# Pickl's Proof of the Quantum Mean-Field Limit and Quantum Klimontovich Solutions

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# PICKL'S PROOF OF THE QUANTUM MEAN-FIELD LIMIT AND QUANTUM KLIMONTOVICH SOLUTIONS

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Abstract. This paper discusses the mean-field limit for the quantum dynamics of $N$ identical bosons in $\mathbf{R}^3$ interacting via a binary potential with Coulomb type singularity. Our approach is based on the theory of quantum Klimontovich solutions defined in [F. Golse, T. Paul, Commun. Math. Phys. **369** (2019), 1021–1053]. Our first main result is a definition of the interaction nonlinearity in the equation governing the dynamics of quantum Klimontovich solutions for a class of interaction potentials slightly less general than those considered in [T. Kato, Trans. Amer. Math. Soc. **70** (1951), 195–211]. Our second main result is a new operator inequality satisfied by the quantum Klimontovich solution in the case of an interaction potential with Coulomb type singularity. When evaluated on an initial bosonic pure state, this operator inequality reduces to a Gronwall inequality for a functional introduced in [P. Pickl, Lett. Math. Phys. **97** (2011), 151–164], resulting in a convergence rate estimate for the quantum mean-field limit leading to the time-dependent Hartree equation.

## 1. Introduction and Notation

In classical mechanics, the motion equations for a system of $N$ identical point particles of mass $m$ with positions $q_j(t) \in \mathbf{R}^3$ and momenta $p_j(t) \in \mathbf{R}^3$ for all $j = 1, \ldots, N$ is

$$\left\{\begin{aligned} &\dot{q}_j(t) = \tfrac{1}{m} p_j(t) = \nabla_{p_j} H_N(p_1(t), \ldots, q_N(t)), \\ &\dot{p}_j(t) = -\sum_{\substack{k=1 \\ k\neq j}}^{N} \nabla V(q_j(t) - q_k(t)) = -\nabla_{p_j} H_N(p_1(t), \ldots, q_N(t)), \end{aligned}\right. \tag{1}$$

where the $N$-particle classical Hamiltonian is

$$H_N(p_1, \ldots, q_N) := \sum_{j=1}^{N} \tfrac{1}{2m} |p_j|^2 + \sum_{1\leq j<k\leq N} V(q_j - q_k).$$

Assuming that $V \in C^{1,1}(\mathbf{R}^3)$, this differential system has a unique global solution for all initial data. If $V$ is even[1], the phase space empirical measure

$$\mu_N(t, dxd\xi) := \tfrac{1}{N} \sum_{j=1}^{N} \delta_{q_j(t/N), p_j(t/N)}(dxd\xi), \qquad Nm = 1, \tag{2}$$

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[1] In this case, the exclusion $j \neq k$ in the right-hand side of Newton's second law for $\dot{p}_j(t)$ is useless since $V$ even $\implies \nabla V(0) = 0$.

is an *exact*, weak solution of the Vlasov equation

$$\partial_t \mu_N + \xi \cdot \nabla_x \mu_N - \nabla_x (V \star \mu_N(t)) \cdot \nabla_\xi \mu_N = 0 \tag{3}$$

with self-consistent, mean-field potential

$$V \star_{x,\xi} \mu_N(t,x) = \frac{1}{N} \sum_{k=1}^{N} V(x - q_k(t))$$

This remarkable observation is due to Klimontovich, and solutions of the Vlasov equation (3) of the form (2) are referred to as “Klimontovich solutions”. Thus, if $\mu_N(0) \to f^{in} dx d\xi$ weakly in the sense of probability measures as $N \to \infty$, where $f^{in}$ is a probability density on $\mathbf{R}^3_x \times \mathbf{R}^3_\xi$, one has

$$\mu_N(t, dx d\xi) \to f(t,x,\xi) dx d\xi \text{ weakly in the sense of probability measures}$$

for all $t \geq 0$ as $N \to \infty$, where $f$ is the solution of the Vlasov equation

$$\partial_t f + \xi \cdot \nabla_x f - \nabla_x (V \star_{x,\xi} f(t,\cdot,\cdot)) \cdot \nabla_\xi f = 0\,, \qquad f\big|_{t=0} = f^{in}\,. \tag{4}$$

Thus, the mean-field limit in classical mechanics is equivalent to the continuous dependence for the weak topology of probability measures of solutions of the Vlasov equation in terms of their initial data. See [4] for a proof of this result. For instance, the weak convergence of the initial data can be realized by a random choice of $(q_j(0), p_j(0))$, independent and identically distributed with distribution $f^{in}$.

The mean-field limit for bosonic systems in quantum mechanics has been formulated in different settings, by using the so-called BBGKY hierarchy [20, 2, 1, 6], or in the second quantization setting [18]. Interestingly, these techniques allow considering singular potentials such as the Coulomb potential, instead of $C^{1,1}$ potentials as in the classical case. (The mean-field limit with Coulomb potentials in classical mechanics is still an open problem at the time of this writing; see however [19] in the special case of monokinetic particle distributions. See also [9, 10] for potentials less singular than the Coulomb potential).

The quantum mean-field equation analogous to the Vlasov equation (4) is the (time-dependent) Hartree equation

$$i\hbar \partial_t \psi(t,x) = -\tfrac{1}{2}\hbar^2 \Delta_x \psi(t,x) + (V \star |\psi(t,\cdot)|^2)(x) \psi(t,x) = 0\,, \qquad \psi\big|_{t=0} = \psi^{in}\,. \tag{5}$$

In [16, 14], an original method, close to the second quantization approach in [18], but avoiding the rather heavy formalism of Fock spaces, was proposed and successfully applied to singular potentials including the Coulomb potential.

All these approaches noticeably differ from the classical setting used in [4] for lack of a quantum notion of phase-space empirical measures. However, a quantum analogue of the notion of phase-space empirical measure was recently proposed in [8], along with an equation analogous to (3) governing their evolution. This notion was used in [8] to prove the uniformity of the mean-field limit in the Planck constant $\hbar > 0$. However, the discussion in [8] only considers regular potentials (specifically $\partial^\alpha V \in \mathcal{F}L^1(\mathbf{R}^d)$ for $|\alpha| \leq 3 + [d/2]$). Even writing the equation analogous to (3) satisfied by the quantum analogue of the phase-space empirical measure requires $V \in \mathcal{F}L^1(\mathbf{R}^d)$ in the setting of [8].

The purpose of the present paper is twofold:

(a) to extend the formalism of quantum empirical measures considered in [8] to treat the case of singular potentials including the Coulomb potential, which is of particular interest for applications to atomic physics, and

(b) to explain how the ideas in [16, 14] can be couched in terms of the formalism of quantum empirical measures defined in [8].

Specifically, we prove an inequality *between operators* on the $N$-particle Hilbert space, of which the key estimates in [16, 14] leading to the quantum mean-field limit are straightforward consequences.

The next section briefly recalls only the essential part of [8] used in the sequel. The main results obtained in the present paper are then stated in section 4. The proofs of these results are given in the subsequent sections.

## 2. Quantum Klimontovich Solutions

Consider the quantum $N$-body Hamiltonian

$$\mathcal{H}_N := \sum_{j=1}^{N} -\tfrac{1}{2}\hbar^2\Delta_{x_j} + \tfrac{1}{N}\sum_{1\le j<k\le N} V(x_j - x_k) \tag{6}$$

on $\mathfrak{H}_N := \mathfrak{H}^{\otimes N} \simeq L^2(\mathbf{R}^{3N})$, where $\mathfrak{H} := L^2(\mathbf{R}^3)$. Henceforth it is assumed that $V$ is a real-valued function such that $\mathcal{H}_N$ has a (unique) self-adjoint extension to $\mathfrak{H}_N$, still denoted $\mathcal{H}_N$. A well-known sufficient condition for this to be true has been found by Kato (see condition (5) in [12]): there exists $R > 0$ such that

$$\int_{|z|\le R} V(z)^2 dz + \operatorname{esssup}_{|z|>R} |V(z)| < \infty\,. \tag{7}$$

In particular, these conditions include the (repulsive) Coulomb potential in $\mathbf{R}^3$. In fact, $\mathcal{H}_N$ has a self-adjoint extension to $\mathfrak{H}_N$ under a condition slightly more general than Kato's original assumption recalled above:

$$V \in L^2(\mathbf{R}^3) + L^\infty(\mathbf{R}^3) \tag{8}$$

(see Theorem X.16 and Example 2 in [17], and Theorem V.9 with $m = 1$ in [15]).

In the sequel, we adopt the notation in [8]. In particular, we set

$$J_k A := I_{\mathfrak{H}}^{\otimes(k-1)} \otimes A \otimes I_{\mathfrak{H}}^{\otimes(N-k)}\,, \quad 1 \le n \le N\,, \tag{9}$$

and

$$\mathcal{M}_N^{in} := \tfrac{1}{N}\sum_{k=1}^{N} J_k \in \mathcal{L}(\mathcal{L}(\mathfrak{H}), \mathcal{L}(\mathfrak{H}_N))\,. \tag{10}$$

The dynamics of the morphism $\mathcal{M}_N^{in}$ is defined by conjugation with the $N$-particle dynamics as follows: for each $A \in \mathcal{L}(\mathfrak{H})$,

$$\mathcal{M}_N(t)A := \mathcal{U}_N(t)^*(\mathcal{M}_N^{in}A)\mathcal{U}_N(t)\,, \quad \text{with } \mathcal{U}_N(t) := \exp(-it\mathcal{H}_N/\hbar)\,. \tag{11}$$

Since $\mathcal{H}_N$ is self-adjoint, $t \mapsto \mathcal{U}_N(t)$ is a unitary group by Stone's theorem. The time-dependent morphism $t \mapsto \mathcal{M}_N(t) \in \mathcal{L}(\mathcal{L}(\mathfrak{H}), \mathcal{L}(\mathfrak{H}_N))$ is henceforth referred to as *the quantum Klimontovich solution.*

Assume henceforth that $V$ is even:

$$V(x) = V(-x)\,, \qquad x \in \mathbf{R}^d\,. \tag{12}$$

The first main result in [8] (Theorem 3.3) is that, if $\hat{V} \in L^1(\mathbf{R}^d)$, the quantum Klimontovich solution $\mathcal{M}_N(t)$ satisfies

$$i\hbar\partial_t\mathcal{M}_N(t) = \mathbf{ad}^*(K)\mathcal{M}_N(t) - \mathcal{C}(V, \mathcal{M}_N(t), \mathcal{M}_N(t))\,, \tag{13}$$

where $K=-\frac{1}{2}\hbar^2\Delta$ is the quantum kinetic energy, and where

$$(\mathbf{ad}^*(T)\Lambda)A:=-\Lambda([T,A])\tag{14}$$

for each unbounded self-adjoint operator $T$ on $\mathfrak{H}$, each $A\in\mathcal{L}(\mathfrak{H})$ satisfying the condition $[T,A]\in\mathcal{L}(\mathfrak{H})$, and each $\Lambda\in\mathcal{L}(\mathcal{L}(\mathfrak{H}),\mathcal{L}(\mathfrak{H}_N))$. Moreover

$$\mathcal{C}(V,\Lambda_1,\Lambda_2)(A):=\tfrac{1}{(2\pi)^d}\int_{\mathbf{R}^d}\hat{V}(\omega)((\Lambda_1E_\omega^*)\Lambda_2(E_\omega A)-\Lambda_2(AE_\omega)(\Lambda_1E_\omega^*))d\omega\tag{15}$$

for each $A\in\mathcal{L}(\mathfrak{H})$ and each $\Lambda_1,\Lambda_2\in\mathcal{L}(\mathcal{L}(\mathfrak{H}),\mathcal{L}(\mathfrak{H}_N))$, where $E_\omega\in\mathcal{L}(\mathfrak{H})$ is the operator defined by

$$(E_\omega\phi)(x):=e^{i\omega\cdot x}\phi(x)\quad\text{ for each }\phi\in\mathfrak{H}\text{ and }\omega\in\mathbf{R}^d\,.\tag{16}$$

Since the integrand of the right-hand side of (15) takes its values in the non separable space $\mathcal{L}(\mathfrak{H}_N)$, it is worth mentioning that this integral is a weak integral for the ultraweak topology in $\mathcal{L}(\mathfrak{H}_N)$ (see footnote 3 on p. 1032 in [8]).

At variance with the classical case recalled in (3), the differential equation (13) satisfied by the quantum Klimontovich solution $t\mapsto\mathcal{M}_N(t)$ is not formally identical to the mean-field, time-dependent Hartree equation (5). The relation between (5) and (13) is explained in Theorem 3.5, the second main result in [8], recalled below.

If $\psi$ is a solution of the the time-dependent Hartree equation (5) satisfying the normalization condition

$$\|\psi(t,\cdot)\|_{\mathfrak{H}}=1\qquad\text{for all }t\in\mathbf{R}\,,$$

the time-dependent morphism $t\mapsto\mathcal{R}(t)\in\mathcal{L}(\mathcal{L}(\mathfrak{H}),\mathcal{L}(\mathfrak{H}_N))$ defined by the formula[2]

$$\mathcal{R}(t)A:=\langle\psi(t,\cdot)|A|\psi(t,\cdot)\rangle I_{\mathfrak{H}_N}$$

is a solution of (13).

## 3. Extending the Definition of $\mathcal{C}(V,\mathcal{M}_N(t),\mathcal{M}_N(t))$ when $V\notin\mathcal{F}L^1(\mathbf{R}^3)$

Our first task is to extend the definition (15) of the term $\mathcal{C}(V,\mathcal{M}_N(t),\mathcal{M}_N(t))$ to a more general class of potentials $V$, including the Coulomb potential in $\mathbf{R}^3$.

Since

$$\begin{aligned}&\mathcal{M}_N(t)(E_\omega^*)\mathcal{M}_N(t)(E_\omega|\phi\rangle\langle\phi|)-\mathcal{M}_N(t)(|\phi\rangle\langle\phi|E_\omega)\mathcal{M}_N(t)(E_\omega^*)\\&=\mathcal{U}_N(t)^*(\mathcal{M}_N^{in}(E_\omega^*)\mathcal{M}_N^{in}(E_\omega|\phi\rangle\langle\phi|)-\mathcal{M}_N^{in}(|\phi\rangle\langle\phi|E_\omega)\mathcal{M}_N^{in}(E_\omega^*))\mathcal{U}_N(t)\,,\end{aligned}$$

the idea is to define

$$\begin{aligned}&\langle\Phi_N^{in}|\mathcal{C}(V,\mathcal{M}_N(t),\mathcal{M}_N(t))(|\phi\rangle\langle\phi|)|\Psi_N^{in}\rangle\\&:=\tfrac{1}{(2\pi)^3}\int_{\mathbf{R}^3}\hat{V}(\omega)\langle\mathcal{U}_N(t)\Phi_N^{in}|S_N[\phi](\omega)|\mathcal{U}_N(t)\Psi_N^{in}\rangle d\omega\end{aligned}$$

for all $\Phi_N,\Psi_N^{in}\in\mathfrak{H}_N$, where

$$S_N[\phi](\omega):=\mathcal{M}_N^{in}(E_\omega^*)\mathcal{M}_N^{in}(E_\omega|\phi\rangle\langle\phi|)-\mathcal{M}_N^{in}(|\phi\rangle\langle\phi|E_\omega)\mathcal{M}_N^{in}(E_\omega^*)$$

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[2]Throughout this paper, we adopt the Dirac bra-ket notation. Thus a wave function $\psi\in\mathfrak{H}$ viewed as a vector of the linear space $\mathfrak{H}$ is denoted $|\psi\rangle$, whereas $\langle\psi|$ designates the linear functional

$$\langle\psi|:\ \mathfrak{H}\ni\phi\mapsto\int_{\mathbf{R}^d}\overline{\psi(x)}\phi(x)dx\in\mathbf{C}\,.$$

If $A\in\mathcal{L}(\mathfrak{H})$, we denote

$$\langle\psi|A|\phi\rangle:=\int_{\mathbf{R}^d}\overline{\psi(x)}(A\phi)(x)dx$$

and $\langle\psi|\phi\rangle:=\langle\psi|I_{\mathfrak{H}}|\phi\rangle$ is the inner product on $\mathfrak{H}$.

and to take advantage of the decay of $S_N[\phi]$ in $\omega$, assuming that $\phi$ is regular enough. Our argument does not use any regularity on $\Phi_N^{in}$ or $\Psi_N^{in}$. This is quite natural, since anyway Kato's condition (8) on the interaction potential $V$ does not entail higher than (Sobolev) $H^2$ regularity for $\mathcal{U}_N(t)\Phi_N^{in}$ or $\mathcal{U}_N(t)\Psi_N^{in}$, as observed in Note V.10 of [15].

Our first main result in this paper is the following result, leading to a definition of $\mathcal{C}(V,\mathcal{M}_N(t),\mathcal{M}_N(t))(|\phi\rangle\langle\phi|)$ in the case of singular, Coulomb-like potentials $V$, and for bounded wave functions $\phi$. This theorem can be regarded as an extension to the case of singular, Coulomb like potentials $V$ of the formalism of quantum Klimontovich solutions in [8].

**Theorem 3.1.** *Assume that $V$ is a real-valued measurable function on $\mathbf{R}^3$ satisfying the parity condition* (12)*, and*

$$V \in L^2(\mathbf{R}^3) + \mathcal{F}L^1(\mathbf{R}^3)\,. \tag{17}$$

*For each $\phi \in L^2 \cap L^\infty(\mathbf{R}^3)$ and each $\Psi_N \in \mathfrak{H}_N$, the function*

$$\omega \mapsto \langle \Psi_N | S_N[\phi](\omega) | \Psi_N \rangle \text{ belongs to } L^2 \cap L^\infty(\mathbf{R}^3)\,.$$

*The interaction operator $\mathcal{C}(V,\mathcal{M}_N(t),\mathcal{M}_N(t))(|\phi\rangle\langle\phi|)$ is defined by the formula*

$$\mathcal{C}(V,\mathcal{M}_N(t),\mathcal{M}_N(t))(|\phi\rangle\langle\phi|) := \tfrac{1}{(2\pi)^3}\int_{\mathbf{R}^3} \hat{V}(\omega)\mathcal{U}_N(t)^* S_N[\phi](\omega)\mathcal{U}_N(t)d\omega$$

*The integral on the right-hand side of the equality above is to be understood as a weak integral and defines*

$$t \mapsto \mathcal{C}(V,\mathcal{M}_N(t),\mathcal{M}_N(t))(|\phi\rangle\langle\phi|)$$

*as a continuous map from $\mathbf{R}$ to $\mathcal{L}(\mathfrak{H}_N)$ endowed with the ultraweak topology, which is moreover bounded on $\mathbf{R}$ for the operator norm on $\mathcal{L}(\mathfrak{H}_N)$.*

Obviously, condition (17) is stronger than Kato's condition (8). In particular, $\mathcal{H}_N$ has a self-adjoint extension to $\mathfrak{H}_N$ under condition (17)

*Proof.* Assuming that $\Psi_N^{in} \in \mathfrak{H}_N$, one has

$$\mathcal{U}_N(t)\Psi_N^{in} \in \mathfrak{H}_N \text{ with } \|\mathcal{U}_N(t)\Psi_N^{in}\|_{\mathfrak{H}_N} = \|\Psi_N^{in}\|_{\mathfrak{H}_N}\,.$$

Therefore, we henceforth forget the time dependence in $\Psi_N(t,\cdot) = \mathcal{U}_N(t)\Psi_N^{in}$, which will be henceforth denoted $\Psi_N \equiv \Psi_N(x_1,\dots,x_N)$.

