsymbol{\rho}}$ such that

$$\boldsymbol{\upsilon}_{N,\boldsymbol{\rho}} = U_{N,\boldsymbol{\rho}}|\boldsymbol{\upsilon}_{N,\boldsymbol{\rho}}|$$

with $\|U_{N,\boldsymbol{\rho}}\psi\|_{\mathcal{F}} = \|\psi\|_{\mathcal{F}}$ if $\psi \in (\ker \boldsymbol{\upsilon}_{N,\boldsymbol{\rho}})^\perp$ and $\|U_{N,\boldsymbol{\rho}}\psi\|_{\mathcal{F}} = 0$ if $\psi \in \ker \boldsymbol{\upsilon}_{N,\boldsymbol{\rho}}$ (see e.g. [65, Theorem VI.10]). Then we define

$$\boldsymbol{\upsilon}_N := U_{N,\boldsymbol{\rho}}|\sqrt{\boldsymbol{\rho}_N}|,$$

and $\Phi = \mathsf{I}_{\mathcal{G}}(\boldsymbol{\upsilon}_N)$, $\Psi := \mathsf{R}_{\boldsymbol{\rho}}^*\Phi$. In particular, $\boldsymbol{\rho}_N = |\boldsymbol{\upsilon}_N|^2$, so (185) is satisfied. Now from Lemma 9.3, 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, $\mathcal{N}_l\Phi = \mathsf{I}_{\mathcal{G}}(\mathcal{N}\boldsymbol{\upsilon}_N)$, $\mathcal{N}_r\Phi = \mathsf{I}_{\mathcal{G}}(\boldsymbol{\upsilon}_N\mathcal{N})$ and $\boldsymbol{\upsilon}_N$ commutes with $\mathcal{N}$, we deduce that

$$\|\mathcal{N}^s\Psi\|_{\mathcal{G}} \leq C_s\|(\mathcal{N} + N)^s(\boldsymbol{\upsilon}_N - \boldsymbol{\upsilon}_{N,\boldsymbol{\rho}})\|_{\mathcal{L}^2(\mathcal{F})}.$$

By our choice of $U_{N,\boldsymbol{\rho}}$,

$$(\mathcal{N}+N)^s(\boldsymbol{v}_N-\boldsymbol{v}_{N,\boldsymbol{\rho}}) = U_{N,\boldsymbol{\rho}}\big(|(\mathcal{N}+N)^s\boldsymbol{v}_N|-|(\mathcal{N}+N)^s\boldsymbol{v}_{N,\boldsymbol{\rho}}|\big)$$

with $\|U_{N,\boldsymbol{\rho}}\|_\infty \leq 1$. Now recall the Powers–Størmer inequality [64, Lemma 4.1]: if A and B are nonnegative operators, then

$$\operatorname{Tr}(|A-B|^2) \leq \operatorname{Tr}(|A^2-B^2|).$$

Hence,

$$\begin{aligned}\|\mathcal{N}^s\Psi\|_{\mathcal{G}}^2 &\leq C_s^2\big\||\boldsymbol{v}_N(\mathcal{N}+N)^s|^2-\big|\boldsymbol{v}_{N,\boldsymbol{\rho}}(\mathcal{N}+N)^s\big|^2\big\|_{\mathfrak{L}^1(\mathcal{F})}\\ &\leq C_s^2\|(\mathcal{N}+N)^s(\boldsymbol{\rho}_N-\boldsymbol{\rho}_{N,\boldsymbol{\rho}})(\mathcal{N}+N)^s\|_{\mathfrak{L}^1(\mathcal{F})}.\end{aligned}$$

■

Proof of Theorem 3.4. In the setting of Theorem 3.4, since $a<1/2$, we can take $\alpha=0$ in Theorem 4.1, and the hypothesis for q implies that condition (80) is satisfied. With this choice, Theorem 4.1 yields, for any $k_1\in\mathbb{N}$,

$$\|\boldsymbol{\rho}_{N:1}-\boldsymbol{\rho}\|_{\mathfrak{L}^p} \leq \frac{Ce^{\lambda t}}{\min(N^{1/2},Nh^{3/p'})}\|\Psi\|_{\mathcal{G}_{3k_1/2+\frac{1}{2p}}}^2\left(1+\frac{h^{-2k_1}}{N^{k_1-1/p}}\right).$$

Taking $k=3k_1/2+\frac{1}{2p}$, the hypothesis on k implies that $\frac{h^{-2k_1}}{N^{k_1-1/p}}\leq C$. Finally, by Lemma 11.1 we get

$$\|\Psi\|_{\mathcal{G}_k}^2 \leq 2^{k+1}(\|\Psi\|_{\mathcal{G}}^2+\|\mathcal{N}^k\Psi\|_{\mathcal{G}}^2) \leq C_k(1+\|\boldsymbol{\rho}_N-\boldsymbol{\rho}_{N,\boldsymbol{\rho}}\|_{\mathfrak{L}^1_k(\mathcal{F})})$$

for some k-dependent constant $C_k>0$. ■

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. Therefore, to simplify the presentation, we set $\hbar\equiv 1$. By (172), the time-dependent operator $\tilde{\mathsf{G}}$ defined in (159) can be written as

$$\tilde{\mathsf{G}} = \mathrm{d}\Gamma_l(H_\omega)-\mathrm{d}\Gamma_r(\overline{H}_\omega)+\tilde{\mathsf{Q}}+\tilde{\mathsf{Q}}^*+\mathsf{D}+\tilde{\mathsf{P}}+\tilde{\mathsf{P}}^*, \tag{187}$$

where $\tilde{\mathsf{Q}}^*$ and D have already been defined after (159) and

$$\begin{aligned}\tilde{\mathsf{P}}^* = \frac{1}{N}\int_{\mathbb{R}^6}\big(&a_r^*(\bar{v}_x)a_l^*(u_x)\mathrm{d}\Gamma_l(u[K_x,u])+a_r^*(\bar{u}_x)a_l^*(v_x)\mathrm{d}\Gamma_l(v[K_x,v])\\ &+\mathrm{d}\Gamma_{l,r}^+([u,K_x]v+[K_x,v]u)\mathrm{d}\Gamma_l(\omega_x)\\ &+a_l^*(v_x)a_r^*(\bar{u}_x)\mathrm{d}\Gamma_r(\bar{u}[K_x,\bar{u}])+a_l^*(u_x)a_r^*(\bar{v}_x)\mathrm{d}\Gamma_r(\bar{v}[K_x,\bar{v}])\\ &+\mathrm{d}\Gamma_{r,l}^+([\bar{u},K_x]\bar{v}+[K_x,\bar{v}]\bar{u})\mathrm{d}\Gamma_r(\bar{\omega}_x)\big)\,\mathrm{d}x.\end{aligned}$$

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

$$i\,\partial_t \tilde{\mathsf{U}}_{t,s}\Psi = \tilde{\mathsf{G}}_t \tilde{\mathsf{U}}_{t,s}\Psi \quad \text{with} \quad \tilde{\mathsf{U}}_{s,s}\Psi = \Psi, \tag{188}$$

for sufficiently smooth $\Psi \in \mathscr{G}$. 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 $\mathsf{L}_0 = \mathrm{d}\Gamma_r(\Delta) - \mathrm{d}\Gamma_l(\Delta)$ 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 (188).