Observe first that

$$S_N[\phi](\omega) = \tfrac{1}{N^2}\sum_{1\le k\ne l\le N} \left(J_k(E_\omega^*)J_l(E_\omega|\phi\rangle\langle\phi|) - J_l(|\phi\rangle\langle\phi|E_\omega)J_k(E_\omega^*)\right)$$

since

$$\begin{aligned}J_k(E_\omega^*)J_k(E_\omega|\phi\rangle\langle\phi|) &- J_k(|\phi\rangle\langle\phi|E_\omega)J_k(E_\omega^*)\\ &= J_k(E_\omega^*E_\omega|\phi\rangle\langle\phi|) - J_k(|\phi\rangle\langle\phi|E_\omega E_\omega^*)\\ &= J_k(|\phi\rangle\langle\phi|) - J_k(|\phi\rangle\langle\phi|) = 0\,.\end{aligned}$$

Without loss of generality, consider the term

$$\begin{aligned}\langle \Psi_N | J_1(E_\omega^*)J_2(E_\omega|\phi\rangle\langle\phi|)|\Psi_N\rangle &= \int_{\mathbf{R}^6} e^{-i\omega\cdot(x_1-x_2)}\phi(x_2)\\ \times\left(\int_{\mathbf{R}^{3N-6}} \overline{\Psi_N(x_1,x_2,Z)}\left(\int_{\mathbf{R}^3}\Psi_N(x_1,y_2,Z)\overline{\phi(y_2)}dy_2\right)dZ\right)&dx_1dx_2\\ &= \hat{F}(-\omega)\end{aligned}$$

where

$$F(X) := \int_{\mathbf{R}^3} \phi(X+x_1) f(x_1, x_1+X, x_1) dx_1 \, ,$$

with the notation

$$f(x_1,x_2,y_1) := \int_{\mathbf{R}^{3N-6}} \overline{\Psi_N(x_1,x_2,Z)} \left( \int_{\mathbf{R}^3} \Psi_N(y_1,y_2,Z) \overline{\phi(y_2)} dy_2 \right) dZ \, .$$

We shall prove that $F \in L^1(\mathbf{R}^3) \cap L^2(\mathbf{R}^3)$, so that $\hat{F} \in L^2(\mathbf{R}^3) \cap C_0(\mathbf{R}^3)$.

First

$$\begin{aligned}
\int_{\mathbf{R}^3} |F(X)| dX &\le \int_{\mathbf{R}^6} |\phi(X+x_1)||f(x_1,x_1+X,x_1)| dx_1 dX \\
&= \int_{\mathbf{R}^3} \left( \int_{\mathbf{R}^3} |\phi(x_2)||f(x_1,x_2,x_1)| dx_2 \right) dx_2 \\
&\le \int_{\mathbf{R}^{3N-3}} \left( \int_{\mathbf{R}^3} |\phi(x_2)||\Psi_N(x_1,x_2,Z)| dx_2 \right) \\
&\qquad \times \left( \int_{\mathbf{R}^3} |\Psi_N(x_1,y_2,Z)||\phi(y_2)| dy_2 \right) dZ dx_1 \\
&= \int_{\mathbf{R}^{3N-3}} \left( \int_{\mathbf{R}^3} |\phi(x_2)||\Psi_N(x_1,x_2,Z)| dx_2 \right)^2 dZ dx_1 \\
&\le \|\phi\|^2_{L^2(\mathbf{R}^3)} \int_{\mathbf{R}^{3N-3}} \int_{\mathbf{R}^3} |\Psi_N(x_1,x_2,Z)|^2 dx_2 dZ dx_1 \\
&= \|\phi\|^2_{L^2(\mathbf{R}^3)} \|\Psi_N\|^2_{L^2(\mathbf{R}^{3N})} < \infty \, .
\end{aligned}$$

where the last inequality is the Cauchy-Schwarz inequality for the inner integral.

On the other hand

$$\int_{\mathbf{R}^3} |F(X)|^2 dX \le \|\phi\|^2_{L^\infty(\mathbf{R}^3)} \int_{\mathbf{R}^3} \left( \int_{\mathbf{R}^3} |f(x_1,x_1+X,x_1)| dx_1 \right)^2 dX \, ,$$

and

$$\int_{\mathbf{R}^3} |f(x_1,x_1+X,x_1)| dx_1 \le \int_{\mathbf{R}^{3N-3}} |\Psi_N(x_1,x_1+X,Z)| \Phi_N(x_1,Z) dZ dx_1 \, ,$$

with

$$\Phi(x_1,Z) := \int_{\mathbf{R}^3} |\Psi_N(x_1,y_2,Z)||\phi(y_2)| dy_2 \, ,$$

so that

$$\Phi_N(x_1,Z_N)^2 \le \|\phi\|^2_{L^2(\mathbf{R}^3)} \int_{\mathbf{R}^3} |\Psi_N(x_1,y_2,Z)|^2 dy_2 \, ,$$

and

$$\begin{aligned}
\int_{\mathbf{R}^{3N-3}} \Phi_N(x_1,Z)^2 dZ dx_1 &\le \|\phi\|^2_{L^2(\mathbf{R}^3)} \int_{\mathbf{R}^3} |\Psi_N(x_1,y_2,Z)|^2 dx_1 dy_2 dZ \\
&= \|\phi\|^2_{L^2(\mathbf{R}^3)} \|\Psi_N\|^2_{L^2(\mathbf{R}^{3N})} \, .
\end{aligned}$$

Hence

$$\begin{aligned}
\left( \int_{\mathbf{R}^3} |f(x_1,x_1+X,x_1)| dx_1 \right)^2 &\le \left( \int_{\mathbf{R}^{3N-3}} |\Psi_N(x_1,x_1+X,Z)| \Phi_N(x_1,Z) dZ dx_1 \right)^2 \\
&\le \int_{\mathbf{R}^{3N-3}} |\Psi_N(x_1,x_1+X,Z)|^2 dZ dx_1 \int_{\mathbf{R}^{3N-3}} \Phi_N(x_1,Z)^2 dZ dx_1 \\
&\le \int_{\mathbf{R}^{3N-3}} |\Psi_N(x_1,x_1+X,Z)|^2 dZ dx_1 \|\phi\|^2_{L^2(\mathbf{R}^3)} \|\Psi_N\|^2_{L^2(\mathbf{R}^{3N})} \, ,
\end{aligned}$$

so that

$$\begin{aligned}&\int_{\mathbf{R}^3}\left(\int_{\mathbf{R}^3}|f(x_1,x_1+X,x_1)|dx_1\right)^2dX\\ \le\|\phi\|^2_{L^2(\mathbf{R}^3)}\|\Psi_N\|^2_{L^2(\mathbf{R}^{3N})}&\int_{\mathbf{R}^3}\int_{\mathbf{R}^{3N-3}}|\Psi_N(x_1,x_1+X,Z)|^2dZdx_1dX\\ =\|\phi\|^2_{L^2(\mathbf{R}^3)}\|\Psi_N\|^2_{L^2(\mathbf{R}^{3N})}&\int_{\mathbf{R}^3}\int_{\mathbf{R}^{3N-3}}|\Psi_N(x_1,x_2,Z)|^2dZdx_1dx_2\\ &=\|\phi\|^2_{L^2(\mathbf{R}^3)}\|\Psi_N\|^4_{L^2(\mathbf{R}^{3N})}\,.\end{aligned}$$

Therefore

$$\int_{\mathbf{R}^3}|F(X)|^2dX\le\|\phi\|^2_{L^\infty(\mathbf{R}^3)}\|\phi\|^2_{L^2(\mathbf{R}^3)}\|\Psi_N\|^4_{L^2(\mathbf{R}^{3N})}<\infty$$

so that $\omega\mapsto\hat F(-\omega)$ belongs to $L^2(\mathbf{R}^d)$ by Plancherel's theorem. Hence, for each $k\ne l\in\{1,\dots,N\}$, one has

$$\hat V\in L^1(\mathbf{R}^d)+L^2(\mathbf{R}^d)\implies\begin{cases}\int_{\mathbf{R}^3}|\hat V(\omega)||\langle\Psi_N|J_k(E^*_\omega)J_l(E_\omega|\phi\rangle\langle\phi|)|\Psi_N\rangle|d\omega<\infty\,,\\ \int_{\mathbf{R}^3}|\hat V(\omega)||\langle\Psi_N|J_l(|\phi\rangle\langle\phi|E_\omega)J_k(E^*_\omega)|\Psi_N\rangle|d\omega<\infty\,.\end{cases}$$

Hence

$$(t,\omega)\mapsto\hat V(\omega)\langle\mathcal{U}_N(t)\Psi_N^{in}|S_N[\phi](\omega)|\mathcal{U}_N(t)\Psi_N^{in}\rangle\text{ belongs to }C_b(\mathbf{R}_t,L^1(\mathbf{R}^3_\omega))\,.$$

Since $S_N[\phi](\omega)^*=-S_N[\phi](\omega)\in\mathcal{L}(\mathfrak{H}_N)$ for each $\omega\in\mathbf{R}^3$ and $\hat V$ is even because of (12), the formula

$$\begin{aligned}&\langle\Psi_N^{in}|\mathcal{C}(V,\mathcal{M}_N(t),\mathcal{M}_N(t))(|\phi\rangle\langle\phi|)|\Psi_N^{in}\rangle\\ :=\tfrac{1}{(2\pi)^3}&\int_{\mathbf{R}^3}\hat V(\omega)\langle\mathcal{U}_N(t)^*\Psi_N^{in}|S_N[\phi](\omega)|\mathcal{U}_N(t)^*\Psi_N^{in}\rangle d\omega\end{aligned}$$

defines

$$\mathcal{C}(V,\mathcal{M}_N(t),\mathcal{M}_N(t))(|\phi\rangle\langle\phi|)=-\mathcal{C}(V,\mathcal{M}_N(t),\mathcal{M}_N(t))(|\phi\rangle\langle\phi|)^*\in\mathcal{L}(\mathfrak{H}_N)$$

for each $t\in\mathbf{R}$ by polarization, and the function

$$t\mapsto\mathcal{C}(V,\mathcal{M}_N(t),\mathcal{M}_N(t))$$

is bounded on $\mathbf{R}$ with values in $\mathcal{L}(\mathfrak{H}_N)$ for the norm topology, and continuous on $\mathbf{R}$ with values in $\mathcal{L}(\mathfrak{H}_N)$ endowed with the weak operator topology, and therefore for the ultraweak topology (since the weak operator and the ultraweak topologies coincide on norm bounded subsets of $\mathcal{L}(\mathfrak{H}_N)$). □

**Remark.** In the sequel, we shall also need to consider terms of the form

$$\begin{aligned}(I)&:=\tfrac{1}{(2\pi)^3}\int_{\mathbf{R}^3}\hat V(\omega)\langle\Psi_N|J_1(E^*_\omega|\phi\rangle\langle\phi|)J_2(E_\omega|\phi\rangle\langle\phi|)|\Psi_N\rangle d\omega\\ (II)&:=\tfrac{1}{(2\pi)^3}\int_{\mathbf{R}^3}\hat V(\omega)\langle\Psi_N|J_1(|\phi\rangle\langle\phi|E^*_\omega)J_2(E_\omega|\phi\rangle\langle\phi|)|\Psi_N\rangle d\omega\\ (III)&:=\tfrac{1}{(2\pi)^3}\int_{\mathbf{R}^3}\hat V(\omega)\langle\Psi_N|J_1(|\phi\rangle\langle\phi|E^*_\omega|\phi\rangle\langle\phi|)J_2(AE_\omega B)|\Psi_N\rangle d\omega\end{aligned}$$

where $A,B\in\mathcal{L}(\mathfrak{H})$.

The term (III) is the easiest of all. Indeed,

$$\begin{aligned}(III) =&\frac{1}{(2\pi)^3}\int_{\mathbf{R}^3}\hat V(\omega)\widehat{|\phi|^2}(\omega)\langle\Psi_N|J_1(|\phi\rangle\langle\phi|)J_2(AE_\omega B)|\Psi_N\rangle d\omega\\ =&\langle\Psi_N|J_1(|\phi\rangle\langle\phi|)J_2(A(V\star|\phi|^2)B)|\Psi_N\rangle\end{aligned}$$

and since $V\in L^2(\mathbf{R}^3)+C_b(\mathbf{R}^3)$ while $\phi\in L^1\cap L^\infty(\mathbf{R}^3)$, one has $V\star|\phi|^2\in C_b(\mathbf{R}^3)$, so that $A(V\star|\phi|^2)B\in\mathcal{L}(\mathfrak{H})$.

The terms (I) and (II) are slightly more delicate, but can be treated by the same method already used in the proof of the theorem above. First,

$$\langle\Psi_N|J_1(E^*_\omega|\phi\rangle\langle\phi|)J_2(E_\omega|\phi\rangle\langle\phi|)|\Psi_N\rangle=\hat F_1(\omega)\,,$$

with

$$\begin{aligned}F_1(Y)&:=\int_{\mathbf{R}^{3N-6}}A_1(Y,Z)A_2(Z)dZ\,,\\ A_1(Y,Z)&:=\int_{\mathbf{R}^3}\phi(X+\tfrac{Y}{2})\phi(X-\tfrac{Y}{2})\overline{\Psi_N(X+\tfrac{Y}{2},X-\tfrac{Y}{2},Z)}dX\,,\\ A_2(Z)&:=\int_{\mathbf{R}^6}\Psi_N(y_1,y_2,Z)\overline{\phi(y_1)\phi(y_2)}dy_1dy_2\,,\end{aligned}$$

so that

$$(I)=\frac{1}{(2\pi)^3}\int_{\mathbf{R}^3}\hat V(\omega)\hat F_1(\omega)d\omega\,.$$

Then

$$\begin{aligned}&\left(\int_{\mathbf{R}^3}|F_1(Y)|dY\right)^2\\ &\le\|A_2\|^2_{L^2(\mathbf{R}^{3N-6})}\int_{\mathbf{R}^{3N-6}}\left(\int_{\mathbf{R}^3}|A_1(Y,Z)|dY\right)^2dZ\le\|A_2\|^2_{L^2(\mathbf{R}^{3N-6})}\\ &\times\int_{\mathbf{R}^{3N-6}}\left(\int_{\mathbf{R}^6}|\phi(X+\tfrac{Y}{2})||\phi(X-\tfrac{Y}{2})||\Psi_N(X+\tfrac{Y}{2},X-\tfrac{Y}{2},Z)|dXdY\right)^2dZ\\ &\le\|A_2\|^2_{L^2(\mathbf{R}^{3N-6})}\int_{\mathbf{R}^6}|\phi(X+\tfrac{Y}{2})|^2|\phi(X-\tfrac{Y}{2})|^2dXdY\\ &\times\int_{\mathbf{R}^{3N}}|\Psi_N(X+\tfrac{Y}{2},X-\tfrac{Y}{2},Z)|^2dXdYdZ\\ &=\|A_2\|^2_{L^2(\mathbf{R}^{3N-6})}\int_{\mathbf{R}^6}|\phi(x_1)|^2|\phi(x_2)|^2dx_1dx_2\\ &\times\int_{\mathbf{R}^{3N}}|\Psi_N(x_1,x_2,Z)|^2dx_1dx_2dZ\\ &=\|A_2\|^2_{L^2(\mathbf{R}^{3N-6})}\|\phi\|^4_{L^2(\mathbf{R}^3)}\|\Psi_N\|^2_{\mathfrak{H}_N}\,.\end{aligned}$$

Besides

$$\begin{aligned}\|A_2\|^2_{L^2(\mathbf{R}^{3N-6})}\le&\int_{\mathbf{R}^6}|\phi(y_1)|^2|\phi(y_2)|^2dy_1dy_2\int_{\mathbf{R}^{3N-6}}|\Psi_N(y_1,y_2,Z)|^2dy_1dy_2dZ\\ =&\|\phi\|^4_{L^2(\mathbf{R}^3)}\|\Psi_N\|^2_{\mathfrak{H}_N}\,,\end{aligned}$$

so that

$$\|F_1\|_{L^1(\mathbf{R}^3)}\le\|\phi\|^4_{L^2(\mathbf{R}^3)}\|\Psi_N\|^2_{\mathfrak{H}_N}<\infty\,.$$

On the other hand

$$\int_{\mathbf{R}^3}|F_1(Y)|^2dY\le\|A_2\|^2_{L^2(\mathbf{R}^{3N-6})}\|A_1\|^2_{L^2(\mathbf{R}^{3N-3})}\,,$$

where

$$\begin{aligned}\|A_1\|^2_{L^2(\mathbf{R}^{3N-3})} \le &\sup_{Y\in\mathbf{R}^3}\int_{\mathbf{R}^3}|\phi(X+\tfrac{Y}{2})|^2|\phi(X-\tfrac{Y}{2})|^2dX\\ &\times\int_{\mathbf{R}^{3N}}|\Psi_N(X+\tfrac{Y}{2},X-\tfrac{Y}{2},Z)|^2dXdYdZ\\ \le&\|\phi\|^4_{L^4(\mathbf{R}^3)}\|\Psi_N\|^2_{\mathfrak{H}_N}\,,\end{aligned}$$

so that

$$\int_{\mathbf{R}^3}|F_1(Y)|^2dY \le \|\phi\|^4_{L^4(\mathbf{R}^3)}\|\phi\|^4_{L^2(\mathbf{R}^3)}\|\Psi_N\|^4_{\mathfrak{H}_N}<\infty\,.$$

Thus, we have proved that $F_1\in L^1\cap L^2(\mathbf{R}^d)$, and since $\hat V\in L^2(\mathbf{R}^d)+L^1(\mathbf{R}^d)$, the product $\hat V\hat F\in L^1(\mathbf{R}^d)$, which leads to a definition of (I).

The case of (II) is essentially similar. Observe that

$$\langle\Psi_N|J_1(|\phi\rangle\langle\phi|E^*_\omega)J_2(E_\omega|\phi\rangle\langle\phi|)|\Psi_N\rangle = \int_{\mathbf{R}^{3N-6}}\hat F_2(\omega,Z)\hat F_3(\omega,Z)dZ\,,$$

where

$$\begin{aligned}F_2(y_1,Z):=&\overline{\phi(y_1)}\int_{\mathbf{R}^3}\overline{\phi(y_2)}\Psi_N(y_1,y_2,Z)dy_2\\ F_3(x_2,Z):=&\phi(x_2)\int_{\mathbf{R}^3}\phi(x_1)\overline{\Psi_N(x_1,x_2,Z)}dx_1\,.\end{aligned}$$

And

$$(II):=\frac{1}{(2\pi)^3}\int_{\mathbf{R}^3}\hat V(\omega)\left(\int_{\mathbf{R}^{3N-6}}\hat F_2(\omega,Z)\hat F_3(\omega,Z)dZ\right)d\omega\,.$$

Observe that

$$\begin{aligned}\left(\int|F_2(y_1,Z)|dy_1\right)^2\le&\left(\int_{\mathbf{R}^6}|\phi(y_1)||\phi(y_2)||\Psi_N(y_1,y_2,Z)|dy_1dy_2\right)^2\\ \le&\|\phi\|^4_{L^2(\mathbf{R}^3)}\int_{\mathbf{R}^6}|\Psi_N(y_1,y_2,Z)|^2dy_1dy_2\,,\end{aligned}$$

so that

$$\begin{aligned}&\sup_{\omega\in\mathbf{R}^3}\left|\int_{\mathbf{R}^{3N-6}}\hat F_2(\omega,Z)\hat F_3(\omega,Z)dZ\right|^2\\ &\le\left(\int_{\mathbf{R}^{3N-6}}\sup_{\omega\in\mathbf{R}^3}|\hat F_2(\omega,Z)|\sup_{\omega\in\mathbf{R}^3}|\hat F_3(\omega,Z)|dZ\right)^2\\ &\le\int_{\mathbf{R}^{3N-6}}\sup_{\omega\in\mathbf{R}^3}|\hat F_2(\omega,Z)|^2dZ\int_{\mathbf{R}^{3N-6}}\sup_{\omega\in\mathbf{R}^3}|\hat F_3(\omega,Z)|^2dZ\\ &\le\int_{\mathbf{R}^{3N-6}}\left(\int|F_2(y_1,Z)|dy_1\right)^2dZ\int_{\mathbf{R}^{3N-6}}\left(\int|F_3(x_2,Z)|dx_2\right)^2dZ\\ &\le\|\phi\|^8_{L^2(\mathbf{R}^3)}\|\Psi_N\|^4_{\mathfrak{H}_N}\,,\end{aligned}$$

while

$$\int_{\mathbf{R}^{3N-6}}\left(\int|F_2(y_1,Z)|dy_1\right)^2dZ\le\|\phi\|^4_{L^2(\mathbf{R}^3)}\|\Psi_N\|^2_{\mathfrak{H}_N}\,,$$

with a similar conclusion for $F_3$. On the other hand

$$\begin{aligned}\int_{\mathbf{R}^3}|F_2(y_1,Z)|^2dy_1\le&\int_{\mathbf{R}^3}|\phi(y_1)|^2\left(\int_{\mathbf{R}^3}\overline{\phi(y_2)}\Psi_N(y_1,y_2,Z)dy_2\right)^2dy_1\\ \le&\|\phi\|^2_{L^2(\mathbf{R}^3)}\int_{\mathbf{R}^3}|\phi(y_1)|^2\left(\int_{\mathbf{R}^3}|\Psi_N(y_1,y_2,Z)|^2dy_2\right)dy_1\\ \le&\|\phi\|^2_{L^2(\mathbf{R}^3)}\|\phi\|^2_{L^\infty(\mathbf{R}^3)}\int_{\mathbf{R}^6}|\Psi_N(y_1,y_2,Z)|^2dy_1dy_2\,,\end{aligned}$$

so that

$$\begin{aligned}
&\int_{\mathbf{R}^3}\left|\int_{\mathbf{R}^{3N-6}}\hat{F}_2(\omega,Z)\hat{F}_3(\omega,Z)dZ\right|^2 d\omega\\
&\le\int_{\mathbf{R}^3}\int_{\mathbf{R}^{3N-6}}|\hat{F}_2(\omega,Z)|^2\left(\int_{\mathbf{R}^{3N-6}}|\hat{F}_3(\omega,Z)|^2dZ\right)dZd\omega\\
&\le\sup_{\omega\in\mathbf{R}^3}\int_{\mathbf{R}^{3N-6}}|\hat{F}_3(\omega,Z)|^2dZ\int_{\mathbf{R}^{3N-6}}\int_{\mathbf{R}^3}|\hat{F}_2(\omega,Z)|^2dZd\omega\\
&\le\int_{\mathbf{R}^{3N-6}}\sup_{\omega\in\mathbf{R}^3}|\hat{F}_3(\omega,Z)|^2dZ\int_{\mathbf{R}^{3N-6}}(2\pi)^3\left(\int_{\mathbf{R}^3}|F_2(y_1,Z)|^2dy_1\right)dZ\\
&\le(2\pi)^3\int_{\mathbf{R}^{3N-6}}\left(\int_{\mathbf{R}^3}|\hat{F}_3(x_2,Z)|dx_2\right)^2dZ\int_{\mathbf{R}^{3N-6}}\int_{\mathbf{R}^3}|F_2(y_1,Z)|^2dy_1dZ\\
&\le(2\pi)^3\|\phi\|^6_{L^2(\mathbf{R}^3)}\|\phi\|^2_{L^\infty(\mathbf{R}^3)}\|\Psi_N\|^4_{\mathfrak{H}_N}\,.
\end{aligned}$$

Therefore the map

$$\omega\mapsto\int_{\mathbf{R}^{3N-6}}\hat{F}_2(\omega,Z)\hat{F}_3(\omega,Z)dZ$$

belongs to $L^2\cap L^\infty(\mathbf{R}^3)$. Since $\hat{V}\in L^2(\mathbf{R}^3)+L^1(\mathbf{R}^3)$, this implies that

$$\omega\mapsto\hat{V}\int_{\mathbf{R}^{3N-6}}\hat{F}_2(\omega,Z)\hat{F}_3(\omega,Z)dZ$$

belongs to $L^1(\mathbf{R}^3)$, thereby leading to a definition of (II).

## 4. An Operator Inequality. Application to the Mean-Field Limit

First consider the Cauchy problem for the time dependent Hartree equation (5). Assuming that the potential $V$ satisfies (8) and (12), for each $\phi^{in}\in H^2(\mathbf{R}^3)$, there exists a unique solution $\phi\in C(\mathbf{R},H^2(\mathbf{R}^3))$ of (5) by Theorems 1.4 and 1.3 of [11].

Pickl's key idea in his proof of the mean-field limit in quantum mechanics is to consider the following functional (see Definition 2.2 and formula (6) in [16], with the choice $n(k):=k/N$, in the notation of [16]):

$$\alpha_N(\Psi_N,\psi):=\langle\Psi_N|\mathcal{M}_N^{in}(I_{\mathfrak{H}}-|\psi\rangle\langle\psi|)|\Psi_N\rangle$$

for all $\Psi_N\in\mathfrak{H}_N$ and $\psi\in\mathfrak{H}$.

Assuming that $\psi\equiv\psi(t,x)$ is a solution of (5) while $\Psi_N(t,\cdot):=\mathcal{U}_N(t)\Psi_N^{in}$, Pickl studies in section 2.1 of [16] the time-dependent function $t\mapsto\alpha_N(\Psi_N(t,\cdot),\psi(t,\cdot))$, and proves that it satisfies some Gronwall inequality.

Observe first that Pickl's functional $\alpha_N(\Psi_N(t,\cdot),\psi(t,\cdot))$ can be recast in terms of the quantum Klimontovich solution $\mathcal{M}_N(t)$ as follows

$$\begin{aligned}
\alpha_N(\mathcal{U}_N(t)\Psi_N^{in},\psi(t,\cdot))&=\langle\mathcal{U}_N(t)\Psi_N^{in}|\mathcal{M}_N^{in}(I_{\mathfrak{H}}-|\psi(t,\cdot)\rangle\langle\psi(t,\cdot)|)\mathcal{U}_N(t)|\Psi_N^{in}\rangle\\
&=\langle\Psi_N^{in}|\mathcal{U}_N(t)\left(\mathcal{M}_N^{in}(I_{\mathfrak{H}}-|\psi(t,\cdot)\rangle\langle\psi(t,\cdot)|)\right)\mathcal{U}_N(t)|\Psi_N^{in}\rangle\\
&=\langle\Psi_N^{in}|\mathcal{M}_N(t)(I_{\mathfrak{H}}-|\psi(t,\cdot)\rangle\langle\psi(t,\cdot)|)|\Psi_N^{in}\rangle\,.
\end{aligned}\tag{18}$$

This identity suggests therefore to deduce from (13) and (5) the expression of

$$\tfrac{d}{dt}\mathcal{M}_N(t)(I_{\mathfrak{H}}-|\psi(t,\cdot)\rangle\langle\psi(t,\cdot)|)$$

in terms of the interaction operator $\mathcal{C}$ defined in (15).

This is done in the first part of the next theorem, which is our second main result in this paper.

**Theorem 4.1.** *Assume that the (real-valued) interaction potential $V$, viewed as an (unbounded) multiplication operator acting on $\mathfrak{H} := L^2(\mathbf{R}^3)$, satisfies the parity condition* (12) *and* (17).

*Let $\psi^{in} \in H^2(\mathbf{R}^3)$ satisfy $\|\psi^{in}\|_{\mathfrak{H}} = 1$, let $\psi$ be the solution of the Cauchy problem* (5) *for the time-dependent Hartree equation, and set*

$$R(t) := |\psi(t,\cdot)\rangle\langle\psi(t,\cdot)|\,, \qquad \text{and} \qquad P(t) := I_{\mathfrak{H}} - R(t)\,. \tag{19}$$

*Then*

*(1) the $N$-body quantum Klimontovich solution $t \mapsto \mathcal{M}_N(t)$ satisfies*

$$i\hbar\partial_t(\mathcal{M}_N(t)(P(t))) = \mathcal{C}(V, \mathcal{M}_N(t) - \mathcal{R}(t), \mathcal{M}_N(t))(R(t))\,,$$

*where*

$$\mathcal{R}(t)A := \langle\psi(t,\cdot)|A|\psi(t,\cdot)\rangle I_{\mathfrak{H}_N} = \operatorname{trace}_{\mathfrak{H}}(R(t)A)I_{\mathfrak{H}_N}\,;$$

*(2) the operator $\mathcal{C}(V, \mathcal{M}_N(t) - \mathcal{R}(t), \mathcal{M}_N(t))(P(t))$ is skew-adjoint on $\mathfrak{H}_N$ and satisfies the operator inequality*

$$\pm i\mathcal{C}(V, \mathcal{M}_N(t) - \mathcal{R}(t), \mathcal{M}_N(t))(R(t)) \le 6L(t)\left(\mathcal{M}_N(t)(P(t)) + \tfrac{2}{N} I_{\mathfrak{H}_N}\right)\,,$$

*where*[3]

$$L(t) := 2\max(1, C_S)\|V\|_{L^2(\mathbf{R}^3)+L^\infty(\mathbf{R}^3)}\|\psi(t,\cdot)\|_{H^2(\mathbf{R}^3)}\,, \tag{20}$$

*and where $C_S$ is the norm of the Sobolev embedding $H^2(\mathbf{R}^3) \subset L^\infty(\mathbf{R}^3)$.*

The operator inequality for quantum Klimontovich solutions in the case of potentials with Coulomb type singularity obtained in part (2) of Theorem 4.1 can be thought of as the reformulation of Pickl's argument in terms of the quantum Klimontovich solution $\mathcal{M}_N(t)$.

Indeed, we deduce from parts (1) and (2) in Theorem 4.1 the operator inequality

$$\tfrac{d}{dt}\mathcal{M}_N(t)(P(t)) \le \tfrac{6L(t)}{\hbar}\left(\mathcal{M}_N(t)(P(t)) + \tfrac{2}{N} I_{\mathfrak{H}_N}\right)\,. \tag{21}$$

Then, evaluating both sides of this inequality on the initial $N$-particle state $\Psi_N^{in}$, and taking into account the identity (18) leads to the Gronwall inequality

$$\tfrac{d}{dt}\alpha_N(\mathcal{U}_N(t)\Psi_N^{in}, \psi(t,\cdot)) \le \tfrac{6L(t)}{\hbar}\left(\alpha_N(\mathcal{U}_N(t)\Psi_N^{in}, \psi(t,\cdot)) + \tfrac{2}{N}\right)$$

satisfied by Pickl's functional $\alpha_N(\mathcal{U}_N(t)\Psi_N^{in}, \psi(t,\cdot))$. This last inequality corresponds to inequality (11) and Lemma 3.2 in [16].

In the sequel, we shall denote by $\mathcal{L}^p(\mathfrak{H})$ for $p \ge 1$ the Schatten two-sided ideal of $\mathcal{L}(\mathfrak{H})$ consisting of operators $T$ such that

$$\|T\|_p := \left(\operatorname{trace}_{\mathfrak{H}}((T^*T)^{p/2})\right)^{1/p} < \infty\,.$$

In particular $\mathcal{L}^1(\mathfrak{H})$ is set of trace-class operators on $\mathfrak{H}$ and $\|\cdot\|_1$ the trace norm, while $\mathcal{L}^2(\mathfrak{H})$ is set of Hilbert-Schmidt operators on $\mathfrak{H}$ and $\|\cdot\|_2$ the Hilbert-Schmidt norm.

---

[3] We recall that, if $E, F*$ are Banach spaces

$$\|v\|_{E\cap F} := \max(\|v\|_E, \|v\|_F)\,,$$

and

$$\|f\|_{L^p(\mathbf{R}^d)+L^q(\mathbf{R}^d)} = \inf\{\|f_1\|_{L^p(\mathbf{R}^d)} + \|f_2\|_{L^q(\mathbf{R}^d)} \text{ s.t. } f = f_1 + f_2 \text{ with } f_1 \in L^p(\mathbf{R}^d),\ f_2 \in L^q(\mathbf{R}^d)\}\,.$$

**Corollary 4.2.** *Under the same assumptions and with the same notations as in Theorem 4.1, consider the $N$-body wave function $\Psi_N(t,\cdot) := \mathcal{U}_N(t)(\psi^{in})^{\otimes N}$, and the $N$-body density operator $F_N(t) := |\Psi_N(t,\cdot)\rangle\langle\Psi_N(t,\cdot)|$. For each $m = 1,\dots,N$, the $m$-particle reduced density operator $F_{N:m}(t)$, defined by the identity*

$$\operatorname{trace}_{\mathfrak{H}_m}(F_{N:m}(t)A_1\otimes\ldots\otimes A_m) = \langle\Psi_N(t,\cdot)|A_1\otimes\ldots\otimes A_m\otimes I_{\mathfrak{H}_{N-m}}|\Psi_N(t,\cdot)\rangle$$

*for all $A_1,\dots,A_m\in\mathcal{L}(\mathfrak{H})$, satisfies*

$$\|F_{N:m}(t) - R(t)^{\otimes m}\|_1 \le 4\sqrt{\frac{m}{N}}\exp\left(\tfrac{3}{\hbar}\int_0^t L(s)ds\right),$$

*with $L$ given by* (20).

Let us briefly indicate how one arrives at the operator inequality in part (2) of Theorem 4.1. Let $\Lambda_1,\Lambda_2\in\mathcal{L}(\mathcal{L}(\mathfrak{H}),\mathcal{L}(\mathfrak{H}_N))$ be such that

$$\omega\mapsto\langle\Psi_N|\Lambda_1(E_\omega^*)\Lambda_2(E_\omega)|\Psi_N\rangle\text{belongs to } L^1\cap L^2(\mathbf{R}^3) \tag{22}$$

for all $\Psi_N\in\mathfrak{H}_N$. For all $V$ satisfying (12) and (17), define $\mathcal{T}(V,\Lambda_1,\Lambda_2)\in\mathcal{L}(\mathfrak{H}_N)$ by polarization of the formula

$$\langle\Psi_N|\mathcal{T}(V,\Lambda_1,\Lambda_2)|\Psi_N\rangle := \tfrac{1}{(2\pi)^d}\int_{\mathbf{R}^d}\hat{V}(\omega)\langle\Psi_N|\Lambda_1(E_\omega^*)\Lambda_2(E_\omega)|\Psi_N\rangle d\omega\,.$$

In other words,

$$\mathcal{T}(V,\Lambda_1,\Lambda_2) := \tfrac{1}{(2\pi)^d}\int_{\mathbf{R}^d}\hat{V}(\omega)\Lambda_1(E_\omega^*)\Lambda_2(E_\omega)d\omega \tag{23}$$

where the integral on the right hand is to be understood in the ultraweak sense (see footnote 3 on p. 1032 in [8]).