Since much of the result in this appendix is similar to that of the appendix of [11], we will only focus on the part that relies explicitly on the regularity of the potential and refer the reader to [11] for a more complete proof. Hence, the rest of this section will be devoted to proving 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

$$\|\Psi\|_{\dot{\mathscr{H}}^s_k} := \|\mathcal{N}^{k-1/2}\mathrm{d}\Gamma((-\Delta)^s)^{1/2}\Psi\|_{\mathscr{G}}. \tag{189}$$

In particular, $\|\Psi\|_{\dot{\mathscr{H}}^0_k} = \|\mathcal{N}^k\Psi\|_{\mathscr{G}}$. 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 (39a), (39b), and $\int_{\mathbb{R}^3}\rho^{\mathrm{in}}(x)(1+|x|^3)\,\mathrm{d}x \le C$. Then there exists $T>0$ and a constant C_T depending on $\boldsymbol{\rho}^{\mathrm{in}}$ such that for any $(t,s)\in[0,T]^2$,*

$$\|(\widehat{\mathsf{G}}_t - \widehat{\mathsf{G}}_s)\Psi\|_{\mathscr{G}} \le C_T|t-s|^{\frac{3-2a}{7}}(\|\Psi\|_{\mathscr{G}_2} + \|\Psi\|_{\dot{\mathscr{H}}^{3/2}_2}).$$

Remark A.2. For a fixed $\hbar$, the global-in-time well-posedness of solutions to the Hartree–Fock equation is a standard result (see for instance [21]). However, the bounds on 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.3. We know from Part II that the conditions (39a) and (39b) remain satisfied on $[0,T]$. In particular, $\|\sqrt{\boldsymbol{\rho}}\|^2_{\mathscr{L}^2(|\boldsymbol{p}|^n)} = \mathrm{Tr}(\boldsymbol{\rho}|\boldsymbol{p}|^{2n})$ is uniformly bounded on $[0,T]$. To see that the third-order spatial moment $\int_{\mathbb{R}^3}\rho^{\mathrm{in}}(x)|x|^3\,\mathrm{d}x = \mathrm{Tr}(\boldsymbol{\rho}|x|^3)$ remains bounded, one can notice that

$$i\,\frac{\mathrm{d}}{\mathrm{d}t}\mathrm{Tr}(\boldsymbol{\rho}|x|^3) = \mathrm{Tr}([|\boldsymbol{p}|^2/2, |x|^3]\boldsymbol{\rho}) + \mathrm{Tr}([\mathsf{X}_{\boldsymbol{\rho}}, |x|^3]\boldsymbol{\rho}).$$

The first term is controlled, using [48, (42)], by a term proportional to

$$\operatorname{Tr}\big(\boldsymbol{\rho}(|x|^3 + |\boldsymbol{p}|^3 + 1)\big).$$

The second term is zero since

$$\operatorname{Tr}([\mathsf{X}_{\boldsymbol{\rho}}, |x|^3]\boldsymbol{\rho}) = \iint_{\mathbb{R}^6} |\boldsymbol{\rho}(x,y)|^2 \frac{|y|^3 - |x|^3}{|x-y|^a}\, \mathrm{d}x\, \mathrm{d}y$$

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 (189) controls quantities of the form $\|\mathrm{d}\Gamma(A\nabla)\Psi\|_{\mathscr{G}}$ as stated in the following lemma.

Lemma A.4. *Let $A \in \mathscr{L}^\infty$ and $\Psi \in \dot{\mathscr{H}}^1_1$. Then $\|\mathrm{d}\Gamma(A\nabla)\Psi\|_{\mathscr{G}} \le \|A\|_\infty \|\Psi\|_{\dot{\mathscr{H}}^1_1}$.*

Proof. Using the fact that A is a bounded operator, we obtain

$$\|\mathrm{d}\Gamma(A\nabla)\Psi\|^2_{\mathscr{G}} \le \|A\|^2_\infty \sum_{n=1}^{\infty} \Big(\sum_{j\le n} \|\nabla_{x_j} \Psi^{(n)}\|_{L^2}\Big)^2.$$

By the Cauchy–Schwarz inequality and integration by parts,

$$\sum_{n=1}^{\infty} \Big(\sum_{j\le n} \|\nabla_{x_j} \Psi^{(n)}\|_{L^2}\Big)^2 \le \langle \mathscr{N}_l \Psi^{(n)} \,|\, \mathrm{d}\Gamma_l(-\Delta)\Psi^{(n)}\rangle_{\mathscr{G}} = \|\mathrm{d}\Gamma_l(-\Delta)^{1/2}\mathscr{N}_l^{1/2}\Psi\|^2_{\mathscr{G}},$$

which is bounded above by $\|\Psi\|_{\dot{\mathscr{H}}^1_1}$. ■

To simplify some of the calculation, it will also be convenient to employ the following lemma.

Lemma A.5. *For any self-adjoint integral operator A on $\mathfrak{h} = L^2(\mathbb{R}^3)$, we have the identities*

$$\mathsf{U}_t^{(0)*} \mathrm{d}\Gamma_l(A) \mathsf{U}_t^{(0)} = \mathrm{d}\Gamma_l(A_I), \tag{190a}$$

$$\mathsf{U}_t^{(0)*} \mathrm{d}\Gamma^+_{l,r}(A) \mathsf{U}_t^{(0)} = \mathrm{d}\Gamma^+_{l,r}(A_I), \tag{190b}$$

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

$$[\mathsf{L}_0, a_{x,l}] = [\mathrm{d}\Gamma_l(-\Delta), a_{x,l}] = \Delta_x a_{x,l}. \tag{191}$$

Therefore, using the Baker–Campbell–Hausdorff formula

$$e^X Y e^{-X} = Y + [X,Y] + \frac{1}{2!}[X,[X,Y]] + \cdots$$

and (191), 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

$$\begin{aligned}\mathsf{U}_t^{(0)*}\mathrm{d}\Gamma_l(A)\mathsf{U}_t^{(0)} &= \int_{\mathbb{R}^6} A(z_1,z_2)\mathsf{U}_t^{(0)*}a_{z_1,l}^*a_{z_2,r}\mathsf{U}_t^{(0)}\,\mathrm{d}z_1\,\mathrm{d}z_2\\ &= \int_{\mathbb{R}^6} e^{-it\Delta_{z_1}}A(z_1,z_2)e^{it\Delta_{z_2}}a_{z_1,l}^*a_{z_2,r}\,\mathrm{d}z_1\,\mathrm{d}z_2.\end{aligned}$$

This establishes (190a). The proof of (190b) is similar. ∎

Proof of Proposition A.1. First notice that $[\mathsf{U}_t^{(0)},\mathrm{d}\Gamma(-\Delta)]=0$, which using (187) allows us to write

$$\begin{aligned}\widehat{\mathsf{G}}_t &= \mathsf{U}_t^{(0)*}\big(\mathrm{d}\Gamma_l(V_{\boldsymbol{\rho}}-\mathsf{X}_{\boldsymbol{\rho}})-\mathrm{d}\Gamma_r(V_{\boldsymbol{\rho}}-\mathsf{X}_{\boldsymbol{\rho}})\big)\mathsf{U}_t^{(0)}\\ &\quad+\mathsf{U}_t^{(0)*}(\tilde{\mathsf{Q}}+\tilde{\mathsf{Q}}^*)\mathsf{U}_t^{(0)}+\mathsf{U}_t^{(0)*}\mathsf{D}\mathsf{U}_t^{(0)}+\mathsf{U}_t^{(0)*}(\tilde{\mathsf{P}}+\tilde{\mathsf{P}}^*)\mathsf{U}_t^{(0)}\\ &=: \mathrm{I}_t+\mathrm{II}_t+\mathrm{III}_t+\mathrm{IV}_t.\end{aligned}$$

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 Lemmas A.6–A.9 below. Combining these lemmas leads to the result. ∎

Lemma A.6. *Under the conditions of Proposition* A.1, *there exists a constant C_T depending on the initial conditions such that*

$$\|\partial_t\mathrm{I}_t\Psi\|_{L^\infty((0,T),\mathscr{G})}\leq C_T(\|\Psi\|_{\mathscr{G}_1}+\|\Psi\|_{\dot{\mathscr{H}}_1^1}).$$

Proof. 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 (190a), we see that

$$\begin{aligned}i\frac{\mathrm{d}}{\mathrm{d}t}\big(\mathsf{U}_t^{(0)*}\mathrm{d}\Gamma_l(V_{\boldsymbol{\rho}})\mathsf{U}_t^{(0)}\big) &= \mathsf{U}_t^{(0)*}\big(\mathrm{d}\Gamma_l([V_{\boldsymbol{\rho}},-\Delta])+\mathrm{d}\Gamma_l(i\partial_t\rho*K)\big)\mathsf{U}_t^{(0)}\\ &=: \mathsf{J}_1+\mathsf{J}_2.\end{aligned}$$

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

$$\|\mathsf{U}_t^{(0)*}\mathrm{d}\Gamma_l(\nabla V_{\boldsymbol{\rho}}\cdot\nabla)\mathsf{U}_t^{(0)}\Psi\|_{\mathscr{G}}\leq\|\nabla V_{\boldsymbol{\rho}}\|_{L^\infty}\|\Psi\|_{\dot{\mathscr{H}}_1^1},$$

where since $\nabla K\in L^{\mathfrak{b},\infty}$, we have

$$\|\nabla V_{\boldsymbol{\rho}}\|_{L^\infty}\leq\sup_{x\in\mathbb{R}^3}\int_{\mathbb{R}^3}|\nabla K(x-y)|\rho(y)\,\mathrm{d}y\leq\|\nabla K\|_{L^{\mathfrak{b},\infty}}\|\rho\|_{L^{\mathfrak{b}',1}}.$$

Similarly, for the second term, by Lemma 8.1 and since $\nabla K\in L^{\mathfrak{b},\infty}$, we have

$$\|\mathsf{U}_t^{(0)*}\mathrm{d}\Gamma_l(\Delta V_{\boldsymbol{\rho}})\mathsf{U}_t^{(0)}\Psi\|_{\mathscr{G}}\leq\|\Delta V_{\boldsymbol{\rho}}\|_{L^\infty}\|\Psi\|_{\mathscr{G}_1}\leq\|\nabla K\|_{L^{\mathfrak{b},\infty}}\|\nabla\rho\|_{L^{\mathfrak{b}',1}}\|\Psi\|_{\mathscr{G}_1}.$$

By Proposition 6.1, the norm of ρ in $L^{\mathfrak{b}',1}$ remains bounded for $t \in [0,T]$. When $\mathfrak{b}' \geq 2$, the same holds for $\nabla\rho$. Moreover, since $\hbar = 1$, $\|\nabla\rho\|_{L^1} \leq C\,\mathrm{Tr}((1-\Delta)\boldsymbol{\rho})$ 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,

$$\|\mathsf{J}_1\Psi\|_{\mathcal{G}} \leq C_T(\|\Psi\|_{\mathcal{G}_1} + \|\Psi\|_{\dot{\mathcal{H}}_1^1}). \tag{192}$$

For the J_2 term, let us begin by recalling that ρ satisfies the equation

$$\partial_t\rho + \nabla\cdot j_{\boldsymbol{\rho}} = 0$$

where $j_{\boldsymbol{\rho}} = \frac{1}{2}\,\mathrm{diag}(\boldsymbol{\rho}\boldsymbol{p} + \boldsymbol{p}\boldsymbol{\rho})$ is known as the probability current. Similarly to J_1, we have the estimate

$$\|\mathsf{J}_2\Psi\|_{\mathcal{G}} = \big\|\mathsf{U}_t^{(0)*}\mathrm{d}\Gamma_l\big(\nabla\cdot(j_{\boldsymbol{\rho}} * K)\big)\mathsf{U}_t^{(0)}\Psi\big\|_{\mathcal{G}} \leq \|j_{\boldsymbol{\rho}}\|_{L^{\mathfrak{b}',1}}\|\nabla K\|_{L^{\mathfrak{b},\infty}}\|\Psi\|_{\mathcal{G}_1}. \tag{193}$$

The term $\|j_{\boldsymbol{\rho}}\|_{L^{\mathfrak{b}',1}}$ is bounded as for ρ by Proposition 6.11 and the kinetic energy of $\boldsymbol{\rho}$.

Now let us handle the exchange term $\mathsf{X}_{\boldsymbol{\rho}}$ in I_t. Note that

$$i\frac{\mathrm{d}}{\mathrm{d}t}\big(\mathsf{U}_t^{(0)*}\mathrm{d}\Gamma_l(\mathsf{X}_{\boldsymbol{\rho}})\mathsf{U}_t^{(0)}\big) = \mathsf{U}_t^{(0)*}\big(\mathrm{d}\Gamma_l([\mathsf{X}_{\boldsymbol{\rho}}, -\Delta]) + \mathrm{d}\Gamma_l(i\partial_t\mathsf{X}_{\boldsymbol{\rho}})\big)\mathsf{U}_t^{(0)} =: \mathsf{J}_3 + \mathsf{J}_4.$$

We start by rewriting the J_3 term. Observe 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 manner as before. We will only deal with the second term. By Lemma 8.1 and (112),

$$\|\mathsf{U}_t^{(0)*}\mathrm{d}\Gamma_l(\mathsf{X}_{\boldsymbol{\Delta}_x\boldsymbol{\rho}})\mathsf{U}_t^{(0)}\Psi\|_{\mathcal{G}} \leq \|\mathsf{X}_{\boldsymbol{\Delta}_x\boldsymbol{\rho}}\|_2\|\Psi\|_{\mathcal{G}_1} \leq \|\boldsymbol{\Delta}_x\boldsymbol{\rho}\,|\boldsymbol{p}|^a\|_2\|\Psi\|_{\mathcal{G}_1}, \tag{194}$$

and since $\hbar = 1$, we have $\boldsymbol{\Delta}_x\boldsymbol{\rho} = -\sum_{\mathrm{j}=1}^3[\boldsymbol{p}_\mathrm{j}, [\boldsymbol{p}_\mathrm{j}, \boldsymbol{\rho}]]$ and so by Lemma 6.9, $\|\boldsymbol{\Delta}_x\boldsymbol{\rho}|\boldsymbol{p}|^a\|_2 \leq C\|\boldsymbol{\rho}|\boldsymbol{p}|^{a+2}\|_2$, which remains bounded on $[0,T]$ by Proposition 6.1. Hence

$$\|\mathsf{J}_3\Psi\|_{\mathcal{G}} \leq C_T(\|\Psi\|_{\mathcal{G}_1} + \|\Psi\|_{\dot{\mathcal{H}}_1^1}). \tag{195}$$

For the J_4 term, we have

$$\mathsf{J}_4 = \mathsf{U}_t^{(0)*}\big(\mathrm{d}\Gamma_l(\mathsf{X}_{[-\Delta,\boldsymbol{\rho}]}) + \mathrm{d}\Gamma_l(\mathsf{X}_{[V_{\boldsymbol{\rho}},\boldsymbol{\rho}]}) - \mathrm{d}\Gamma_l(\mathsf{X}_{[\mathsf{X}_{\boldsymbol{\rho}},\boldsymbol{\rho}]})\big)\mathsf{U}_t^{(0)}.$$