For each $A\in\mathcal{L}(\mathfrak{H})$, denote by $\Lambda_j(\bullet A)$ and $\Lambda_j(A\bullet)$ the linear maps

$$\Lambda_j(\bullet A):\mathcal{L}(\mathfrak{H})\ni B\mapsto\Lambda_j(BA)\in\mathcal{L}(\mathfrak{H}_N)$$
$$\Lambda_j(A\bullet):\mathcal{L}(\mathfrak{H})\ni B\mapsto\Lambda_j(AB)\in\mathcal{L}(\mathfrak{H}_N)$$

respectively. If $A\in\mathcal{L}(\mathfrak{H})$ is such that $\Lambda_1,\Lambda_2(\bullet A)$ and $\Lambda_2(A\bullet),\Lambda_1$ satisfy (22), then one has

$$\mathcal{C}(V,\Lambda_1,\Lambda_2)A = \mathcal{T}(V,\Lambda_1,\Lambda_2(\bullet A)) - \mathcal{T}(V,\Lambda_2(A\bullet),\Lambda_1)\,. \tag{24}$$

**Lemma 4.3.** *Let $\Lambda_1,\Lambda_2\in\mathcal{L}(\mathcal{L}(\mathfrak{H}),\mathcal{L}(\mathfrak{H}_N))$ be $*$-homomorphisms, in other words*

$$\Lambda_j(A^*) = \Lambda_j(A)^*\,,\qquad j=1,2$$

*for all $A\in\mathcal{L}(\mathfrak{H})$. Assume that $\Lambda_1,\Lambda_2$ satisfy* (22). *Then*

$$\mathcal{T}(V,\Lambda_2,\Lambda_1) = \mathcal{T}(V,\Lambda_1,\Lambda_2)^*\,.$$

*Proof.* Indeed

$$\begin{aligned}\mathcal{T}(V,\Lambda_2,\Lambda_1) &= \tfrac{1}{(2\pi)d}\int_{\mathbf{R}^d}\hat{V}(\omega)\Lambda_2(E_\omega^*)\Lambda_1(E_\omega)d\omega\\ &= \tfrac{1}{(2\pi)d}\int_{\mathbf{R}^d}\hat{V}(\omega)\Lambda_2(E_\omega)^*\Lambda_1(E_\omega^*)^*d\omega = \mathcal{T}(V,\Lambda_1,\Lambda_2)^*\end{aligned}$$

where the first equality follows from the fact that $\Lambda_1$ and $\Lambda_2$ are $^*$-homomorphisms, while the second equality uses the fact that $\hat{V}$ is real-valued, since $V$ is real-valued and even. □

An easy consequence of (24) and of this lemma is that, for each $A = A^* \in \mathcal{L}(\mathfrak{H})$ such that $\Lambda_1, \Lambda_2 \in \mathcal{L}(\mathcal{L}(\mathfrak{H}), \mathcal{L}(\mathfrak{H}_N))$ are $*$-homomorphisms such that $\Lambda_1, \Lambda_2(\bullet A)$ satisfy (22), then

$$(\mathcal{C}(V, \Lambda_1, \Lambda_2)A)^* = -\mathcal{C}(V, \Lambda_1, \Lambda_2)A\,. \tag{25}$$

The key observations leading to Theorem 4.1 are summarized in the two following lemmas. In the first of these two lemmas, the interaction operator is decomposed into a sum of four terms.

**Lemma 4.4.** *Under the same assumptions and with the same notations as in Theorem 4.1, the interaction operator satisfies the identity*

$$\mathcal{C}(V, \mathcal{M}_N(t) - \mathcal{R}(t), \mathcal{M}_N(t))(R(t)) = T_1 + T_2 + T_3 + T_4\,,$$

*with*

$$\begin{aligned}
T_1 :=& \mathcal{T}(V, \mathcal{M}_N(t)(P(t)\bullet P(t)), \mathcal{M}_N(t)(P(t)\bullet R(t)) \\
&- \mathcal{T}(V, \mathcal{M}_N(t)(R(t)\bullet P(t)), \mathcal{M}_N(t)(P(t)\bullet P(t))\,, \\
T_2 :=& \mathcal{M}_N(t)(R(t)V_{R(t)}P(t))\mathcal{M}_N(t)(P(t)) \\
&- \mathcal{M}_N(t)(P(t))\mathcal{M}_N(t)(P(t)V_{R(t)}R(t))\,, \\
T_3 :=& \mathcal{T}(V, \mathcal{M}_N(t)(P(t)\bullet R(t)), \mathcal{M}_N(t)(P(t)\bullet R(t)) \\
&- \mathcal{T}(V, \mathcal{M}_N(t)(R(t)\bullet P(t)), \mathcal{M}_N(t)(R(t)\bullet P(t))\,, \\
T_4 :=& \tfrac{1}{N}\mathcal{M}_N(t)[V_{R(t)}, R(t)]\,.
\end{aligned}$$

All the terms involved in this decomposition can be defined by the same method already used in the proof of Theorem 3.1. Indeed, one can check that all these terms involve only expressions of the type (I), (II) or (III) in the Remark following Theorem 3.1. This easy verification is left to the reader, and we shall henceforth consider this matter as settled by the detailed explanations concerning (I), (II) and (III) given in the previous section.

Each term in this decomposition satisfies an operator inequality involving only the operator norm of the "mean-field squared potential" $(V^2)_{R(t)}$, instead of the "bare" interaction potential $V$ itself.

**Lemma 4.5.** *Under the same assumptions and with the same notations as in Theorem 4.1, set*

$$\ell(t) := \|V^2 \star |\psi(t,\cdot)|^2\|^{\frac{1}{2}}\,. \tag{26}$$

*Then*

$$\begin{aligned}
\pm iT_1 \le& 2\ell(t)\left((1 - \tfrac{1}{N})\mathcal{M}_N(t)(P(t)) + \tfrac{4}{N}I_{\mathfrak{H}_N}\right)\,, \\
\pm iT_2 \le& 2\ell(t)(\mathcal{M}_N(t)(P(t)) + \tfrac{1}{N}I_{\mathfrak{H}_N})\,, \\
\pm iT_3 \le& 2\ell(t)((1 - \tfrac{1}{N})\mathcal{M}_N(t)(P(t)) + \tfrac{1}{N}I_{\mathfrak{H}_N})\,, \\
\pm iT_4 \le& \tfrac{2}{N}\ell(t)I_{\mathfrak{H}_N}\,.
\end{aligned}$$

**Remarks on $\ell(t)$ in (26) and $L(t)$ in (20).**

(1) If $V$ satisfies condition (17) in Theorem 3.1, then $V \in L^2(\mathbf{R}^3) + L^\infty(\mathbf{R}^3)$, so that $V^2 \in L^1(\mathbf{R}^d) + L^\infty(\mathbf{R}^d)$. Thus $(V^2)_{R(t)}$, which is the multiplication operator by the

function $V^2 \star |\psi(t,\cdot)|^2$, satisfies

$$\ell(t)^2 := \|V^2 \star |\psi(t,\cdot)|^2\|_{L^\infty(\mathbf{R}^3} \le \|V^2\|_{L^1(\mathbf{R}^3)+L^\infty(\mathbf{R}^3)}\|\psi(t,\cdot)\|^2_{L^1\cap L^\infty(\mathbf{R}^3)}$$
$$\le 2\|V\|^2_{L^1(\mathbf{R}^3)+L^\infty(\mathbf{R}^3)}\max(1,\|\psi(t,\cdot)\|_{L^\infty(\mathbf{R}^3)})^2$$
$$\le 2C_S^2\|V\|^2_{L^1(\mathbf{R}^3)+L^\infty(\mathbf{R}^3)}\|\psi(t,\cdot)\|^2_{H^2(\mathbf{R}^3)}$$

where we recall that $C_S$ is the norm of the Sobolev embedding $H^2(\mathbf{R}^3) \subset L^\infty(\mathbf{R}^3)$.
(2) If $V$ satisfies (8), then $\|V(I-\Delta)^{-1}\| \le M$ for some positive constant $M$ (see the discussion in §5.3 of chapter V in [13], so that

$$V^2 \le M^2(I-\Delta)^2\,.$$

In this remark, we shall make a slightly more restrictive assumption, namely that $V^2$ satisfies

$$V^2 \le C(I-\Delta)\,. \tag{27}$$

In space dimension $d=3$, the Hardy inequality, which can be put in the form[4]

$$\frac{1}{|x|^2} \le 4(-\Delta)$$

implies that the Coulomb potential satisfies the assumption above on $V$. If the potential $V$ satisfies the (operator) inequality (27), then

$$0 \le (V^2)_{R(t)}(x) = \int_{\mathbf{R}^d} V^2(y)|\psi(t,x-y)|^2dy = \langle\psi(t,x-\cdot)|V^2|\psi(t,x-\cdot)\rangle$$
$$\le C\langle\psi(t,x-\cdot)|(I-\Delta)|\psi(t,x-\cdot)\rangle = C\|\psi(t,x-\cdot)\|^2_{L^2} + C\|\nabla\psi(t,x-\cdot)\|^2_{L^2}$$
$$= C\|\psi(t,\cdot)\|^2_{L^2} + C\|\nabla\psi(t,\cdot)\|^2_{L^2}\,.$$

Thus, if $\psi \in C(\mathbf{R}; H^1(\mathbf{R}^d))$ is a solution of the Hartree equation,

$$\ell(t) \le \sqrt{C}\|\psi(t,\cdot)\|_{H^1(\mathbf{R}^3)}\,.$$

(3) A bound on $\ell(t)$ in terms of $\|\psi(t,\cdot)\|_{H^1(\mathbf{R}^3)}$ instead of $\|\psi(t,\cdot)\|_{H^2(\mathbf{R}^3)}$ is advantageous since the former quantity can be controlled rather explicitly by means of the conservation of energy for the Hartree equation (5). This explicit control is useful in particular to assess the dependence in $\hbar$ of the convergence rate for the mean-field limit obtained in Corollary (4.2).

Clearly, the convergence rate for the quantum mean-field limit in Corollary 4.2 is not uniform in the semiclassical regime, in the first place because of the factor $3/\hbar$ on the right hand side of the upper bound for $\|F_{N:m}(t) - R(t)^{\otimes m}\|_1$, which comes from the $i\hbar\partial_t$ part of the quantum dynamical equation.

However, one should expect that the function $\ell(t)$, or at least the upper bound for $\ell(t)$ obtained in (2), grows at least as $1/\hbar$, since it involves $\|\nabla_x\psi(t,\cdot)\|_{L^2}$, expected to be of order $1/\hbar$ for semiclassical wave functions $\psi$ (think for instance of a WKB wave function, or of a Schrödinger coherent state).

[4]To see that 4 is optimal, minimize in $\alpha > 0$ the expression

$$\int_{\mathbf{R}^3}\left|\nabla u + \alpha\frac{x}{|x|^2}u\right|^2 dx\,.$$

We shall discuss this issue by means of the conservation of energy satisfied by the Hartree solution $\psi$ (see formula (5.2) in [3]):

$$\begin{aligned}&\tfrac{1}{2}\hbar^2\|\nabla\psi(t,\cdot)\|_{L^2}^2+\tfrac{1}{2}\int_{\mathbf{R}^d}|\psi(t,x)|^2(V\star|\psi(t,x)|^2)dx\\&=\tfrac{1}{2}\hbar^2\|\nabla\psi^{in}\|_{L^2}^2+\tfrac{1}{2}\int_{\mathbf{R}^d}|\psi^{in}(x)|^2(V\star|\psi^{in}(x)|^2)dx\,.\end{aligned}$$

Observe that

$$|V\star|\psi(t,x)|^2|\le\|\psi(t,\cdot)\|_{L^2}(V^2\star|\psi(t,x)|^2)^{1/2}=\ell(t)\,,\tag{28}$$

so that

$$\begin{aligned}&\tfrac{1}{2}\hbar^2\|\nabla\psi^{in}\|_{L^2}^2+\tfrac{1}{2}\int_{\mathbf{R}^d}|\psi^{in}(x)|^2(V\star|\psi^{in}(x)|^2)dx\\&\le\tfrac{1}{2}\hbar^2\|\psi^{in}\|_{H^1}^2+\tfrac{1}{2}\ell(t)\le\tfrac{1}{2}\hbar^2\|\psi^{in}\|_{H^1}^2+\tfrac{1}{2}\sqrt{C}\|\psi^{in}\|_{H^1}\,.\end{aligned}$$

Thus, if $V\ge0$, or if $\hat{V}\ge0$, one has

$$\int_{\mathbf{R}^d}|\psi(t,x)|^2(V\star|\psi(t,x)|^2)dx=\tfrac{1}{(2\pi)^d}\int_{\mathbf{R}^d}\hat{V}(\omega)|\mathcal{F}(|\psi(t,\cdot)|^2)|^2(\omega)d\omega\ge0$$

(where $\mathcal{F}$ designates the Fourier transform on $\mathbf{R}^d$), so that the conservation of mass and energy for the Hartree solution implies that

$$\hbar^2\|\psi(t,\cdot)\|_{H^1}^2\le\hbar^2\|\psi^{in}\|_{H^1}^2+\sqrt{C}\|\psi^{in}\|_{H^1}\,.$$

In that case

$$\ell(t)\le\tfrac{1}{\hbar}\sqrt{C(\hbar^2\|\psi^{in}\|_{H^1}^2+\sqrt{C}\|\psi^{in}\|_{H^1})}\,.$$

Typical states used in the semiclassical regime (WKB or coherent states, for instance) satisfy $\hbar\|\nabla\psi^{in}\|_{L^2}=O(1)$. Thus, in that case

$$\ell(t)\le\hbar^{-3/2}\sqrt{C(\hbar^3\|\psi^{in}\|_{H^1}^2+\sqrt{C}\hbar\|\psi^{in}\|_{H^1})}=O(\hbar^{-3/2})\,.$$

Things become worse if the potential energy is a priori of indefinite sign. With (28), the energy conservation implies that

$$\begin{aligned}\hbar^2\|\psi(t,\cdot)\|_{H^1}^2&\le\hbar^2\|\psi^{in}\|_{H^1}^2+\sqrt{C}\|\psi^{in}\|_{H^1}+\sqrt{C}\|\psi(t,\cdot)\|_{H^1}\\&\le\hbar^2\|\psi^{in}\|_{H^1}^2+\sqrt{C}\|\psi^{in}\|_{H^1}+\tfrac{C}{2\hbar^2}+\tfrac{1}{2}\hbar^2\|\psi(t,\cdot)\|_{H^1}^2\,,\end{aligned}$$

so that

$$\hbar^2\|\psi(t,\cdot)\|_{H^1}^2\le2\left(\hbar^2\|\psi^{in}\|_{H^1}^2+\sqrt{C}\|\psi^{in}\|_{H^1}+\tfrac{C}{2\hbar^2}\right)\le3\hbar^2\|\psi^{in}\|_{H^1}^2+2\tfrac{C}{\hbar^2}\,,$$

and thus

$$\ell(t)\le\hbar^{-2}\sqrt{C(3\hbar^4\|\psi^{in}\|_{H^1}^2+2C)}=O(\hbar^{-2})\,.$$

Therefore, the exponential amplifying factor in Corollary 4.2 is $\exp(Kt/\hbar^{5/2})$ in the first case, and $\exp(Kt/\hbar^3)$ in the second. These elementary remarks suggest that Pickl's clever method for proving the quantum mean-field limit with singular potentials including the Coulomb potential (see [16, 14]) is not expected to give uniform convergence rates (as in [7, 8] in the case of regular interaction potentials) for the mean field limit in the semiclassical regime.

## 5. Proof of part (1) in Theorem 4.1

For each $\sigma \in \mathfrak{S}_N$ and each $\Psi_N \in \mathfrak{H}_N$, set

$$(U_\sigma \Psi_N)(x_1, \dots, x_N) = \Psi_N(x_{\sigma^{-1}(1)}, \dots, x_{\sigma^{-1}(N)}) .$$

Since $\psi(t,\cdot) \in H^2(\mathbf{R}^3)$, the commutator $[\Delta, R(t)]$ is a bounded operator on $\mathfrak{H}$. According to formula (25) in [8], denoting by $V_{kl}$ the multiplication operator

$$(V_{kl}\Psi_N)(x_1, \dots, x_N) = V(x_k - x_l)\Psi_N(x_1, \dots, x_N) , \tag{29}$$

one has

$$\begin{aligned} &\operatorname{trace}_{\mathfrak{H}_N}((i\hbar\partial_t \mathcal{M}_N(t) - \mathbf{ad}^*(-\tfrac{1}{2}\hbar^2\Delta)\mathcal{M}_N(t))(P(t))F_N) \\ &\qquad = -\operatorname{trace}_{\mathfrak{H}_N}(\tfrac{N-1}{N}([V_{12}, J_1 P(t)])F_N) = \operatorname{trace}_{\mathfrak{H}_N}(\tfrac{N-1}{N}([V_{12}, J_1 R(t)])F_N) \end{aligned} \tag{30}$$

for all $F_N \in \mathcal{L}(\mathfrak{H}_N)$ such that

$$F_N = F_N^* \geq 0 , \quad \operatorname{trace}_{\mathfrak{H}_N}(F_N) = 1 , \quad \text{and} \quad U_\sigma F_N U_\sigma^* = F_N \text{ for all } \sigma \in \mathfrak{S}_N . \tag{31}$$

The core result in the proof of Theorem 3.1 is that the function

$$\omega \mapsto \langle \Psi_N | J_k([E_\omega, R(t)]) J_l(E_\omega^*) | \Psi_N \rangle \in L^2 \cap L^\infty(\mathbf{R}^3)$$

for each $k \neq l \in \{1, \dots, N\}$. Since $\hat{V} \in L^1(\mathbf{R}^3) + L^2(\mathbf{R}^3)$, this has led us to define

$$\langle \Psi_N | [V_{kl}, J_k R(t)] | \Psi_N \rangle := \frac{1}{(2\pi)^3} \int_{\mathbf{R}^3} \hat{V}(\omega) \langle \Psi_N | J_k([E_\omega, R(t)]) J_l(E_\omega^*) | \Psi_N \rangle d\omega ,$$

and more generally, using a spectral decomposition of the trace-class operator $F_N$,

$$\operatorname{trace}_{\mathfrak{H}_N}([V_{kl}, J_k R(t)] F_N) := \frac{1}{(2\pi)^3} \int_{\mathbf{R}^3} \hat{V}(\omega) \operatorname{trace}_{\mathfrak{H}_N}(J_k([E_\omega, R(t)]) J_l(E_\omega^*) F_N) d\omega$$

with

$$\omega \mapsto \operatorname{trace}_{\mathfrak{H}_N}(|J_k([E_\omega, R(t)]) J_l(E_\omega^*) F_N) \in L^2 \cap L^\infty(\mathbf{R}^3) .$$

Since $U_\sigma F_N U_\sigma^* = F_N$ for all $\sigma \in \mathfrak{S}_N$, for each $m \neq n \in \{1, \dots, N\}$, one has

$$\begin{aligned} \operatorname{trace}_{\mathfrak{H}_N}(\tfrac{N-1}{N}([V_{12}, J_1 R(t)])F_N) &= \operatorname{trace}_{\mathfrak{H}_N}(\tfrac{N-1}{N}([V_{mn}, J_m R(t)])F_N) \\ = \frac{1}{N^2} \sum_{1 \leq k \neq l \leq N} &\frac{1}{(2\pi)^3} \int_{\mathbf{R}^3} \hat{V}(\omega) \operatorname{trace}_{\mathfrak{H}_N}(J_k([E_\omega, R(t)]) J_l(E_\omega^*) F_N) d\omega \\ &= \frac{1}{(2\pi)^3} \int_{\mathbf{R}^3} \hat{V}(\omega) \operatorname{trace}_{\mathfrak{H}_N}(S_N[\psi(t,\cdot)](\omega) F_N) d\omega . \end{aligned}$$