To estimate the term with the Laplacian, we proceed as in (194) and use the fact that since $\hbar = 1$, we have $[-\Delta, \boldsymbol{\rho}] = |\boldsymbol{p}|^2\boldsymbol{\rho} - \boldsymbol{\rho}|\boldsymbol{p}|^2$. To estimate the second term, we use (112) to get

$$\|\mathsf{X}_{[V_{\boldsymbol{\rho}},\boldsymbol{\rho}]}\|_\infty \leq \|[V_{\boldsymbol{\rho}}, \boldsymbol{\rho}]|\boldsymbol{p}|^a\|_\infty \leq \|[V_{\boldsymbol{\rho}}, \boldsymbol{\rho}](1 + |\boldsymbol{p}|^2)\|_\infty.$$

Then similarly to 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 Propositions 6.13 and 6.15 with $V_{\boldsymbol{\rho}}$ instead of $E_{\boldsymbol{\rho}}$. Similarly, to bound the last term, we use (112) and then Proposition 6.23. Hence we have the estimate

$$\|\mathsf{J}_4\Psi\|_{\mathcal{G}} \leq C_T\|\Psi\|_{\mathcal{G}_1}. \tag{196}$$

The bound on $\partial_t\mathrm{I}_t$ now follows by combining the inequalities for each part, i.e. (192), (193), (195) and (196). ∎

Lemma A.7. *Under the conditions of Proposition A.1, there exists a constant C_T depending on the initial conditions such that for any $(t,s) \in [0,T]^2$,*

$$\|(\mathrm{II}_t - \mathrm{II}_s)\Psi\|_{\mathscr{G}} \leq C_T |t-s|^{\frac{3-2a}{7}} \|\Psi\|_{\mathscr{G}_{3/2}}.$$

Proof. 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:

$$K = K_R^L + K_R^S := C_a \left(\int_0^{R^{-2}} s^{a/2-1} \varphi_s \, \mathrm{d}s + \int_{R^{-2}}^{\infty} s^{a/2-1} \varphi_s \, \mathrm{d}s \right) \tag{197}$$

for some R which we will determine shortly, and with $\varphi_s(x) = e^{-\pi |x|^2 s}$. Consequently, we have the decomposition

$$N\tilde{\mathsf{Q}}_1^* = \int_{\mathbb{R}^6} (K_R^L + K_R^S)(x-y) \mathrm{d}\Gamma_{l,r}^+(u\delta_x v) \mathrm{d}\Gamma_{l,r}^+(u\delta_y v) \, \mathrm{d}x \, \mathrm{d}y =: \tilde{\mathsf{Q}}_{1,R}^{L*} + \tilde{\mathsf{Q}}_{1,R}^{S*}.$$

For the long-range part, we follow the proof of the bounded potential case in [11] and show that $\tilde{\mathsf{Q}}_{1,R}^{L*}$ is time differentiable. Applying Lemma A.5 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

$$\mathsf{U}_t^{(0)*} \tilde{\mathsf{Q}}_{1,R}^{L*} \mathsf{U}_t^{(0)} = \int_{\mathbb{R}^3} \widehat{K_R^L}(y) \mathrm{d}\Gamma_{l,r}^+(u_I e^{iy\cdot(x-2it\nabla)} v_I) \mathrm{d}\Gamma_{l,r}^+(u_I e^{-iy\cdot(x-2it\nabla)} v_I) \, \mathrm{d}y,$$

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

$$\begin{aligned} i\partial_t (u_I e^{iy\cdot(x-2it\nabla)} v_I) &= e^{-it\Delta}(u[e^{iy\cdot x}, -\Delta]v) e^{it\Delta} \\ &\quad + e^{-it\Delta}([V_{\boldsymbol{\rho}} - \mathsf{X}_{\boldsymbol{\rho}}, u] e^{iy\cdot x} v + u e^{iy\cdot x}[V_{\boldsymbol{\rho}} - \mathsf{X}_{\boldsymbol{\rho}}, v]) e^{it\Delta}. \end{aligned}$$

Applying Lemma 8.1, we have the estimates

$$\begin{aligned} \|\mathrm{d}\Gamma_{l,r}^+(u_I e^{iy\cdot(x-2it\nabla)} v_I)\Psi\|_{\mathscr{G}} &\leq 2\|u\|_\infty \|v\|_2 \|\Psi\|_{\mathscr{G}_1}, \\ \left\|\mathrm{d}\Gamma_{l,r}^+\left(\partial_t(u_I e^{iy\cdot(x-2it\nabla)} v_I)\right)\Psi\right\|_{\mathscr{G}} &\leq C_T \langle y\rangle^2 \|u\|_\infty \|\langle\nabla\rangle v\|_2 \|\Psi\|_{\mathscr{G}_1}, \end{aligned} \tag{198}$$

where $C_T = C \sup_{t\in[0,T]}(1 + \|V_{\boldsymbol{\rho}}\|_{L^\infty} + \|\mathsf{X}_{\boldsymbol{\rho}}\|_\infty)$ is finite, and $\langle y\rangle^2 = 1 + |y|^2$. In particular, it follows from (198) that

$$\left\| \frac{\mathrm{d}}{\mathrm{d}t} \mathsf{U}_t^{(0)*} \tilde{\mathsf{Q}}_{1,R}^{L*} \mathsf{U}_t^{(0)} \Psi \right\|_{\mathscr{G}} \leq C_T \int_{\mathbb{R}^3} |\widehat{K_R^L}(y)| \langle y\rangle^2 \, \mathrm{d}y \, \|\Psi\|_{\mathscr{G}_1}.$$

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 $\widehat{\varphi}_s = s^{-3/2}\varphi_{1/s}$, we have

$$\int_{\mathbb{R}^3} |\widehat{K_R^L}| \langle y\rangle^2 \, \mathrm{d}y = \int_0^{R^{-2}} \int_{\mathbb{R}^3} s^{\frac{a-5}{2}} e^{-\frac{\pi}{s}|y|^2} \langle y\rangle^2 \, \mathrm{d}y \, \mathrm{d}s = \frac{3}{\pi} \left(\frac{R^{-(a+2)}}{a+2} + \frac{R^{-a}}{a} \right). \tag{199}$$

Therefore, provided $R < 1$, we obtain

$$\left\| \frac{\mathrm{d}}{\mathrm{d}t} (\mathsf{U}_t^{(0)*} \tilde{\mathsf{Q}}_{1,R}^{L*} \mathsf{U}_t^{(0)} \Psi) \right\|_{\mathscr{G}} \leq \frac{6}{\pi a} R^{-(a+2)} \|\Psi\|_{\mathscr{G}_1},$$

which implies that for any $(t, s) \in [0, T]^2$,

$$\|(\mathsf{U}_t^{(0)*} \tilde{\mathsf{Q}}_{1,R}^{L*} \mathsf{U}_t^{(0)} - \mathsf{U}_s^{(0)*} \tilde{\mathsf{Q}}_{1,R}^{L*} \mathsf{U}_s^{(0)}) \Psi\|_{\mathscr{G}} \leq \frac{6}{\pi a} R^{-(a+2)} |t - s| \, \|\Psi\|_{\mathscr{G}_1}. \tag{200}$$

For the singular part, by the Cauchy–Schwarz inequality, we have

$$\begin{aligned} |\langle \Psi_1 \,|\, \tilde{\mathsf{Q}}_{1,R}^{S*} \Psi_2 \rangle| &= \left| \int_{\mathbb{R}^3} \langle a_l(u_x) \Psi_1 \,|\, a_r^*(\overline{v}_x) \mathrm{d}\Gamma_{l,r}^+(u K_{R,x}^S v) \Psi_2 \rangle \, \mathrm{d}x \right| \\ &\leq \left(\int_{\mathbb{R}^3} \|a_l(u_x) \Psi_1\|_{\mathscr{G}}^2 \, \mathrm{d}x \right)^{1/2} \left(\int_{\mathbb{R}^3} \|a_r^*(\overline{v}_x) \mathrm{d}\Gamma_{l,r}^+(u K_{R,x}^S v) \Psi_2\|_{\mathscr{G}}^2 \, \mathrm{d}x \right)^{1/2}. \end{aligned}$$