With the definition of $\mathcal{C}$ in Theorem 3.1, we conclude that the operator

$$S_N = (i\hbar\partial_t \mathcal{M}_N(t) - \mathbf{ad}^*(-\tfrac{1}{2}\hbar^2\Delta)\mathcal{M}_N(t))(P(t)) - \mathcal{C}(V, \mathcal{M}_N(t), \mathcal{M}_N(t))(R(t))$$

satisfies

$$\operatorname{trace}_{\mathfrak{H}_N}(S_N F_N) = 0$$

for each operator $F_N \in \mathcal{L}(\mathfrak{H}_N)$ satisfying (31). One easily checks that

$$U_\sigma^* S_N U_\sigma = S_N \quad \text{for all } \sigma \in \mathfrak{S}_N .$$

Let $D_N \in \mathcal{L}(\mathfrak{H}_N)$ be a density operator on $\mathfrak{H}_N$, i.e.

$$D_N = D_N^* \geq 0 \quad \text{and} \quad \operatorname{trace}_{\mathfrak{H}_N}(D_N) = 1 . \tag{32}$$

Obviously

$$F_N := \frac{1}{N!} \sum_{\sigma \in \mathfrak{S}_N} U_\sigma D_N U_\sigma^*$$

satisfies (31), so that

$$0=\operatorname{trace}_{\mathfrak{H}_N}(S_NF_N)=\tfrac{1}{N!}\sum_{\sigma\in\mathfrak{S}_N}\operatorname{trace}_{\mathfrak{H}_N}(U_\sigma^*S_NU_\sigma D_N)=\operatorname{trace}_{\mathfrak{H}_N}(S_ND_N)$$

for all $D_N\in\mathcal{L}(\mathfrak{H}_N)$ satisfying (32). Since any trace-class operator on $\mathfrak{H}_N$ is a linear combination of 4 density operators, we conclude that

$$\operatorname{trace}_{\mathfrak{H}_N}(S_NT_N)=0\qquad\text{for all }T_N\in\mathcal{L}^1(\mathfrak{H}_N)\,,$$

so that

$$S_N=0\,. \tag{33}$$

On the other hand

$$\begin{aligned}\mathcal{M}_N(t)(i\hbar\partial_tP(t))&=\mathcal{M}_N(t)([-\tfrac12\hbar^2\Delta+V\star|\psi(t,\cdot)|^2,P(t)])\\&=\mathcal{M}_N(t)([-\tfrac12\hbar^2\Delta,P(t)])-\mathcal{M}_N(t)([V\star|\psi(t,\cdot)|^2,R(t)])\end{aligned}$$

so that

$$\begin{aligned}i\hbar\partial_t(\mathcal{M}_N(t)(P(t)))=&\,\mathbf{ad}^*(-\tfrac12\hbar^2\Delta)\mathcal{M}_N(t)(P(t))+\mathcal{C}(V,\mathcal{M}_N(t),\mathcal{M}_N(t))(R(t))\\&+\mathcal{M}_N(t)([-\tfrac12\hbar^2\Delta,P(t)])-\mathcal{M}_N(t)([V\star|\psi(t,\cdot)|^2,R(t)])\\=&\,\mathcal{C}(V,\mathcal{M}_N(t),\mathcal{M}_N(t))(R(t))-\mathcal{M}_N(t)([V\star|\psi(t,\cdot)|^2,R(t)])\,.\end{aligned}\tag{34}$$

Finally, by condition (17) on $V$, one has

$$\psi(t,\cdot)\in H^2(\mathbf{R}^3)\subset L^2\cap L^4(\mathbf{R}^3)\implies V\star|\psi(t,\cdot)|^2\in\mathcal{F}L^1(\mathbf{R}^3)$$

so that

$$\begin{aligned}V\star|\psi(t,\cdot)|^2&=\tfrac{1}{(2\pi)^3}\int_{\mathbf{R}^3}\hat V(\omega)\mathcal{F}(|\psi(t,\cdot)|^2)(\omega)E_\omega d\omega\\&=\tfrac{1}{(2\pi)^3}\int_{\mathbf{R}^3}\hat V(\omega)\langle\psi(t,\cdot)|E_\omega^*|\psi(t,\cdot)\rangle E_\omega d\omega\\&=\tfrac{1}{(2\pi)^3}\int_{\mathbf{R}^3}\hat V(\omega)\mathcal{R}(t)(E_\omega^*)E_\omega d\omega\,.\end{aligned}\tag{35}$$

Hence

$$\begin{aligned}\mathcal{M}_N(t)([V\star|\psi(t,\cdot)|^2,R(t)])&=\tfrac{1}{(2\pi)^3}\int_{\mathbf{R}^3}\hat V(\omega)\mathcal{R}(t)(E_\omega^*)\mathcal{M}_N(t)[E_\omega,R(t)]d\omega\\&=\mathcal{C}(V,\mathcal{R}(t),\mathcal{M}_N(t))(R(t))\end{aligned}\tag{36}$$

so that, returning to (34), one arrives at the equality

$$i\hbar\partial_t(\mathcal{M}_N(t)(P(t)))=\mathcal{C}(V,\mathcal{M}_N(t),\mathcal{M}_N(t))(R(t))-\mathcal{C}(V,\mathcal{R}(t),\mathcal{M}_N(t))(R(t))\,,$$

which proves part (1) in Theorem 4.1.

**Remark.** In [8], the equality

$$i\hbar\partial_t\mathcal{M}_N(t)(A)=\mathbf{ad}^*(-\tfrac12\hbar^2\Delta)\mathcal{M}_N(t)(A)-\mathcal{C}(V,\mathcal{M}_N(t),\mathcal{M}_N(t))(A)$$

is proved for all $A\in\mathcal{L}(\mathfrak{H})$ such that $[\Delta,A]\in\mathcal{L}(\mathfrak{H})$ assuming that $V\in\mathcal{F}L^1(\mathbf{R}^3)$. This argument cannot be used here since $V\notin\mathcal{F}L^1(\mathbf{R}^3)$. Besides, the definition of the operator $\mathcal{C}(V,\mathcal{M}_N(t),\mathcal{M}_N(t))(R(t))$ in Theorem 3.1 makes critical use of the fact that $R(t)=|\psi(t,\cdot)\rangle\langle\psi(t,\cdot)|$ with $\psi(t,\cdot)\in L^2\cap L^\infty(\mathbf{R}^3)$. This is the reason for the rather lengthy justification of (33) in this section.

## 6. Proof of Lemma 4.4

In the sequel, we seek to "simplify" the expression of the interaction operator

$$\mathcal{C}(V,\mathcal{M}_N(t)-\mathcal{R}(t),\mathcal{M}_N(t))(R(t))\,.$$

This will lead to rather involved computations which do not seem much of a simplification. However, we shall see that the final result of these computations, reported in Lemma 4.4, although algebraically more cumbersome, has better analytical properties.

6.1. **A First Simplification.** First we decompose $E_\omega R(t)$ and $R(t)E_\omega$ in the terms $\mathcal{M}_N(t)(E_\omega R(t))$ and $\mathcal{M}_N(t)(R(t)E_\omega)$ as

$$E_\omega R(t)=P(t)E_\omega R(t)+R(t)E_\omega R(t)\,,$$

and observe that

$$\begin{aligned}&\mathcal{C}(V,\mathcal{M}_N(t)-\mathcal{R}(t),\mathcal{M}_N(t))(R(t))\\ &=\tfrac{1}{(2\pi)^3}\int_{\mathbf{R}^3}\hat V(\omega)((\mathcal{M}_N(t)-\mathcal{R}(t))(E_\omega^*)\mathcal{M}_N(t)(P(t)E_\omega R(t))\\ &\qquad-\mathcal{M}_N(t)(R(t)E_\omega P(t))(\mathcal{M}_N(t)-\mathcal{R}(t))(E_\omega^*))d\omega\\ &+\tfrac{1}{(2\pi)^3}\int_{\mathbf{R}^3}\hat V(\omega)[(\mathcal{M}_N(t)-\mathcal{R}(t))(E_\omega^*),\mathcal{M}_N(t)(R(t)E_\omega R(t))]d\omega\,.\end{aligned}$$

All the terms in the right hand side of the equality above are either similar to the one considered in Theorem 3.1, or of the type denoted (III) in the Remark following Theorem 3.1.

An elementary computation shows that, for all $\omega\in\mathbf{R}^d$,

$$\begin{aligned}&[(\mathcal{M}_N(t)-\mathcal{R}(t))(E_\omega^*),\mathcal{M}_N(t)(R(t)E_\omega R(t))]\\ &=[\mathcal{M}_N(t)(E_\omega^*),\mathcal{M}_N(t)(R(t)E_\omega R(t))]\\ &=\tfrac{1}{N}\mathcal{M}_N(t)[E_\omega^*,R(t)E_\omega R(t)]\,.\end{aligned}$$

Recall indeed that, for each $A,B\in\mathcal{L}(\mathfrak{H})$, one has

$$[\mathcal{M}_N(t)A,\mathcal{M}_N(t)B]=\tfrac{1}{N}\mathcal{M}_N(t)([A,B])$$

— see formula before (41) on p. 1041 in [8]. On the other hand

$$R(t)E_\omega R(t)=|\psi(t,\cdot)\rangle\langle\psi(t,\cdot)|E_\omega|\psi(t,\cdot)\rangle\langle\psi(t,\cdot)|=\mathcal{F}(|\psi(t,\cdot)|^2)(-\omega)R(t)\,,\tag{37}$$

so that

$$\begin{aligned}&[(\mathcal{M}_N(t)-\mathcal{R}(t))(E_\omega^*),\mathcal{M}_N(t)(R(t)E_\omega R(t))]\\ &=\tfrac{1}{N}\mathcal{F}(|\psi(t,\cdot)|^2)(-\omega)\mathcal{M}_N(t)[E_\omega^*,R(t)]\,.\end{aligned}$$

Besides

$$\begin{aligned}(\mathcal{M}_N(t)-\mathcal{R}(t))(E_\omega^*)=&\mathcal{M}_N(t)E_\omega^*-\langle\psi(t,\cdot)|E_\omega^*\psi(t,\cdot)|\rangle\, I_{\mathfrak{H}_N}\\ =&\mathcal{M}_N(t)E_\omega^*-\mathcal{F}(|\psi(t,\cdot)|^2)(\omega)I_{\mathfrak{H}_N}\\ =&\mathcal{M}_N(t)(E_\omega^*-\mathcal{F}(|\psi(t,\cdot)|^2)(\omega)I_{\mathfrak{H}})\,.\end{aligned}$$

Indeed

$$\mathcal{M}_N^{in}I_{\mathfrak{H}}=I_{\mathfrak{H}_N}\implies\mathcal{M}_N(t)I_{\mathfrak{H}}=\mathcal{U}_N(t)^*(\mathcal{M}_N^{in}I_{\mathfrak{H}})\mathcal{U}_N(t)=I_{\mathfrak{H}_N}\tag{38}$$

where we recall that $\mathcal{U}_N(t):=e^{-it\mathcal{H}_N/\hbar}$, while $\mathcal{H}_N$ is the $N$-body Hamiltonian.

Therefore

$$\begin{aligned}&\mathcal{C}(V,\mathcal{M}_N(t)-\mathcal{R}(t),\mathcal{M}_N(t))(R(t))\\ &=\tfrac{1}{(2\pi)^3}\int_{\mathbf{R}^3}\hat{V}(\omega)((\mathcal{M}_N(t)(E^*_\omega-\mathcal{F}(|\psi(t,\cdot)|^2)(\omega)I_{\mathfrak{H}})\mathcal{M}_N(t)(P(t)E_\omega R(t))\\ &\quad-\mathcal{M}_N(t)(R(t)E_\omega P(t))(\mathcal{M}_N(t)(E^*_\omega-\mathcal{F}(|\psi(t,\cdot)|^2)(\omega)I_{\mathfrak{H}}))d\omega\\ &\quad+\tfrac{1}{(2\pi)^3}\int_{\mathbf{R}^3}\hat{V}(\omega)\mathcal{F}(|\psi(t,\cdot)|^2)(\omega)\tfrac{1}{N}\mathcal{M}_N(t)[E_\omega,R(t)]d\omega\,,\end{aligned}$$

in view of (12). With the formula (36), we conclude that

(39)

$$\begin{aligned}&\mathcal{C}(V,\mathcal{M}_N(t)-\mathcal{R}(t),\mathcal{M}_N(t))R(t)\\ &=\tfrac{1}{(2\pi)^3}\int_{\mathbf{R}^3}\hat{V}(\omega)((\mathcal{M}_N(t)(E^*_\omega-\mathcal{F}(|\psi(t,\cdot)|^2)(\omega)I_{\mathfrak{H}})\mathcal{M}_N(t)(P(t)E_\omega R(t))\\ &\quad-\mathcal{M}_N(t)(R(t)E_\omega P(t))(\mathcal{M}_N(t)(E^*_\omega-\mathcal{F}(|\psi(t,\cdot)|^2)(\omega)I_{\mathfrak{H}}))d\omega\\ &\quad+\tfrac{1}{N}\mathcal{M}_N(t)[V\star|\psi(t,\cdot)|^2,R(t)]\,.\end{aligned}$$

6.2. **A Second Simplification.** Next we decompose $E^*_\omega$ in $\mathcal{M}_N(t)(E^*_\omega)$ as

$$E^*_\omega=P(t)E^*_\omega P(t)+P(t)E^*_\omega R(t)+R(t)E^*_\omega P(t)+R(t)E^*_\omega R(t)\,.$$

The identity (37) shows that

$$R(t)E^*_\omega R(t)=\mathcal{F}(|\psi(t,\cdot)|^2)(\omega)R(t)\,,$$

and hence

$$R(t)(E^*_\omega-\mathcal{F}(|\psi(t,\cdot)|^2)(\omega)I_{\mathfrak{H}})R(t)=0\,.$$

Therefore

$$\begin{aligned}\mathcal{M}_N(t)(E^*_\omega-\mathcal{F}(|\psi(t,\cdot)|^2)(\omega)I_{\mathfrak{H}})=&\mathcal{M}_N(t)(P(t)E^*_\omega P(t)-\mathcal{F}(|\psi(t,\cdot)|^2)(\omega)P(t))\\ &+\mathcal{M}_N(t)(P(t)E^*_\omega R(t)+R(t)E^*_\omega P(t))\,,\end{aligned}$$

since $R(t)P(t)=P(t)R(t)=0$. Thus

$$\begin{aligned}&\mathcal{C}(V,\mathcal{M}_N(t)-\mathcal{R}(t),\mathcal{M}_N(t))(R(t))\\ &=\int_{\mathbf{R}^3}\hat{V}(\omega)((\mathcal{M}_N(t)(P(t)E^*_\omega P(t)-\mathcal{F}(|\psi(t,\cdot)|^2)(\omega)P(t))\mathcal{M}_N(t)(P(t)E_\omega R(t))\\ &\quad-\mathcal{M}_N(t)(R(t)E_\omega P(t))(\mathcal{M}_N(t)(P(t)E^*_\omega P(t)-\mathcal{F}(|\psi(t,\cdot)|^2)(\omega)P(t)))\tfrac{d\omega}{(2\pi)^3}\\ &\quad+\int_{\mathbf{R}^3}\hat{V}(\omega)(\mathcal{M}_N(t)(P(t)E^*_\omega R(t)+R(t)E^*_\omega P(t))\mathcal{M}_N(t)(P(t)E_\omega R(t))\\ &\quad-\mathcal{M}_N(t)(R(t)E_\omega P(t))\mathcal{M}_N(t)(P(t)E^*_\omega R(t)+R(t)E^*_\omega P(t)))\tfrac{d\omega}{(2\pi)^3}\\ &\quad+\tfrac{1}{N}\mathcal{M}_N(t)[(V\star|\psi(t,\cdot)|^2),R(t)]\,.\end{aligned}$$

Using again (12) implies that

$$\begin{aligned}&\int_{\mathbf{R}^3}\hat{V}(\omega)(\mathcal{M}_N(t)(R(t)E^*_\omega P(t))\mathcal{M}_N(t)(P(t)E_\omega R(t))d\omega\\ &=\int_{\mathbf{R}^3}\hat{V}(\omega)(\mathcal{M}_N(t)(R(t)E_\omega P(t))\mathcal{M}_N(t)(P(t)E^*_\omega R(t))d\omega\,,\end{aligned}$$

so that

$$
\begin{aligned}
&\mathcal{C}(V,\mathcal{M}_N(t)-\mathcal{R}(t),\mathcal{M}_N(t))(R(t))\\
=&\int_{\mathbf{R}^3}\hat V(\omega)((\mathcal{M}_N(t)(P(t)E_\omega^*P(t)-\mathcal{F}(|\psi(t,\cdot)|^2)(\omega)P(t))\mathcal{M}_N(t)(P(t)E_\omega R(t))\\
&-\mathcal{M}_N(t)(R(t)E_\omega P(t))(\mathcal{M}_N(t)(P(t)E_\omega^*P(t)-\mathcal{F}(|\psi(t,\cdot)|^2)(\omega)P(t)))\tfrac{d\omega}{(2\pi)^3}\\
&+\int_{\mathbf{R}^3}\hat V(\omega)(\mathcal{M}_N(t)(P(t)E_\omega^*R(t))\mathcal{M}_N(t)(P(t)E_\omega R(t))\\
&-\mathcal{M}_N(t)(R(t)E_\omega P(t))\mathcal{M}_N(t)(R(t)E_\omega^*P(t)))\tfrac{d\omega}{(2\pi)^3}\\
&+\tfrac{1}{N}\mathcal{M}_N(t)[(V\star|\psi(t,\cdot)|^2),R(t)]\,.
\end{aligned}
$$

By (35), one can further simplify the term

$$
\begin{aligned}
\int_{\mathbf{R}^3}&\hat V(\omega)\mathcal{F}(|\psi(t,\cdot)|^2)(\omega)\mathcal{M}_N(t)(P(t))\mathcal{M}_N(t)(P(t)E_\omega R(t))\\
&-\mathcal{M}_N(t)(R(t)E_\omega P(t))(\mathcal{M}_N(t)(P(t)))\tfrac{d\omega}{(2\pi)^3}\\
&=\mathcal{M}_N(t)(P(t))\mathcal{M}_N(t)(P(t)(V\star|\psi(t,\cdot)|^2)R(t))\\
&-\mathcal{M}_N(t)(R(t)(V\star|\psi(t,\cdot)|^2)P(t))\mathcal{M}_N(t)(P(t))\,.
\end{aligned}
$$

Finally

$$
\mathcal{C}(V,\mathcal{M}_N(t)-\mathcal{R}(t),\mathcal{M}_N(t))(R(t))=T_1+T_2+T_3+T_4
$$

with

$$
\begin{aligned}
T_1:=&\int_{\mathbf{R}^3}\hat V(\omega)((\mathcal{M}_N(t)(P(t)E_\omega^*P(t))\mathcal{M}_N(t)(P(t)E_\omega R(t))\\
&-\mathcal{M}_N(t)(R(t)E_\omega P(t))(\mathcal{M}_N(t)(P(t)E_\omega^*P(t)))\tfrac{d\omega}{(2\pi)^3}\\
T_2:=&\mathcal{M}_N(t)(R(t)(V\star|\psi(t,\cdot)|^2)P(t))\mathcal{M}_N(t)(P(t))\\
&-\mathcal{M}_N(t)(P(t))\mathcal{M}_N(t)(P(t)(V\star|\psi(t,\cdot)|^2)R(t))\\
T_3:=&\int_{\mathbf{R}^3}\hat V(\omega)(\mathcal{M}_N(t)(P(t)E_\omega^*R(t))\mathcal{M}_N(t)(P(t)E_\omega R(t))\\
&-\mathcal{M}_N(t)(R(t)E_\omega P(t))\mathcal{M}_N(t)(R(t)E_\omega^*P(t)))\tfrac{d\omega}{(2\pi)^3}\\
T_4:=&\tfrac{1}{N}\mathcal{M}_N(t)[(V\star|\psi(t,\cdot)|^2),R(t)]\,.
\end{aligned}
$$

Observe again that all the integrals in the right hand side of the equalities defining $T_1$ and $T_3$ are of the form defined in Theorem 3.1, or of the form (I), (II) or (III), or their adjoint, in the Remark following Theorem 3.1.

That

$$
\begin{aligned}
T_1=&\mathcal{T}(V,\mathcal{M}_N(t)(P(t)\bullet P(t)),\mathcal{M}_N(t)(P(t)\bullet R(t)))\\
&-\mathcal{T}(V,\mathcal{M}_N(t)(R(t)\bullet P(t)),\mathcal{M}_N(t)(P(t)\bullet P(t)))\\
T_3=&\mathcal{T}(V,\mathcal{M}_N(t)(P(t)\bullet R(t)),\mathcal{M}_N(t)(P(t)\bullet R(t)))\\
&-\mathcal{T}(V,\mathcal{M}_N(t)(R(t)\bullet P(t)),\mathcal{M}_N(t)(R(t)\bullet P(t)))
\end{aligned}
$$

follows from (12) and the definition (23). This concludes the proof of Lemma 4.4.

## 7. Proof of Lemma 4.5

In the sequel, we shall estimate these four terms in increasing order of technical difficulty.

7.1. **Bound for $T_4$.** The easiest term to treat is obviously $T_4$. We first recall that

$$\|\mathcal{M}_N(t)(A)\| \le \|A\| \qquad \text{for each } A \in \mathcal{L}(\mathfrak{H}) \tag{40}$$

— see the formula following (41) on p. 1041 in [8]. Thus

$$\begin{aligned}\|T_4\| \le& \tfrac{1}{N}\|[V\star|\psi(t,\cdot)|^2, R(t)]\| \le \tfrac{1}{N}(\|R(t)V\star|\psi(t,\cdot)|^2\| + \|(V\star|\psi(t,\cdot)|^2)R(t)\|)\\ =& \tfrac{2}{N}\|(V\star|\psi(t,\cdot)|^2)R(t)\|,\end{aligned}$$

where the equality follows from the fact that $R(t) = R(t)^*$, which implies that

$$((V\star|\psi(t,\cdot)|^2)R(t))^* = R(t)(V\star|\psi(t,\cdot)|^2). \tag{41}$$

On the other hand, by Jensen's inequality

$$(|V|\star|\psi(t,\cdot)|^2)^2 \le V^2\star|\psi(t,\cdot)|^2,$$

so that

$$\begin{aligned}\|(V\star|\psi(t,\cdot)|^2)R(t)\|^2 \le& \|V\star|\psi(t,\cdot)|^2\|_{L^\infty}^2\\ \le& \|\,|V|\star|\psi(t,\cdot)|^2\,\|_{L^\infty}^2 \le \|(V^2)\star|\psi(t,\cdot)|^2\|_{L^\infty} = \ell(t)^2,\end{aligned} \tag{42}$$

and therefore

$$\|T_4\| \le \tfrac{2}{N}\ell(t). \tag{43}$$

Finally, we recall that

$$(\mathcal{M}_N^{in}A)^* = \frac{1}{N}\sum_{k=1}^N (J_kA)^* = \frac{1}{N}\sum_{k=1}^N J_k(A^*) = \mathcal{M}_N^{in}(A^*)$$

for each $A \in \mathcal{L}(\mathfrak{H})$, so that

$$\begin{aligned}(\mathcal{M}_N(t)A)^* = (\mathcal{U}_N(t)^*(\mathcal{M}_N^{in}A)\mathcal{U}_N(t))^* =& \mathcal{U}_N(t)^*(\mathcal{M}_N^{in}A)^*\mathcal{U}_N(t)\\ =& \mathcal{U}_N(t)^*\mathcal{M}_N^{in}(A^*)\mathcal{U}_N(t) = \mathcal{M}_N(t)(A^*).\end{aligned} \tag{44}$$

Then (41) and (44) imply that

$$\begin{aligned}(\mathcal{M}_N(t)[V\star|\psi(t,\cdot)|^2, R(t)])^* =& \mathcal{M}_N(t)([V\star|\psi(t,\cdot)|^2, R(t)]^*)\\ =& \mathcal{M}_N(t)(-[V\star|\psi(t,\cdot)|^2, R(t)])\\ =& -\mathcal{M}_N(t)([V\star|\psi(t,\cdot)|^2, R(t)])\end{aligned}$$

so that $T_4^* = -T_4$. Hence $\pm iT_4$ are self-adjoint operators on $\mathfrak{H}_N$, so that

$$\|T_4\| \le \tfrac{2}{N}\ell(t) \implies \pm iT_4 \le \tfrac{2}{N}\ell(t)I_{\mathfrak{H}_N}. \tag{45}$$

7.2. **Bound for $T_2$.** Set

$$S_2 := \mathcal{M}_N(t)(P(t))\mathcal{M}_N(t)(P(t)(V\star|\psi(t,\cdot)|^2)R(t)). \tag{46}$$

One has

$$\begin{aligned}S_2 =& \mathcal{U}_N(t)^*\mathcal{M}_N^{in}(P(t))\mathcal{M}_N^{in}(P(t)(V\star|\psi(t,\cdot)|^2)R(t))\mathcal{U}_N(t)\\ =& \frac{1}{N}\sum_{k=1}^N \mathcal{U}_N(t)^*(J_kP(t))\mathcal{M}_N^{in}(P(t)(V\star|\psi(t,\cdot)|^2)R(t))(J_kP(t))\mathcal{U}_N(t)\\ &+ \frac{1}{N}\sum_{k=1}^N \mathcal{U}_N(t)^*(J_kP(t))[J_kP(t), \mathcal{M}_N^{in}(P(t)(V\star|\psi(t,\cdot)|^2)R(t))]\mathcal{U}_N(t).\end{aligned}$$

Then

$$\begin{aligned}&[J_kP(t),\mathcal{M}_N^{in}(P(t)(V\star|\psi(t,\cdot)|^2)R(t))]\\&=\tfrac{1}{N}[J_kP(t),J_k(P(t)(V\star|\psi(t,\cdot)|^2)R(t))]\\&=\tfrac{1}{N}J_k(P(t)(V\star|\psi(t,\cdot)|^2)R(t))\,,\end{aligned}$$

so that

$$\begin{aligned}S_2=&\tfrac{1}{N}\sum_{k=1}^N\mathcal{U}_N(t)^*(J_kP(t))\mathcal{M}_N^{in}(P(t)(V\star|\psi(t,\cdot)|^2)R(t))(J_kP(t))\mathcal{U}_N(t)\\&+\tfrac{1}{N^2}\sum_{k=1}^N\mathcal{U}_N(t)^*J_k(P(t)(V\star|\psi(t,\cdot)|^2)R(t))\mathcal{U}_N(t)\,.\end{aligned}$$

By cyclicity of the trace, for each $F_N^{in}$ satisfying (31), denoting

$$F_N(t):=\mathcal{U}_N(t)F_N^{in}\mathcal{U}_N(t)^*\,,$$

one has

$$\begin{aligned}&\operatorname{trace}_{\mathfrak{H}_N}(S_2F_N^{in})\\&=\tfrac{1}{N}\sum_{k=1}^N\operatorname{trace}_{\mathfrak{H}_N}(\mathcal{M}_N^{in}(P(t)(V\star|\psi(t,\cdot)|^2)R(t))(J_kP(t))F_N(t)(J_kP(t)))\\&\quad+\tfrac{1}{N^2}\sum_{k=1}^N\operatorname{trace}_{\mathfrak{H}_N}(J_k(P(t)(V\star|\psi(t,\cdot)|^2)R(t))F_N(t))\end{aligned}$$

so that

$$\begin{aligned}&|\operatorname{trace}_{\mathfrak{H}_N}(S_2F_N^{in})|\\&\le\tfrac{1}{N}\sum_{k=1}^N\|\mathcal{M}_N^{in}(P(t)(V\star|\psi(t,\cdot)|^2)R(t))\|\|(J_kP(t))F_N(t)(J_kP(t))\|_1\\&\quad+\tfrac{1}{N^2}\sum_{k=1}^N\|J_k(P(t)(V\star|\psi(t,\cdot)|^2)R(t))\|\|F_N(t)\|_1\\&\le\|(V\star|\psi(t,\cdot)|^2)R(t)\|\tfrac{1}{N}\sum_{k=1}^N\operatorname{trace}_{\mathfrak{H}_N}((J_kP(t))F_N(t)(J_kP(t))))\\&\quad+\|(V\star|\psi(t,\cdot)|^2)R(t)\|\tfrac{1}{N^2}\sum_{k=1}^N\|F_N(t)\|_1\\&=\|(V\star|\psi(t,\cdot)|^2)R(t)\|(\operatorname{trace}_{\mathfrak{H}_N}(\mathcal{M}_N(t)(P(t))F_N^{in})+\tfrac{1}{N}\|F_N^{in}\|_1)\,.\end{aligned}\tag{47}$$

By (44),

$$S_2^*=\mathcal{M}_N(t)(R(t)(V\star|\psi(t,\cdot)|^2)P(t))\mathcal{M}_N(t)(P(t))\,,$$

so that

$$T_2=S_2^*-S_2=-T_2^*\,.$$

Thus

$$\begin{aligned}|\operatorname{trace}_{\mathfrak{H}_N}(T_2F_N^{in})|\le&|\operatorname{trace}_{\mathfrak{H}_N}(S_2^*F_N^{in})|+|\operatorname{trace}_{\mathfrak{H}_N}(S_2F_N^{in})|\\=&|\operatorname{trace}_{\mathfrak{H}_N}(F_N^{in}S_2)|+|\operatorname{trace}_{\mathfrak{H}_N}(S_2F_N^{in})|=2|\operatorname{trace}_{\mathfrak{H}_N}(S_2F_N^{in})|\,,\end{aligned}$$

so that

$$\begin{aligned}&|\operatorname{trace}_{\mathfrak{H}_N}(T_2F_N^{in})|\\ &\le 2\|(V\star|\psi(t,\cdot)|^2)R(t)\|(\operatorname{trace}_{\mathfrak{H}_N}(\mathcal{M}_N(t)(P(t))F_N^{in})+\tfrac{1}{N}\|F_N^{in}\|_1)\\ &\le 2\ell(t)(\operatorname{trace}_{\mathfrak{H}_N}(\mathcal{M}_N(t)(P(t))F_N^{in})+\tfrac{1}{N}\operatorname{trace}_{\mathfrak{H}_N}(F_N^{in}))\end{aligned}\tag{48}$$

by (42).

Next we use the following elementary observation.

**Lemma 7.1.** *Let $T=T^*\in\mathcal{L}(\mathfrak{H}_N)$ satisfy*

$$U_\sigma T U_\sigma^*=T \text{ for all } \sigma\in\mathfrak{S}_N\,,\qquad \text{and } \operatorname{trace}_{\mathfrak{H}_N}(TF)\ge 0$$

*for each $F\in\mathcal{L}(\mathfrak{H}_N)$ satisfying* (31)*. Then $T\ge 0$.*

*Proof.* Indeed, we seek to prove that

$$\langle\Psi|T|\Psi\rangle\ge 0\qquad\text{for each } \Psi\in\mathfrak{H}_N\,.$$

For each $\Psi\in\mathfrak{H}_N$ such that $\|\Psi_N\|_{\mathfrak{H}_N}=1$, set

$$F=\tfrac{1}{N!}\sum_{\sigma\in\mathfrak{S}_N}|U_\sigma\Psi\rangle\langle U_\sigma\Psi|\,.$$

Then $F$ satisfies (31), so that

$$0\le\operatorname{trace}(TF)=\tfrac{1}{N!}\sum_{\sigma\in\mathfrak{S}_N}\langle U_\sigma\Psi|T|U_\sigma\Psi\rangle=\tfrac{1}{N!}\sum_{\sigma\in\mathfrak{S}_N}\langle\Psi|U_\sigma^*TU_\sigma|\Psi\rangle=\langle\Psi|T|\Psi\rangle$$

since $U_\sigma^*TU_\sigma=T$ for each $\sigma\in\mathfrak{S}_N$. Thus $\langle\Psi|T|\Psi\rangle\ge 0$ for each $\Psi\in\mathfrak{H}_N$ such that $\|\Psi_N\|_{\mathfrak{H}_N}=1$, and thus for each $\Psi\in\mathfrak{H}_N\setminus\{0\}$ by normalization. □

The inequality (48) implies that

$$\begin{aligned}2\ell(t)\operatorname{trace}_{\mathfrak{H}_N}((\mathcal{M}_N(t)(P(t))+\tfrac{1}{N}I_{\mathfrak{H}_N})F_N^{in})\ge&|\operatorname{trace}_{\mathfrak{H}_N}(T_2F_N^{in})|\\ \ge&\operatorname{trace}_{\mathfrak{H}_N}(\pm iT_2F_N^{in})\,,\end{aligned}$$

and we conclude from Lemma 7.1 that

$$\pm iT_2\le 2\ell(t)(\mathcal{M}_N(t)(P(t))+\tfrac{1}{N}I_{\mathfrak{H}_N})\,.\tag{49}$$

7.3. **Bound for $T_1$.** Next we estimate

$$\begin{aligned}S_1:=&\mathcal{T}(V,\mathcal{M}_N(t)(P(t)\bullet P(t)),\mathcal{M}_N(t)(P(t)\bullet R(t)))\\ =&\mathcal{U}_N(t)^*\mathcal{T}(V,\mathcal{M}_N^{in}(P(t)\bullet P(t)),\mathcal{M}_N^{in}(P(t)\bullet R(t)))\mathcal{U}_N(t)\\ =&\tfrac{1}{N}\sum_{k=1}^N\mathcal{U}_N(t)^*\mathcal{T}(V,J_k(P(t)\bullet P(t)),\mathcal{M}_N^{in}(P(t)\bullet R(t)))\mathcal{U}_N(t)\,.\end{aligned}$$

Observe that

$$\begin{aligned}&\mathcal{T}(V,J_k(P(t)\bullet P(t)),\mathcal{M}_N^{in}(P(t)\bullet R(t)))\\ =&\int_{\mathbf{R}^3}\hat V(\omega)(J_kP(t))J_k(P(t)E_\omega^*P(t))\mathcal{M}_N^{in}(P(t)E_\omega R(t))(J_kP(t))\tfrac{d\omega}{(2\pi)^3}\\ &+\tfrac{1}{N}\int_{\mathbf{R}^3}\hat V(\omega)(J_kP(t))J_k(P(t)E_\omega^*P(t))[J_kP(t),J_k(P(t)E_\omega R(t))]\tfrac{d\omega}{(2\pi)^3}\,,\end{aligned}$$

since $P(t)=P(t)^2$, so that $J_kP(t)=(J_kP(t))^2$. Then

$$[J_kP(t),J_k(P(t)E_\omega R(t))]=J_k(P(t)E_\omega R(t))\,,$$

so that

$$J_k(P(t)E_\omega^* P(t))[J_k P(t), J_k(P(t)E_\omega R(t))] = J_k(P(t)E_\omega^* P(t)E_\omega R(t))$$
$$= J_k(P(t)E_\omega^*(I - R(t))E_\omega R(t)) = -\mathcal{F}(|\psi(t,\cdot)|^2)(-\omega)J_k(P(t)E_\omega^* R(t))\,.$$

Hence (12) implies that

$$\tfrac{1}{N}\int_{\mathbf{R}^3}\hat{V}(\omega)(J_kP(t))J_k(P(t)E_\omega^*P(t))[J_kP(t),J_k(P(t)E_\omega R(t))]\tfrac{d\omega}{(2\pi)^3}$$
$$= -\tfrac{1}{N}(J_kP(t))J_k(P(t)(V\star|\psi(t,\cdot)|^2)R(t))\,.$$

On the other hand

$$\int_{\mathbf{R}^3}\hat{V}(\omega)(J_kP(t))J_k(P(t)E_\omega^*P(t))\mathcal{M}_N^{in}(P(t)E_\omega R(t))(J_kP(t))\tfrac{d\omega}{(2\pi)^3}$$
$$= \tfrac{1}{N}\int_{\mathbf{R}^3}\hat{V}(\omega)(J_kP(t))J_k(P(t)E_\omega^*P(t))\sum_{\substack{l=1\\ l\neq k}}^N J_l(P(t)E_\omega R(t))J_kP(t)\tfrac{d\omega}{(2\pi)^3}$$
$$= \tfrac{1}{N}\int_{\mathbf{R}^3}\hat{V}(\omega)(J_kP(t))J_k(E_\omega^*)\sum_{\substack{l=1\\ l\neq k}}^N J_l(P(t)E_\omega R(t))J_kP(t)\tfrac{d\omega}{(2\pi)^3}$$
$$= (J_kP(t))\left(\tfrac{1}{N}\sum_{\substack{l=1\\ l\neq k}}^N(J_kP(t))(J_lP(t))V_{kl}(J_lR(t))(J_kP(t))\right)(J_kP(t))\,,$$

since $J_k(P(t)E_\omega R(t))J_k(P(t)) = 0$, with $V_{kl}$ defined as in (29).