Applying Lemma 8.1 and $\|u\|_\infty \leq 1$ yields

$$\|a_r^*(\overline{v}_x) \mathrm{d}\Gamma_{l,r}^+(u K_{R,x}^S v) \Psi_2\|_{\mathscr{G}} \leq (N\rho(x))^{1/2} \|K_{R,x}^S v\|_2 \|\Psi_2\|_{\mathscr{G}_{1/2}},$$

which gives

$$|\langle \Psi_1 \,|\, \tilde{\mathsf{Q}}_{1,R}^{S*} \Psi_2 \rangle| \leq C N^{1/2} \langle \Psi_1 \,|\, \mathscr{N} \Psi_1 \rangle^{1/2} \left(\int_{\mathbb{R}^3} \rho(x) \|K_{R,x}^S v\|_2^2 \, \mathrm{d}x \right)^{1/2} \|\Psi_2\|_{\mathscr{G}_{1/2}}.$$

Since $\operatorname{diag}(v^2) = N\rho$, we see that

$$\begin{aligned} \|K_{R,x}^S v\|_2 &\leq \int_{R^{-2}}^\infty s^{a/2-1} \|\varphi_{s,x} v\|_2 \, \mathrm{d}s \\ &= N^{1/2} \int_{R^{-2}}^\infty s^{a/2-1} (|\varphi_s|^2 * \rho)^{1/2}(x) \, \mathrm{d}s \\ &\leq N^{1/2} \|\rho\|_{L^\infty}^{1/2} \int_{R^{-2}}^\infty s^{a/2-1} \|\varphi_s\|_{L^2} \, \mathrm{d}s \leq C_T N^{1/2} R^{3/2-a}. \end{aligned}$$

Hence, by duality, it follows that $\|\tilde{\mathsf{Q}}_{1,R}^S \Psi\|_{\mathscr{G}} \leq R^{3/2-a} \|\Psi\|_{\mathscr{G}_{3/2}}$. By a similar argument, one can also show the same inequality for the dual operator $\tilde{\mathsf{Q}}_{1,R}^{S*}$. Therefore,

$$\|\tilde{\mathsf{Q}}_{1,R}^{S*} \Psi\|_{\mathscr{G}} \leq C_T N R^{3/2-a} \|\Psi\|_{\mathscr{G}_{3/2}}. \tag{201}$$

Combining (200) and (201), we find that for any $(t, s) \in [0, T]^2$ and any $R \in (0, 1)$,

$$\|(\mathsf{U}_t^{(0)*} \tilde{\mathsf{Q}}_1^* \mathsf{U}_t^{(0)} - \mathsf{U}_s^{(0)*} \tilde{\mathsf{Q}}_1^* \mathsf{U}_s^{(0)}) \Psi\| \leq C_T (R^{-(a+2)} |t - s| + R^{3/2-a}) \|\Psi\|_{\mathscr{G}_{3/2}}.$$

In particular, if $t \neq s$, one can take $R^{7/2} = |t - s|/T \leq 1$, leading to

$$\|(\mathsf{U}_t^{(0)*} \tilde{\mathsf{Q}}_1^* \mathsf{U}_t^{(0)} - \mathsf{U}_s^{(0)*} \tilde{\mathsf{Q}}_1^* \mathsf{U}_s^{(0)}) \Psi\|_{\mathscr{G}} \leq C_T |t - s|^{\frac{3-2a}{7}} \|\Psi\|_{\mathscr{G}_{3/2}}.$$

If $t = s$, we can let $R \to 0$ to obtain the same inequality. ■

Next, let us consider the type III terms.

Lemma A.8. *Under the conditions of Proposition A.1, there exists a constant C_T depending on the initial conditions such that for any $(t,s) \in [0,T]^2$,*

$$\|(\mathrm{III}_t - \mathrm{III}_s)\Psi\|_{\mathscr{G}} \leq C_T |t-s|^{\frac{3-2a}{7}} (\|\Psi\|_{\mathscr{G}_2} + \|\Psi\|_{\dot{\mathscr{H}}_2^{3/2}}).$$

Proof. 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 for $\tilde{\mathsf{Q}}_1$. Using (197), we decompose D_1 into two parts,

$$2N\mathsf{D}_1 = \mathsf{D}_{1,R}^L + \mathsf{D}_{1,R}^S.$$

For the long-range part, we begin by writing

$$\mathsf{U}_t^{(0)*}\mathsf{D}_{1,R}^L\mathsf{U}_t^{(0)} = \int_{\mathbb{R}^3} \widehat{K_R^L}(y) \mathrm{d}\Gamma_l(u_I e^{iy\cdot(x-2it\nabla)} u_I) \mathrm{d}\Gamma_l(u_I e^{-iy\cdot(x-2it\nabla)} u_I) \, \mathrm{d}y.$$

Using the identity

$$i\partial_t(u_I e^{iy\cdot(x-2it\nabla)} u_I) = e^{-it\Delta}(\eta e^{iy\cdot x} u + u e^{iy\cdot x}\eta + u[e^{iy\cdot x}, -\Delta]u) e^{it\Delta},$$

where $\eta = [V_{\boldsymbol{\rho}} - \mathsf{X}_{\boldsymbol{\rho}}, u]$, and Lemma 8.1, we deduce that

$$\begin{aligned} &\|\mathrm{d}\Gamma_l(u_I e^{iy\cdot(x-2it\nabla)} u_I)\Psi\|_{\mathscr{G}} \leq \|\Psi\|_{\mathscr{G}_1}, \\ &\left\|\mathrm{d}\Gamma_l\big(\partial_t(u_I e^{iy\cdot(x-2it\nabla)} u_I)\big)\Psi\right\|_{\mathscr{G}} \leq (\|\eta\|_\infty + |y|^2)\|\Psi\|_{\mathscr{G}_1} + |y|\|\Psi\|_{\dot{\mathscr{H}}_1^1}. \end{aligned} \tag{202}$$

By (202) and (199), provided $R \in (0,1)$, we get

$$\|\frac{\mathrm{d}}{\mathrm{d}t}(\mathsf{U}_t^{(0)*}\mathsf{D}_{1,R}^L\mathsf{U}_t^{(0)})\Psi\|_{\mathscr{G}} \leq C_a(1+\|\eta\|_\infty)R^{-(a+2)}(\|\Psi\|_{\mathscr{G}_2} + \|\Psi\|_{\dot{\mathscr{H}}_2^1}).$$

To handle the singular part, we begin by writing $u = 1 - w$. Then it follows that

$$\begin{aligned} \mathsf{D}_{1,R}^S = &\int_{\mathbb{R}^6} K_R^S(x-y) a_{x,l}^* a_{y,l}^* a_l(u_y) a_l(u_x) \, \mathrm{d}x \, \mathrm{d}y \\ &+ \int_{\mathbb{R}^6} K_R^S(x-y) a_l^*(w_x) a_l^*(w_y) a_l(u_y) a_l(u_x) \, \mathrm{d}x \, \mathrm{d}y \\ &- \int_{\mathbb{R}^6} K_R^S(x-y) a_{x,l}^* a_l^*(w_y) a_l(u_y) a_l(u_x) \, \mathrm{d}x \, \mathrm{d}y \\ &- \int_{\mathbb{R}^6} K_R^S(x-y) a_l^*(w_x) a_{y,l}^* a_l(u_y) a_l(u_x) \, \mathrm{d}x \, \mathrm{d}y \\ =: &\, \mathsf{I}_1 + \mathsf{I}_2 + \mathsf{I}_3 + \mathsf{I}_4. \end{aligned}$$

To estimate I_1, we begin by observing that

$$(\mathsf{I}_1\Psi)^{(n,m)}(\underline{x}_n, \underline{y}_m) = \sum_{1\leq j<k\leq n} K_R^S(x_i - x_j)(\bar{u}^{(x_j)}\bar{u}^{(x_k)}\Psi^{(n,m)})(\underline{x}_n, \underline{y}_m),$$

where $u^{(x_j)}$ is the operator acting on the variable x_j and $\underline{x}_n = (x_1, \ldots, x_n)$. Defining $g(x,y) := \|\bar{u}^{(x)}\bar{u}^{(y)}\Psi^{(n,m)}(x,y,\ldots)\|_{L^2(\mathbb{R}^{3(n+m-2)})}$, it follows from the triangle inequality and the anti-symmetry of Ψ that

$$\|(\mathsf{I}_1\Psi)^{(n,m)}\|_{L^2} \leq n(n-1)\left(\iint_{|z|\leq R} \frac{|g(x+z,x)|^2}{|z|^{2a}}\,\mathrm{d}z\,\mathrm{d}x\right)^{1/2}$$
$$\leq n^2 R^{3/2-a}\left(\int_{\mathbb{R}^3}\left\|\frac{g_{R,x}(z)}{|z|^a}\right\|^2_{L^2_z(B_1)}\mathrm{d}x\right)^{1/2},$$

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

$$T_{B_1} : H^a(B_1) \to H^a(\mathbb{R}^3), \quad \forall x \in B_1, (T_{B_1}g)(x) = g(x),$$

which exists as proved for example in [20, Theorem IX.7] when $a \in \mathbb{N}$; one can proceed by interpolation when $a \in \mathbb{R}$. Then one has

$$\left\|\frac{g_{R,x}(z)}{|z|^a}\right\|_{L^2_z(B_1)} = \left\|\frac{T_{B_1}g_{R,x}(z)}{|z|^a}\right\|_{L^2_z(B_1)} \leq \left\|\frac{T_{B_1}g_{R,x}(z)}{|z|^a}\right\|_{L^2_z(\mathbb{R}^3)}$$

and by Hardy–Rellich's inequality

$$\left\|\frac{T_{B_1}g_{R,x}(z)}{|z|^a}\right\|_{L^2_z(\mathbb{R}^3)} \leq C\|(-\Delta)^{a/2}T_{B_1}g_{R,x}\|_{L^2(\mathbb{R}^3)} \leq C_{T_{B_1}}\|g_{R,x}\|_{H^a(B_1)}.$$

For I_1, this leads to

$$\|(\mathsf{I}_1\Psi)^{(n,m)}\|_{L^2} \leq Cn^2R^{3/2-a}\left(\iint_{|z|\leq 1}[|(-\Delta)^{a/2}g_{R,x}(z)|^2 + |g_{R,x}(z)|^2]\,\mathrm{d}x\,\mathrm{d}z\right)^{1/2}$$
$$\leq Cn^2\left(\iint_{|z|\leq R}[|(-\Delta)_z^{a/2}g|^2 + |R^{-a}g|^2]\,\mathrm{d}z\,\mathrm{d}x\right)^{1/2}.$$

Now by Hölder's inequality and by Sobolev's embedding, for any $\alpha > 0$ and any $f \in H^\alpha$,

$$\int_{|z|\leq R}|f(z)|^2\,\mathrm{d}z \leq \|f\|^2_{L^{2p'}}\|\mathbb{1}_{B_R}\|_{L^p} \leq CR^{2\alpha}\|(-\Delta)^{\alpha/2}f\|^2_{L^2}$$

with $p = \frac{3}{2\alpha}$. In particular, taking $f = (-\Delta)_z^{a/2}g$, $\alpha = 3/2-a$, $f = R^{-a}g$ and $\alpha = 3/2$ we obtain

$$\|(\mathsf{I}_1\Psi)^{(n,m)}\|_{L^2} \leq Cn^2R^{3/2-a}\|(-\Delta)_x^{3/4}g\|_{L^2}.$$

Using $\|u\|_\infty \leq 1$, we can control the L^2 norm on the right-hand side of the above inequality by

$$\|(-\Delta)_x^{3/4}g\|_{L^2} = \left\|\left(\bar{u}^{(y)}(-\Delta)_x^{3/4}\bar{u}^{(x)}\Psi^{(n,m)}\right)(x,y,\ldots)\right\|_{L^2(\mathbb{R}^{3(n+m)})}$$
$$\leq \left\|\left((-\Delta)^{3/4}\bar{u}\right)^{(x)}\Psi^{(n,m)}(x,\ldots)\right\|_{L^2(\mathbb{R}^{3(n+m)})}$$

and using the fact that $\bar{u} = 1 - \bar{w}$, we finally obtain

$$\|\mathsf{I}_1\Psi\|_{\mathscr{G}} \leq \frac{C}{N} R^{3/2-a}\big(\|\Psi\|_{\dot{\mathcal{H}}_2^{3/2}} + \||\boldsymbol{p}|^{\frac{3}{2}} w\|_2\|\Psi\|_{\mathscr{G}_2}\big).$$

The other I_i terms are less singular and treated in the same way, leading to

$$\|\mathsf{U}_t^{(0)*}\mathsf{D}_{1,R}^S\mathsf{U}_t^{(0)}\Psi\|_{\mathscr{G}} \leq C_T R^{3/2-a}(\|\mathcal{N}\Psi\|_{\dot{\mathcal{H}}_2^{3/2}} + \|\Psi\|_{\mathscr{G}_2}).$$

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. ∎

Finally, let us handle type IV terms.

Lemma A.9. *Under the conditions of Proposition A.1, there exists a constant C_T depending on the initial conditions such that for any $(t,s) \in [0,T]^2$,*

$$\|(\mathrm{IV}_t - \mathrm{IV}_s)\Psi\|_{\mathscr{G}} \leq C_T|t-s|^{\frac{3-2a}{7}}(\|\Psi\|_{\mathcal{H}_2^1} + \|\Psi\|_{\mathscr{G}_2}).$$

Proof. For this case, it suffices to consider

$$\begin{aligned} J_1 &= -\int_{\mathbb{R}^3} \mathrm{d}\Gamma_{l,r}^+(u\delta_x v)\mathrm{d}\Gamma_l(u[K_x,u])\,\mathrm{d}x, \\ J_{12} &= -\int_{\mathbb{R}^3} \mathrm{d}\Gamma_{l,r}^+([K_x,u]v + [v,K_x]u)\mathrm{d}\Gamma_l(\omega_x)\,\mathrm{d}x. \end{aligned}$$

Following the same routine as before, we decompose the operators into a long-range part and a singular part using (197). Again, we will denote the decomposition by $J_{1,R}^L + J_{1,R}^S$ and likewise for J_{12}. Applying Lemma A.5, we can now rewrite $J_{1,R}^L$ as

$$\mathsf{U}_t^{(0)*}J_{1,R}^L\mathsf{U}_t^{(0)} = \int_{\mathbb{R}^3} \widehat{K_R^L}(y)\mathrm{d}\Gamma_{l,r}^+(u_I e^{-iy\cdot(x-2it\nabla)}v_I)\mathrm{d}\Gamma_l(u_I[e^{-iy\cdot(x-2it\nabla)},w_I])\,\mathrm{d}y.$$