Hence

$$S_1 = \tfrac{1}{N^2}\sum_{1\le k\neq l\le N}\mathcal{U}_N(t)^*(J_kP(t))^2(J_lP(t))V_{kl}(J_lR(t))(J_kP(t))^2\mathcal{U}_N(t)$$
$$-\tfrac{1}{N^2}\sum_{k=1}^N\mathcal{U}_N(t)^*(J_kP(t))J_k(P(t)(V\star|\psi(t,\cdot)|^2)R(t))\mathcal{U}_N(t)\,.$$

Therefore, by cyclicity of the trace, for each $F_N^{in}\in\mathcal{L}(\mathfrak{H}_N)$ satisfying (31), denoting $F_N(t) := \mathcal{U}_N(t)F_N^{in}\mathcal{U}_N(t)^*$, one has

$$\operatorname{trace}_{\mathfrak{H}_N}(S_1F_N^{in})$$
$$= \tfrac{1}{N^2}\sum_{1\le k\neq l\le N}\operatorname{trace}_{\mathfrak{H}_N}((J_kP(t))(J_lP(t))V_{kl}(J_lR(t))(J_kP(t))^2F_N(t)(J_kP(t)))$$
$$-\tfrac{1}{N^2}\sum_{k=1}^N\operatorname{trace}_{\mathfrak{H}_N}(J_k(P(t)(V\star|\psi(t,\cdot)|^2)R(t))F_N(t)(J_kP(t)))\,,$$

so that

(50)
$$|\operatorname{trace}_{\mathfrak{H}_N}(S_1F_N^{in})|$$
$$\le \tfrac{1}{N^2}\sum_{1\le k\neq l\le N}\|(J_kP(t))(J_lP(t))V_{kl}(J_lR(t))(J_kP(t))\|\|(J_kP(t))F_N(t)(J_kP(t))\|_1$$
$$+\tfrac{1}{N^2}\sum_{k=1}^N\|J_k(P(t)(V\star|\psi(t,\cdot)|^2)R(t))\|\|F_N(t)\|_1\|J_kP(t)\|$$
$$\le (1-\tfrac{1}{N})\|V_{12}J_2R(t)\|\operatorname{trace}_{\mathfrak{H}_N}(F_N^{in}\mathcal{M}_N(t)(P(t)))$$
$$+\tfrac{2}{N}\|(V\star|\psi(t,\cdot)|^2)R(t)\|\|F_N(t)\|_1\,.$$

Finally

$$\begin{aligned}T_1 =&\mathcal{T}(V,\mathcal{M}_N(t)(P(t)\bullet P(t)),\mathcal{M}_N(t)(P(t)\bullet R(t)))\\&-\mathcal{T}(V,\mathcal{M}_N(t)(R(t)\bullet P(t)),\mathcal{M}_N(t)(P(t)\bullet P(t)))=S_1-S_1^*=-T_1^*\end{aligned}$$

because of Lemma 4.3, so that

$$\begin{aligned}|\operatorname{trace}_{\mathfrak{H}_N}(T_1F_N^{in})|\le&2(1-\tfrac{1}{N})\|V_{12}J_2R(t)\|\operatorname{trace}_{\mathfrak{H}_N}(F_N^{in}\mathcal{M}_N(t)(P(t)))\\&+\tfrac{4}{N}\|(V\star|\psi(t,\cdot)|^2)R(t)\|\|F_N(t)\|_1\,.\end{aligned}$$

Since $R(s)$ is a rank-one orthogonal projection

$$\begin{aligned}\|V_{12}(J_2R(t))\|^2=&\|(J_2R(t))V_{12}^2(J_2R(t))\|\\=&\|(V^2\star|\psi(t,\cdot)|^2)\otimes R(s)\|\le\|(V^2\star|\psi(t,\cdot)|^2\|_{L^\infty}=\ell(t)^2\,.\end{aligned}\tag{51}$$

Thus

$$\begin{aligned}|\operatorname{trace}_{\mathfrak{H}_N}(T_1F_N^{in})|\le&2\ell(t)\left((1-\tfrac{1}{N})\operatorname{trace}_{\mathfrak{H}_N}(F_N^{in}\mathcal{M}_N(t)(P(t)))+\tfrac{2}{N}\|F_N^{in}\|_1\right)\\=&2\ell(t)\left((1-\tfrac{1}{N})\operatorname{trace}_{\mathfrak{H}_N}(F_N^{in}\mathcal{M}_N(t)(P(t)))+\tfrac{2}{N}\operatorname{trace}_{\mathfrak{H}_N}(F_N^{in})\right).\end{aligned}\tag{52}$$

In particular

$$2\ell(t)\operatorname{trace}_{\mathfrak{H}_N}\left(F_N^{in}\left((1-\tfrac{1}{N})\mathcal{M}_N(t)(P(t)))+\tfrac{2}{N}I_{\mathfrak{H}_N}\right)\right)\ge\operatorname{trace}_{\mathfrak{H}_N}(\pm iT_1F_N^{in})$$

and since this inequality holds for each $F_N^{in}\in\mathcal{L}_s(\mathfrak{H}_N)$ such that $F_N^{in}=(F_N^{in})^*\ge0$, we conclude from Lemma 7.1 that

$$\pm iT_1\le2\ell(t)\left((1-\tfrac{1}{N})\mathcal{M}_N(t)(P(t)))+\tfrac{2}{N}I_{\mathfrak{H}_N}\right)\tag{53}$$

7.4. **The Operator $\Pi_N$.** In order to treat the last term $T_3$, we need the following auxiliary lemma — see the formula preceding (13) in [16].

**Lemma 7.2.** *Let $R=R^*$ be a rank-one projection on $\mathfrak{H}$ and let $P:=I-R$. Set $\Pi_N:=\mathcal{M}_N^{in}P$. For each $N>1$,*

$$\Pi_N^*=\Pi_N\,,\quad\Pi_N^2\ge\tfrac{1}{N}\Pi_N\,,\qquad\textit{and}\qquad\operatorname{Ker}\Pi_N=\operatorname{Ker}(I-R^{\otimes N})\,,$$

*so that*

$$\Pi_N\ge\tfrac{1}{N}(1-R^{\otimes N})\,.$$

*In particular, there exists a pseudo-inverse $\Pi_N^{-1}:(\operatorname{Ker}\Pi_N)^\perp\to(\operatorname{Ker}\Pi_N)^\perp$, with extension by $0$ on $\operatorname{Ker}\Pi_N$ also (abusively) denoted $\Pi_N$, such that*

$$\Pi_N^{-1}\Pi_N=\Pi_N\Pi_N^{-1}=I-R^{\otimes N}\,.\tag{54}$$

In [16], the definition of the pseudo-inverse of $\Pi_N$ immediately follows from formula (6), which can be viewed as the spectral decomposition of $\Pi_N$. The proof below is quite straightforward and avoids using the clever argument leading to formula (6) in [16], which is not entirely obvious unless one already knows the result.

*Proof.* That $\Pi_N$ is self-adjoint is obvious by definition of $\mathcal{M}_N^{in}$. Then

$$\Pi_N^2=\frac{1}{N^2}\left(\sum_{k=1}^N J_kP+2\sum_{1\le k<l\le N}J_kPJ_lP\right)\ge\frac{1}{N^2}\sum_{k=1}^NJ_kP=\frac{1}{N}\Pi_N\,.$$

If $X \in \operatorname{Ker}\Pi_N$, one has, for each $k = 1, \dots, N$,

$$0 = \sum_{k=1}^{N} \langle X|J_k P|X\rangle \implies \langle X|J_k P|X\rangle = 0 \implies J_k P X = 0\,.$$

Hence

$$X = J_N R X = J_{N-1} R X = \dots = J_2 R X = J_1 R X$$

so that

$$X = J_N R X = J_N R J_{N-1} R X = \dots = J_N R J_{N-1} R \dots J_2 R J_1 R X = R^{\otimes N} X\,.$$

Thus $\operatorname{Ker}\Pi_N = \operatorname{Ker}(I - R^{\otimes N})$. Finally

$$\Pi_N^3 = \Pi_N^{1/2}\Pi_N^2\Pi_N^{1/2} \geq \frac{1}{N}\Pi_N^{1/2}\Pi_N\Pi_N^{1/2} = \frac{1}{N}\Pi_N^2\,.$$

Therefore, for each $X \in \mathfrak{H}_N$, one has

$$\langle \Pi_N X|\Pi_N|\Pi_N X\rangle \geq \frac{1}{N}\|\Pi_N X\|^2\,.$$

Since $\Pi_N = \Pi_N^*$, one has

$$\overline{\operatorname{Im}\Pi_N} = (\operatorname{Ker}\Pi_N)^\perp$$

(see for instance Corollary 2.18 (iv) in chapter 2 of [5]). Since

$$\langle Y|\Pi_N|Y\rangle \geq \frac{1}{N}\|Y\|^2\,, \qquad Y \in \operatorname{Im}\Pi_N\,,$$

and since one has obviously $\|\Pi_N\| \leq 1$, a straightforward density argument shows that

$$\langle Y|\Pi_N|Y\rangle \geq \frac{1}{N}\|Y\|^2\,, \qquad Y \in (\operatorname{Ker}\Pi_N)^\perp\,.$$

Hence

$$\Pi_N \geq \tfrac{1}{N}(1 - R^{\otimes N})\,.$$

The existence of the pseudo-inverse $\Pi_N^{-1}$ follows from this inequality. □

7.5. **Bound for $T_3$.** Finally, we treat the term $T_3$. Set

$$\begin{aligned} S_3 =& \mathcal{T}(V, \mathcal{M}_N(t)(P(t)\bullet R(t)), \mathcal{M}_N(t)(P(t)\bullet R(t))) \\ =& \mathcal{U}_N(t)^*\mathcal{T}(V, \mathcal{M}_N^{in}(P(t)\bullet R(t)), \mathcal{M}_N^{in}(P(t)\bullet R(t)))\mathcal{U}_N(t)\,. \end{aligned}$$

One easily checks that

$$\begin{aligned} &\mathcal{T}(V, \mathcal{M}_N^{in}(P(t)\bullet R(t)), \mathcal{M}_N^{in}(P(t)\bullet R(t))) \\ &= \int_{\mathbf{R}^3} \hat{V}(\omega)\mathcal{M}_N^{in}(P(t)E_\omega^* R(t))\mathcal{M}_N^{in}(P(t)E_\omega R(t))\tfrac{d\omega}{(2\pi)^3} \\ &= \tfrac{1}{N^2}\sum_{1\leq k\neq l\leq N}(J_l P(t))(J_k P(t))V_{kl}(J_k R(t))(J_l R(t))\,. \end{aligned}$$

At this point, we set $\Pi_N(t) := \mathcal{M}_N^{in}P(t)$ and use Lemma 7.2 to define the pseudo-inverse $\Pi_N(t)^{-1}$. One has $\Pi_N(t) = \Pi_N(t)^* \geq 0$, so that $\Pi_N(t)^{-1} = (\Pi_N(t)^{-1})^* \geq 0$ on $\operatorname{Ker}(I - R(t)^{\otimes N})$. Abusing the notation $\Pi_N(t)^{-1/2}$ to designate the linear map $(\Pi_N(t)^{-1})^{1/2}$, we deduce from (54) that

$$\Pi_N(t)^{1/2}\Pi_N(t)^{-1/2} = I - R(t)^{\otimes N}\,,$$

so that

$$(J_k P(t))\Pi_N(t)^{1/2}\Pi_N(t)^{-1/2} = \Pi_N(t)^{1/2}\Pi_N(t)^{-1/2}(J_k P(t)) = J_l P(t)\,.$$

Hence

$$\begin{aligned}&\mathcal{T}(V,\mathcal{M}_N^{in}(P(t)\bullet R(t)),\mathcal{M}_N^{in}(P(t)\bullet R(t)))\\&=\tfrac{1}{N^2}\sum_{1\le k\ne l\le N}(J_lP(t))(J_kP(t))\Pi_N(t)^{-\frac12}\Pi_N(t)^{\frac12}V_{kl}(J_kR(t))(J_lR(t))\,,\end{aligned}$$

and we study the quantity

$$\begin{aligned}&\operatorname{trace}_{\mathfrak{H}_N}(S_3F_N^{in})=\operatorname{trace}_{\mathfrak{H}_N}((F_N^{in})^{\frac12}S_2(F_N^{in})^{\frac12})\\&=\operatorname{trace}_{\mathfrak{H}_N}(F_N(t)^{\frac12}\mathcal{T}(V,\mathcal{M}_N^{in}(P(t)\bullet R(t)),\mathcal{M}_N^{in}(P(t)\bullet R(t)))F_N(t)^{\frac12})\,.\end{aligned}$$

where $F_N(t)=\mathcal{U}_N(t)F_N^{in}\mathcal{U}_N(t)^*$, for each $F_N^{in}\in\mathcal{L}(\mathfrak{H}_N)$ satisfying (31). Observe that

$$\begin{aligned}&|\operatorname{trace}_{\mathfrak{H}_N}(F_N(t)^{\frac12}(J_lP(t))(J_kP(t))\Pi_N(t)^{-\frac12}\Pi_N(t)^{\frac12}V_{kl}(J_kR(t))(J_lR(t))F_N(t)^{\frac12})|\\&\le\|\Pi_N(t)^{-\frac12}(J_kP(t))(J_lP(t))F_N(t)^{\frac12}\|_2\|\Pi_N(t)^{\frac12}V_{kl}(J_kR(t))(J_lR(t))F_N(t)^{\frac12}\|_2,\end{aligned}$$

so that, by the Cauchy-Schwarz inequality,

$$\begin{aligned}|\operatorname{trace}_{\mathfrak{H}_N}(S_3F_N^{in})|\le&\tfrac{1}{N^2}\left(\sum_{1\le k\ne l\le N}\|\Pi_N(t)^{-\frac12}(J_kP(t))(J_lP(t))F_N(t)^{\frac12}\|_2^2\right)^{1/2}\\&\times\left(\sum_{1\le k\ne l\le N}\|\Pi_N(t)^{\frac12}V_{kl}(J_kR(t))(J_lR(t))F_N(t)^{\frac12}\|_2^2\right)^{1/2}.\end{aligned}$$

First, one has

$$\begin{aligned}&\|\Pi_N(t)^{-\frac12}(J_kP(t))(J_lP(t))F_N(t)^{\frac12}\|_2^2\\&=\operatorname{trace}_{\mathfrak{H}_N}(F_N(t)^{\frac12}(J_lP(t))(J_kP(t))\Pi_N(t)^{-1}(J_kP(t))(J_lP(t))F_N(t)^{\frac12})\\&=\operatorname{trace}_{\mathfrak{H}_N}(F_N(t)^{\frac12}\Pi_N(t)^{-1}(J_kP(t))(J_lP(t))F_N(t)^{\frac12})\\&=\operatorname{trace}_{\mathfrak{H}_N}(\Pi_N(t)^{-1}(J_kP(t))(J_lP(t))F_N(t))\,,\end{aligned}$$

(the second equality follows from the fact that $J_k(P(t))$ commutes with $\Pi_N(t)$ and $\Pi_N(t)^{-1}$), so that

$$\begin{aligned}&\sum_{1\le k\ne l\le N}\|\Pi_N(t)^{-\frac12}(J_kP(t))(J_lP(t))F_N(t)^{\frac12}\|_2^2\\&\le\operatorname{trace}_{\mathfrak{H}_N}\left(\Pi_N(t)^{-1}\sum_{1\le k,l\le N}(J_kP(t))(J_lP(t))F_N(t)\right)\\&=N^2\operatorname{trace}_{\mathfrak{H}_N}(\Pi_N(t)^{-1}\Pi_N(t)^2F_N(t))=N^2\operatorname{trace}_{\mathfrak{H}_N}(\Pi_N(t)F_N(t))\,.\end{aligned}$$

The inequality above follows from the fact that

$$\begin{aligned}&\operatorname{trace}_{\mathfrak{H}_N}(\Pi_N(t)^{-1}(J_kP(t))^2F_N(t))\\&=\operatorname{trace}_{\mathfrak{H}_N}(F_N(t)^{\frac12}(J_kP(t))\Pi_N(t)^{-1}(J_kP(t))F_N(t)^{\frac12})\ge0\,.\end{aligned}$$

On the other hand

$$\sum_{1\le k\ne l\le N}\|\Pi_N(t)^{\frac12}V_{kl}(J_kR(t))(J_lR(t))F_N(t)^{\frac12}\|_2^2$$
$$=\sum_{1\le k\ne l\le N}\operatorname{trace}(F_N(t)^{\frac12}(J_lR(t))(J_kR(t))V_{kl}\Pi_N(t)V_{kl}(J_kR(t))(J_lR(t))F_N(t)^{\frac12})$$
$$=\tfrac1N\sum_{1\le k\ne l\le N}\|J_k(P(t))V_{kl}(J_kR(t))(J_lR(t))F_N(t)^{\frac12}\|_2^2$$
$$+\tfrac1N\sum_{1\le k\ne l\le N}\|J_l(P(t))V_{kl}(J_kR(t))(J_lR(t))F_N(t)^{\frac12}\|_2^2$$
$$+\tfrac1N\sum_{1\le m\ne k\ne l\le N}\|(J_mP(t))V_{kl}(J_kR(t))(J_lR(t))F_N(t)^{\frac12}\|_2^2$$
$$\le\tfrac2N\sum_{1\le k\ne l\le N}\|V_{kl}(J_kR(t))(J_lR(t))F_N(t)^{\frac12}\|_2^2$$
$$+\tfrac1N\sum_{1\le m\ne k\ne l\le N}\|(J_mP(t))V_{kl}(J_kR(t))(J_lR(t))F_N(t)^{\frac12}\|_2^2\,.$$

Now, $m\notin\{k,l\}$ implies that $J_mP(t)$ commutes with $V_{kl}$, $J_kR(t)$ and $J_lR(t)$, so that

$$\|(J_mP(t))V_{kl}(J_kR(t))(J_lR(t))F_N(t)^{\frac12}\|_2^2$$
$$=\|V_{kl}(J_kR(t))(J_lR(t))(J_mP(t))F_N(t)^{\frac12}\|_2^2$$
$$\le\|V_{kl}(J_kR(t))(J_lR(t))\|^2\|(J_mP(t))F_N(t)^{\frac12}\|_2^2$$
$$=\|V_{12}R(t)\otimes R(t)\|^2\operatorname{trace}_{\mathfrak H_N}((J_mP(t))F_N(t)(J_mP(t)))$$
$$=\|V_{12}R(t)\otimes R(t)\|^2\operatorname{trace}_{\mathfrak H_N}(\Pi_N(t)F_N(t))\,.$$