Since

$$\begin{aligned} i\partial_t(u_I[e^{-iy\cdot(x-2it\nabla)},w_I]) &= e^{-it\Delta}([V_{\boldsymbol{\rho}} - \mathsf{X}_{\boldsymbol{\rho}},u][e^{-iy\cdot x},w])e^{it\Delta} \\ &\quad + e^{-it\Delta}\big(u\big[[e^{iy\cdot x},-\Delta],w\big] + u\big[e^{-iy\cdot x},[V_{\boldsymbol{\rho}} - \mathsf{X}_{\boldsymbol{\rho}},w]\big]\big)e^{it\Delta} \end{aligned}$$

by Lemma 8.1 we have, since $\|u\|_\infty \leq 1$ and $\|w\|_\infty \leq 1$, the estimates

$$\|\mathrm{d}\Gamma_l(u_I[e^{-iy\cdot(x-2it\nabla)},w_I])\Psi\|_{\mathscr{G}} \leq 2\|\Psi\|_{\mathscr{G}_1}, \tag{203a}$$

$$\big\|\mathrm{d}\Gamma_l\big(\partial_t(u_I[e^{-iy\cdot(x-2it\nabla)},w_I])\big)\Psi\big\|_{\mathscr{G}} \leq \mathscr{C}_T\langle y\rangle^2\|\langle\boldsymbol{p}\rangle^2 w\|_2\|\Psi\|_{\mathscr{G}_1}, \tag{203b}$$

where $\mathscr{C}_T = C\sup_{[0,T]}(1 + \|V_{\boldsymbol{\rho}}\|_\infty + \|\mathsf{X}_{\boldsymbol{\rho}}\|_\infty)$. In particular, by (198), (203), and (199), we have

$$\left\|\frac{\mathrm{d}}{\mathrm{d}t}\mathsf{U}_t^{(0)*}J_{1,R}^L\mathsf{U}_t^{(0)}\Psi\right\|_{\mathscr{G}} \leq C_T R^{-(a+2)}\|\Psi\|_{\mathscr{G}_1}.$$

The singular part follows from Lemma 10.4 and Remark 10.5. More precisely,

$$\|\mathsf{U}_t^{(0)*} J_{1,R}^S \mathsf{U}_t^{(0)} \Psi\|_{\mathscr{G}} \le C_T R^{3/2-a} \|\Psi\|_{\mathscr{G}_1}. \tag{204}$$

Repeating the argument for $\tilde{\mathsf{Q}}_1$ 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

$$\mathsf{U}_t^{(0)*} J_{12} \mathsf{U}_t^{(0)} = \int_{\mathbb{R}^3} \mathrm{d}\Gamma_{l,r}^+([K_{x,I}, w_I]v_I)\mathrm{d}\Gamma_l(\omega_{x,I})\,\mathrm{d}x \tag{205a}$$

$$+ \int_{\mathbb{R}^3} \mathrm{d}\Gamma_{l,r}^+([K_{x,I}, v_I]u_I)\mathrm{d}\Gamma_l(\omega_{x,I})\,\mathrm{d}x. \tag{205b}$$

It suffices to handle (205b) since (205a) can be treated in a similar manner. Taking its time derivative yields

$$\begin{aligned} i\partial_t(205\text{b}) &= \int_{\mathbb{R}^3} \mathrm{d}\Gamma_{l,r}^+(i\partial_t([K_{x,I}, v_I]u_I))\mathrm{d}\Gamma_l(\omega_{x,I})\,\mathrm{d}x \\ &\quad + \int_{\mathbb{R}^3} \mathrm{d}\Gamma_{l,r}^+([K_{x,I}, v_I]u_I)\mathrm{d}\Gamma_l(i\partial_t\omega_{x,I})\,\mathrm{d}x =: \mathsf{I}_5 + \mathsf{I}_6. \end{aligned}$$

Let us first consider I_6. Notice that

$$i\partial_t\omega_{x,I} = e^{-it\Delta}(2\nabla_1\omega_x \cdot \nabla_1 + \Delta_2\omega_x + [V_{\boldsymbol{\rho}} - \mathsf{X}_{\boldsymbol{\rho}}, \omega]_x)e^{it\Delta}.$$

In particular, we can write

$$\begin{aligned} \mathsf{I}_6 &= \mathsf{U}_t^{(0)*} \int_{\mathbb{R}^3} \mathrm{d}\Gamma_{l,r}^+([K_x, v]u)\mathrm{d}\Gamma_l(2\nabla_1\omega_x \cdot \nabla)\,\mathrm{d}x\,\mathsf{U}_t^{(0)} \\ &\quad + \mathsf{U}_t^{(0)*} \int_{\mathbb{R}^3} \mathrm{d}\Gamma_{l,r}^+([K_x, v]u)\mathrm{d}\Gamma_l(\Delta_x\omega_x)\,\mathrm{d}x\,\mathsf{U}_t^{(0)} \\ &\quad + \mathsf{U}_t^{(0)*} \int_{\mathbb{R}^3} \mathrm{d}\Gamma_{l,r}^+([K_x, v]u)\mathrm{d}\Gamma_l([V_{\boldsymbol{\rho}} - \mathsf{X}_{\boldsymbol{\rho}}, \omega]_x)\,\mathrm{d}x\,\mathsf{U}_t^{(0)} \\ &=: \mathsf{J}_1 + \mathsf{J}_2 + \mathsf{J}_3. \end{aligned}$$

To bound J_1, it suffices to estimate the quantity

$$\left\| \int_{\mathbb{R}^3} ([K_x, v]u)(z_1, z_2)\nabla_1\omega(x_n, x) \cdot \nabla\Psi^{(n,m)}(\underline{x}_{n-1}, x_n, \underline{y}_n)\,\mathrm{d}x \right\|_{L^2(\mathrm{d}\underline{z}_2\,\mathrm{d}\underline{x}_n\,\mathrm{d}\underline{y}_n)}, \tag{206}$$

where $\mathrm{d}\underline{x}_n = \mathrm{d}x_1 \ldots \mathrm{d}x_n$ and $\mathrm{d}\underline{z}_2 = \mathrm{d}z_1\,\mathrm{d}z_2$. Let us also break the commutator, that is,

$$\begin{aligned} (206) \le &\left\| \int_{\mathbb{R}^6} \frac{v(z_1, z)u(z, z_2)}{|x - z_1|^a} \nabla_1\omega(x_n, x) \cdot \nabla\Psi^{(n,m)}(\underline{x}_{n-1}, x_n, \underline{y}_n)\,\mathrm{d}x\,\mathrm{d}z \right\|_{L^2(\mathrm{d}\underline{z}_2\,\mathrm{d}\underline{x}_n\,\mathrm{d}\underline{y}_n)} \\ &+ \left\| \int_{\mathbb{R}^6} \frac{v(z_1, z)u(z, z_2)}{|x - z|^a} \nabla_1\omega(x_n, x) \cdot \nabla\Psi^{(n,m)}(\underline{x}_{n-1}, x_n, \underline{y}_n)\,\mathrm{d}x\,\mathrm{d}z \right\|_{L^2(\mathrm{d}\underline{z}_2\,\mathrm{d}\underline{x}_n\,\mathrm{d}\underline{y}_n)}. \end{aligned}$$