Therefore

$$\begin{aligned}
&|\operatorname{trace}_{\mathfrak H_N}(S_3F_N^{in})|\\
&\le\tfrac{1}{N^2}\cdot N\operatorname{trace}_{\mathfrak H_N}(\Pi_N(t)F_N(t))^{\frac12}\Big(\tfrac{2N(N-1)}{N}\|V_{12}R(t)\otimes R(t)\|^2\|F_N(t)\|_1\\
&\qquad+\tfrac{N(N-1)(N-2)}{N}\|V_{12}R(t)\otimes R(t)\|^2\operatorname{trace}_{\mathfrak H_N}(\Pi_N(t)F_N(t))\Big)^{\frac12}\\
&\le\tfrac{1}{\sqrt N}\|V_{12}R(t)\otimes R(t)\|\operatorname{trace}_{\mathfrak H_N}(\mathcal M_N(t)(P(t))F_N^{in})^{\frac12}\\
&\qquad\times\big(2\|F_N(t)\|_1+(N-2)\operatorname{trace}_{\mathfrak H_N}(\mathcal M_N(t)(P(t))F_N^{in})\big)^{\frac12}.
\end{aligned}\tag{55}$$

Now

$$\begin{aligned}T_3=&\mathcal T(V,\mathcal M_N(t)(P(t)\bullet R(t)),\mathcal M_N(t)(P(t)\bullet R(t)))\\
&-\mathcal T(V,\mathcal M_N(t)(R(t)\bullet P(t)),\mathcal M_N(t)(R(t)\bullet P(t)))=S_3-S_3^*=-T_3^*\,,\end{aligned}$$

according to Lemma 4.3. Thus (55) implies that

$$\begin{aligned}|\operatorname{trace}_{\mathfrak H_N}(T_3F_N^{in})|\le&2\|V_{12}R(t)\otimes R(t)\|\operatorname{trace}_{\mathfrak H_N}(\mathcal M_N(t)(P(t))F_N^{in})^{\frac12}\\
&\times\big(\tfrac2N\|F_N(t)\|_1+\tfrac{N-2}{N}\operatorname{trace}_{\mathfrak H_N}(\mathcal M_N(t)(P(t))F_N^{in})\big)^{\frac12}\,.\end{aligned}$$

According to (51)

$$\|V_{12}R(t)\otimes R(t)\|=\|V_{12}(J_1R(t))(J_2R(t))\|\le\|V_{12}J_2R(t)\|\le\ell(t)\,,$$

so that

$$|\operatorname{trace}_{\mathfrak H_N}(T_3F_N^{in})|\le2\ell(t)\big((1-\tfrac1N)\operatorname{trace}_{\mathfrak H_N}(\mathcal M_N(t)(P(t))F_N^{in})+\tfrac2N\|F_N^{in}\|_1\big)\,.\tag{56}$$

In particular

$$\operatorname{trace}_{\mathfrak{H}_N}(\pm iT_3F_N^{in})| \le 2\ell(t)\operatorname{trace}_{\mathfrak{H}_N}\left(F_N^{in}\left((1-\tfrac{1}{N})\mathcal{M}_N(t)(P(t))+\tfrac{1}{N}I_{\mathfrak{H}_N}\right)\right).$$

Since this last inequality holds for each $F_N^{in}\in\mathcal{L}(\mathfrak{H}_N)$ satisfying (31), we deduce from Lemma 7.1 that

$$\pm iT_3 \le 2\ell(t)\left((1-\tfrac{1}{N})\mathcal{M}_N(t)(P(t))+\tfrac{1}{N}I_{\mathfrak{H}_N}\right). \tag{57}$$

## 8. Proofs of part (2) in Theorem 4.1 and Corollary 4.2

8.1. **Proof of part (2) in Theorem 4.1.** Applying Lemma 4.4 shows that

$$\pm i\mathcal{C}(V,\mathcal{M}_N(t)-\mathcal{R}(t),\mathcal{M}_N(t))(R(t)) = \pm i(T_1+T_2+T_3+T_4).$$

With Lemma 4.5, this shows that

$$(\pm i\mathcal{C}(V,\mathcal{M}_N(t)-\mathcal{R}(t),\mathcal{M}_N(t))(R(t)))^* = \pm i\mathcal{C}(V,\mathcal{M}_N(t)-\mathcal{R}(t),\mathcal{M}_N(t))(R(t))$$

and that

$$\pm i\mathcal{C}(V,\mathcal{M}_N(t)-\mathcal{R}(t),\mathcal{M}_N(t))(R(t)) \le 6\ell(t)\left(\mathcal{M}_N(t)(P(t))+\tfrac{2}{N}I_{\mathfrak{H}_N}\right).$$

It remains to bound the function

$$\ell(t) := \|V^2\star|\psi(t,\cdot)|^2\|^{1/2}_{L^\infty(\mathbf{R}^3)}.$$

Since

$$V=V_1+V_2 \text{ with } V_1\in\mathcal{F}L^1(\mathbf{R}^3)\subset L^\infty(\mathbf{R}^3) \text{ and } V_2\in L^2(\mathbf{R}^3)$$

one has

$$\begin{aligned}0\le& V^2\star|\psi(t,\cdot)|^2 \le 2V_1^2\star|\psi(t,\cdot)|^2+2V_2^2\star|\psi(t,\cdot)|^2\\ \le& 2\|V_1\|^2_{L^\infty(\mathbf{R}^3)}\|\psi(t,\cdot)\|^2_{L^2(\mathbf{R}^3)}+2\|V_2\|^2_{L^2(\mathbf{R}^3)}\|\psi(t,\cdot)\|^2_{L^\infty(\mathbf{R}^3)}.\end{aligned}$$

Minimizing $\|V_1\|_{L^\infty(\mathbf{R}^3)}+\|V_2\|_{L^2(\mathbf{R}^3)}$ over all possible decompositions of $V=V_1+V_2$ as above, one has

$$\begin{aligned}0\le V^2\star|\psi(t,\cdot)|^2 \le& 4\|V\|^2_{L^2(\mathbf{R}^3)+L^\infty(\mathbf{R}^3)}\max(\|\psi(t,\cdot)\|^2_{L^2(\mathbf{R}^3)},\|\psi(t,\cdot)\|^2_{L^\infty(\mathbf{R}^3)})\\ \le& 4\|V\|^2_{L^2(\mathbf{R}^3)+L^\infty(\mathbf{R}^3)}\max(\|\psi(t,\cdot)\|^2_{L^2(\mathbf{R}^3)},C_S^2\|\psi(t,\cdot)\|^2_{H^2(\mathbf{R}^3)})\\ \le& 4\max(1,C_S)^2\|V\|^2_{L^2(\mathbf{R}^3)+L^\infty(\mathbf{R}^3)}\|\psi(t,\cdot)\|^2_{H^2(\mathbf{R}^3)} =: L(t)^2.\end{aligned}$$

8.2. **Proof of Corollary 4.2.** In [16], Pickl considers the functional

$$\alpha_N(t) := \operatorname{trace}_{\mathfrak{H}}(F_{N:1}(t)P(t))$$

(see Definition 2.2 and formula (6) in [16]), where $F_{N:1}(t)$ is the single-body reduced density operator deduced from

$$F_N(t) := \mathcal{U}_N(t)F_N^{in}\mathcal{U}_N(t)^*,$$

where $F_N^{in}\in\mathcal{L}(\mathfrak{H}_N)$ satisfies (31). Specifically $F_{N:1}(t)$ is defined by the formula

$$\operatorname{trace}_{\mathfrak{H}}(F_{N:1}(t)A) = \operatorname{trace}_{\mathfrak{H}_N}(F_N(t)J_1A), \qquad \text{for all } A\in\mathcal{L}(\mathfrak{H}).$$

8.2.1. *The Gronwall inequality for Pickl's functional.* One deduces from part (2) in Theorem 4.1 that

$$\begin{aligned}\mathcal{M}_N(t)(P(t)) =&\mathcal{M}_N^{in}(P(0)) + \tfrac{1}{\hbar}\int_0^t -i\mathcal{C}(V,\mathcal{M}_N(s)-\mathcal{R}(s),\mathcal{M}_N(s))(R(s))ds\\ \le&\mathcal{M}_N^{in}(P(0)) + \tfrac{6}{\hbar}\int_0^t L(s)\left(\mathcal{M}_N(s)(P(s)) + \tfrac{2}{N}I_{\mathfrak{H}_N}\right)ds\,.\end{aligned}$$

This inequality implies that

$$\begin{aligned}\operatorname{trace}_{\mathfrak{H}_N}((F_N^{in})^{\frac12}\mathcal{M}_N(t)(P(t))(F_N^{in})^{\frac12}) \le \operatorname{trace}_{\mathfrak{H}_N}((F_N^{in})^{\frac12}\mathcal{M}_N^{in}(P(0))(F_N^{in})^{\frac12})\\ +\tfrac{6}{\hbar}\int_0^t L(s)\left(\operatorname{trace}_{\mathfrak{H}_N}((F_N^{in})^{\frac12}\mathcal{M}_N(s)(P(s))(F_N^{in})^{\frac12}) + \tfrac{2}{N}\operatorname{trace}_{\mathfrak{H}_N}(F_N^{in})\right)ds\,.\end{aligned}$$

Now, by cyclicity of the trace and Lemma 2.3 in [8] (the *raison d'être* of $\mathcal{M}_N(t)$)

$$\begin{aligned}\operatorname{trace}_{\mathfrak{H}_N}((F_N^{in})^{\frac12}\mathcal{M}_N(t)(P(t))(F_N^{in})^{\frac12}) &= \operatorname{trace}_{\mathfrak{H}_N}(F_N^{in}\mathcal{M}_N(t)(P(t)))\\ &= \operatorname{trace}_{\mathfrak{H}}(F_{N:1}(t)P(t)) = \alpha_N(t)\,,\end{aligned}$$

so that, by Gronwall's inequality,

$$\alpha_N(t) \le \alpha_N(0)\exp\left(\tfrac{6}{\hbar}\int_0^t L(s)ds\right) + \tfrac{2}{N}\left(\exp\left(\tfrac{6}{\hbar}\int_0^t L(s)ds\right)-1\right).$$

For instance, if $F_N^{in} = |\psi^{in}\rangle\langle\psi^{in}|^{\otimes N}$ with $\psi^{in}\in\mathfrak{H}$ and $\|\psi^{in}\|_{\mathfrak{H}} = 1$, one has

$$\alpha_N(0) = \operatorname{trace}_{\mathfrak{H}_N}(R(0)^{\otimes N}\mathcal{M}_N^{in}(P(0))) = \operatorname{trace}_{\mathfrak{H}}(R(0)P(0)) = 0\,,$$

so that

$$\alpha_N(t) \le \frac{2}{N}\left(\exp\left(\tfrac{6}{\hbar}\int_0^t L(s)ds\right)-1\right) = O\left(\frac{1}{N}\right).$$

8.2.2. *Pickl's functional and the trace norm.* How the inequality above implies the mean-field limit is explained by the following lemma, which recaps the results stated as Lemmas 2.1 and 2.2 in [14], and whose proof is given below for the sake of keeping the present paper self-contained.

If $F_N^{in}\in\mathcal{L}(\mathfrak{H}_N)$ satisfies (31), for each $m = 1,\dots,N$, we denote by $F_{N:m}(t)$ the $m$-particle reduced density operator deduced from $F_N(t) = \mathcal{U}_N(t)F_N^{in}\mathcal{U}_N(t)^*$, i.e.

$$\operatorname{trace}_{\mathfrak{H}_m}(F_{N:m}(t)A_1\otimes\ldots\otimes A_m) = \operatorname{trace}_{\mathfrak{H}_N}(F_N(t)(J_1A_1)\ldots(J_mA_m))$$

for all $A_1,\dots,A_m\in\mathcal{L}(\mathfrak{H})$.

**Lemma 8.1.** *The Pickl functional satisfies the inequality*

$$\|F_{N:m}(t) - R(t)^{\otimes m}\|_1 \le 2\sqrt{2m\operatorname{trace}_{\mathfrak{H}}(F_{N:1}(t)P(t))}\,,\qquad m = 1,\dots,N\,.$$

*Proof.* Call $\mathcal{P}_-$ the spectral projection on the direct sums of eigenspaces of the trace-class operator $F_{N:m}(t)-R(t)^{\otimes m}$ corresponding to negative eigenvalues. Then the self-adjoint operator

$$\mathcal{P}_-F_{N:m}(t)\mathcal{P}_- - \mathcal{P}_-R(t)^{\otimes m}\mathcal{P}_- = \mathcal{P}_-F_{N:m}(t)\mathcal{P}_- - |\mathcal{P}_-\psi(t,\cdot)^{\otimes m}\rangle\langle\mathcal{P}_-\psi(t,\cdot)^{\otimes m}|$$

must have only negative eigenvalues by definition of $\mathcal{P}_-$, and is obviously nonnegative on the orthogonal complement of $\mathcal{P}_-\psi(t,\cdot)^{\otimes m}$ in the range of $\mathcal{P}_-$. By definition of $\mathcal{P}_-$, this orthogonal complement must be $\{0\}$. Hence $\mathcal{P}_-$ is a rank-one projection, so that $F_{N:m}(t) - R(t)^{\otimes m}$ has only one negative eigenvalue $\lambda_0$, with all its other eigenvalues $\lambda_1,\lambda_2,\dots$ being nonnegative. Since

$$\operatorname{trace}_{\mathfrak{H}_m}(F_{N:m}(t) - R(t)^{\otimes m}) = \sum_{j\ge1}\lambda_j + \lambda_0 = 0\,,$$

one has[5]

$$\begin{aligned}\|F_{N:m}(t) - R(t)^{\otimes m}\|_1 = \sum_{j\geq 1}\lambda_j + |\lambda_0| = 2|\lambda_0| =&2\|F_{N:m}(t) - R(t)^{\otimes m}\|\\ \leq&2\|F_{N:m}(t) - R(t)^{\otimes m}\|_2\,.\end{aligned}$$

Now $F_{N:m}(t)$ is self-adjoint, and therefore

$$\begin{aligned}\|F_{N:m}(t) - R(t)^{\otimes m}\|_2^2 =&\operatorname{trace}_{\mathfrak{H}_m}((F_{N:m}(t) - R(t)^{\otimes m})^2)\\ =&\operatorname{trace}_{\mathfrak{H}_m}(F_{N:m}(t)^2 + R(t)^{\otimes m})\\ &-\operatorname{trace}_{\mathfrak{H}_m}(F_{N:m}(t)R(t)^{\otimes m} + R(t)^{\otimes m}F_{N:m}(t))\\ \leq&2 - 2\operatorname{trace}_{\mathfrak{H}_m}(R(t)^{\otimes m}F_{N:m}(t)R(t)^{\otimes m})\\ =&2\operatorname{trace}_{\mathfrak{H}_m}(F_{N:m}(t)(I_{\mathfrak{H}}^{\otimes m} - R(t)^{\otimes m}))\,.\end{aligned}$$

Hence

$$\|F_{N:m}(t) - R(t)^{\otimes m}\|_1 \leq 2\sqrt{2\operatorname{trace}_{\mathfrak{H}_m}(F_{N:m}(t)(I_{\mathfrak{H}}^{\otimes m} - R(t)^{\otimes m}))}\,.$$

Since $R(t) = |\psi(t,\cdot)\rangle\langle\psi(t,\cdot)|$ is a self-adjoint projection

$$\begin{aligned}&R(t)\otimes I_{\mathfrak{H}}^{\otimes(m-1)} - R(t)^{\otimes m}\\ &= (I_{\mathfrak{H}}^{\otimes m} - I_{\mathfrak{H}}\otimes R(t)^{\otimes(m-1)})R(t)\otimes I_{\mathfrak{H}}^{\otimes(m-1)}(I_{\mathfrak{H}}^{\otimes m} - I_{\mathfrak{H}}\otimes R(t)^{\otimes(m-1)})\\ &\leq (I_{\mathfrak{H}}^{\otimes m} - I_{\mathfrak{H}}\otimes R(t)^{\otimes(m-1)})^2 = (I_{\mathfrak{H}}^{\otimes m} - I_{\mathfrak{H}}\otimes R(t)^{\otimes(m-1)})\end{aligned}$$

so that

$$\begin{aligned}&\operatorname{trace}_{\mathfrak{H}}(F_{N:1}(t)R(t)) - \operatorname{trace}_{\mathfrak{H}_m}(F_{N:m}(t)R(t)^{\otimes m})\\ &= \operatorname{trace}_{\mathfrak{H}_m}(F_{N:m}(t)(R(t)\otimes I_{\mathfrak{H}}^{\otimes(m-1)} - R(t)^{\otimes m}))\\ &\leq \operatorname{trace}_{\mathfrak{H}_m}(F_{N:m}(t)(I_{\mathfrak{H}}^{\otimes m} - I_{\mathfrak{H}}\otimes R(t)^{\otimes(m-1)}))\\ &= 1 - \operatorname{trace}_{\mathfrak{H}_{m-1}}(F_{N:m-1}(t)R(t)^{\otimes(m-1)})\,.\end{aligned}$$

Since $F_N^{in}$ satisfies (31), the reduced $m$-particle operator $F_{N:m}(t) \in \mathcal{L}(\mathfrak{H}_m)$ also satisfies (31) (with $N$ replaced by $m$), and hence

$$\begin{aligned}\operatorname{trace}_{\mathfrak{H}_m}(F_{N:m}(t)(I_{\mathfrak{H}}^{\otimes m} - R(t)^{\otimes m})) \leq&1 - \operatorname{trace}_{\mathfrak{H}}(F_{N:1}(t)R(t))\\ &+ 1 - \operatorname{trace}_{\mathfrak{H}_{m-1}}(F_{N:m-1}(t)R(t)^{\otimes(m-1)})\\ \leq&m(1 - \operatorname{trace}_{\mathfrak{H}}(F_{N:1}(t)R(t)))\\ =&m\operatorname{trace}_{\mathfrak{H}}(F_{N:1}(t)P(t))\,,\end{aligned}$$

by induction, which implies the inequality in the lemma. □

With this lemma, the consequence of the Gronwall inequality above implies that, under the assumptions of Corollary 4.2,

$$\|F_{N:m}(t) - R(t)^{\otimes m}\|_1 \leq \sqrt{8m\alpha_N(t)} \leq 4\sqrt{\frac{m}{N}}\exp\left(\tfrac{3}{\hbar}\int_0^t L(s)ds\right)\,.$$

This completes the proof of Corollary 4.2.

[5]This observation is attributed to Seiringer on p. 35 in [18].

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