Since $u = 1 - w$ where w is a Hilbert–Schmidt operator, we will focus on the identity part. Using $\omega = v^2$ and the Cauchy–Schwarz inequality, we see that

$$\begin{aligned}
&\left\| \int_{\mathbb{R}^3} \frac{v(z_1, z_2)}{|x - z_1|^a} \nabla_1 \omega(x_n, x) \cdot \nabla_{x_n} \Psi^{(n,m)}(\underline{x}_{n-1}, x_n, \underline{y}_n)\, \mathrm{d}x \right\|_{L^2(\mathrm{d}\underline{z}_2\, \mathrm{d}\underline{x}_n\, \mathrm{d}\underline{y}_n)} \\
&= \left\| \int_{\mathbb{R}^6} \frac{v(z, x)}{|x - z_1|^a} v(z_1, z_2) \nabla_1 v(x_n, z) \cdot \nabla_{x_n} \Psi^{(n,m)}(\underline{x}_{n-1}, x_n, \underline{y}_n)\, \mathrm{d}x\, \mathrm{d}z \right\|_{L^2(\mathrm{d}\underline{z}_2\, \mathrm{d}\underline{x}_n\, \mathrm{d}\underline{y}_n)} \\
&\leq \sup_{z_1} \left(\int_{\mathbb{R}^3} \frac{\rho(x)^{1/2}}{|x - z_1|^a}\, \mathrm{d}x \right) \|v\|_2 \|\nabla_1 v\|_{L^\infty_x L^2_z} \|\nabla \Psi^{(n)}\|_{L^2(\mathrm{d}\underline{x}_n\, \mathrm{d}\underline{y}_n)},
\end{aligned}$$

since $\|v_x\|_{L^2} = \rho(x)^{1/2}$. Note that by Young's and Hölder's inequalities,

$$\int_{\mathbb{R}^3} \frac{\rho(x)^{1/2}}{|x - z_1|^a}\, \mathrm{d}x \leq C \|\rho^{1/2}\|_{L^{\frac{3}{3-a}}} \leq C \int_{\mathbb{R}^3} \rho(x) \langle x \rangle^k\, \mathrm{d}x$$

provided $k > 3 - 2a$. Hence,

$$\|\mathsf{J}_1 \Psi\|_{\mathcal{G}} \leq C_T (\|\Psi\|_{\mathcal{H}^1_2} + \|\Psi\|_{\mathcal{G}_2}).$$

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 $\|\mathsf{X}_{\boldsymbol{\rho}}\|_{L^\infty_x L^2_y} \leq C \|\boldsymbol{\rho} |\boldsymbol{p}|^{2+a}\|_2$ are bounded. Thus,

$$\|\mathsf{I}_6 \Psi\|_{\mathcal{G}} \leq C_T (\|\Psi\|_{\mathcal{H}^1_2} + \|\Psi\|_{\mathcal{G}_2}).$$

Lastly, we handle the I_5 term. Since

$$\begin{aligned}
i \partial_t ([K_{x,I}, v_I] u_I) &= e^{-it\Delta} ([K_x, v][V_{\boldsymbol{\rho}} - \mathsf{X}_{\boldsymbol{\rho}}, u]) e^{it\Delta} \\
&\quad + e^{-it\Delta} \big(\big[[\Delta, K_x], v\big] u + \big[K_x, [V_{\boldsymbol{\rho}} - \mathsf{X}_{\boldsymbol{\rho}}, v]\big] u \big) e^{it\Delta},
\end{aligned}$$

we can write

$$\begin{aligned}
\mathsf{I}_5 &= \mathsf{U}_t^{(0)*} \int_{\mathbb{R}^3} \mathrm{d}\Gamma^+_{l,r}([K_x, v][-V_{\boldsymbol{\rho}} + \mathsf{X}_{\boldsymbol{\rho}}, w]) \mathrm{d}\Gamma_l(\omega_x)\, \mathrm{d}x\, \mathsf{U}_t^{(0)} \\
&\quad + \mathsf{U}_t^{(0)*} \int_{\mathbb{R}^3} \mathrm{d}\Gamma^+_{l,r}\big(\big[K_x, [V_{\boldsymbol{\rho}} - \mathsf{X}_{\boldsymbol{\rho}}, v]\big] u\big) \mathrm{d}\Gamma_l(\omega_x)\, \mathrm{d}x\, \mathsf{U}_t^{(0)} \\
&\quad + \mathsf{U}_t^{(0)*} \int_{\mathbb{R}^3} \mathrm{d}\Gamma^+_{l,r}([[\Delta, K_x], v] u) \mathrm{d}\Gamma_l(\omega_x)\, \mathrm{d}x\, \mathsf{U}_t^{(0)} \\
&=: \mathsf{J}_4 + \mathsf{J}_5 + \mathsf{J}_6.
\end{aligned}$$

The terms 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. Thus, it suffices to estimate J_6.

To do so, it suffices to estimate the quantity

$$\left\| \int_{\mathbb{R}^3} [\Delta K_x + 2 \nabla K_x \cdot \nabla, v](z_1, z_2) \omega(x_n, x) \Psi^{(n,m)}(\underline{x}_{n-1}, x_n, \underline{y}_n)\, \mathrm{d}x \right\|_{L^2(\mathrm{d}\underline{z}_2\, \mathrm{d}\underline{x}_n\, \mathrm{d}\underline{y}_n)}. \tag{207}$$

In the case $a = 1$, we have

$$(207) \leq C \left\| \int_{\mathbb{R}^3} (v\delta_x)(z_1, z_2)\omega(x_n, x)\Psi^{(n,m)}(\underline{x}_{n-1}, x_n, \underline{y}_n)\,\mathrm{d}x \right\|_{L^2(\mathrm{d}\underline{z}_2\,\mathrm{d}\underline{x}_n\,\mathrm{d}\underline{y}_n)}$$

$$+ C \left\| \int_{\mathbb{R}^3} \frac{x - z_1}{|x - z_1|^3} \cdot \nabla_1 v(z_1, z_2)\omega(x_n, x)\Psi^{(n,m)}(\underline{x}_{n-1}, x_n, \underline{y}_n)\,\mathrm{d}x \right\|_{L^2(\mathrm{d}\underline{z}_2\,\mathrm{d}\underline{x}_n\,\mathrm{d}\underline{y}_n)}.$$

For the first term, we have

$$\|v(z_1, z_2)\omega(x_n, z_2)\Psi^{(n,m)}(\underline{x}_{n-1}, x_n, \underline{y}_n)\|_{L^2(\mathrm{d}\underline{z}_2\,\mathrm{d}\underline{x}_n\,\mathrm{d}\underline{y}_n)}$$
$$\leq \|v\|_{L^\infty_x L^2_y}\|\omega\|_{L^\infty_x L^2_y}\|\Psi^{(n)}\|_{L^2(\mathrm{d}\underline{x}_n\,\mathrm{d}\underline{y}_n)} \leq C\|\rho\|^{1/2}_{L^\infty}\big\|\omega|\boldsymbol{p}|^2\big\|_2\|\Psi^{(n)}\|_{L^2(\mathrm{d}\underline{x}_n\,\mathrm{d}\underline{y}_n)}.$$

For the second term, we have

$$\left\| \int_{\mathbb{R}^3} \frac{x - z_1}{|x - z_1|^3} \cdot \nabla_1 v(z_1, z_2)\omega(x_n, x)\Psi^{(n,m)}(\underline{x}_{n-1}, x_n, \underline{y}_n)\,\mathrm{d}x \right\|_{L^2(\mathrm{d}\underline{z}_2\,\mathrm{d}\underline{x}_n\,\mathrm{d}\underline{y}_n)}$$
$$\leq C \sup_{z_1}\left(\int_{\mathbb{R}^3} \frac{\rho(x)^{1/2}}{|x - z_1|^2}\,\mathrm{d}x\right)\|\rho\|^{1/2}_{L^\infty}\|\nabla_1 v\|_2\|\Psi^{(n)}\|_{L^2(\mathrm{d}\underline{x}_n\,\mathrm{d}\underline{y}_n)}.$$

where the first integral term is controlled by $\|\rho\|^{1/2}_{L^\infty} + \|\rho\|^{1/2}_{L^1}$. 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

$$\|\mathsf{I}_5\Psi\|_{\mathscr{G}} \leq C_T\|\Psi\|_{\mathscr{G}_2},$$

which completes the proof. ■

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