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Empirical Measures and Quantum Mechanics: Applications to the Mean-Field Limit

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Abstract: In this paper, we define a quantum analogue of the notion of empirical measure in the classical mechanics of N-particle systems. We establish an equation governing the evolution of our quantum analogue of the N-particle empirical measure, and we prove that this equation contains the Hartree equation as a special case. Applications to the mean-field limit of the N-particle Schrödinger equation include an $O(1/\sqrt{N})$ convergence rate in some appropriate dual Sobolev norm for the Wigner transform of the single-particle marginal of the N-particle density operator, uniform in $\hbar \in (0,1]$ provided that V and $(-\Delta)^{3/2+d/4}V$ have integrable Fourier transforms.

1. Introduction and Main Result

1.1. The mean-field limit for the dynamics of N identical particles. In classical mechanics, the dynamics of N identical, interacting point particles is governed by Newton's second law of motion written for each particle. One obtains in this way a system of $6N$ coupled ordinary differential equations, set on a $6N$-dimensional phase space. For large values of N, solving such a differential system becomes impracticable. One way of reducing the complexity of this problem is to solve the Liouville equation for the phase space number density of the "typical particle", replacing the force exerted on that particle by the "self-consistent" force, also called the "mean-field force", computed in terms of the solution of the Liouville equation itself. The mean-field equation so obtained is the Vlasov equation (see equation (10) below). When the force field derives from a $C^{1,1}$ potential, the validity of this approximation has been proved in [10,12,35]. The case of the Coulomb (electric), or of the Newton (gravitational) potential remains open at the time of this writing, in spite of significant progress on this program: see [24,25] for singularities weaker than the Coulomb or Newton $1/r$ singularity at the origin, or [29,30] for the Coulomb potential with a vanishing regularization as the particle number N tends to infinity.

All these results are based on a remarkable property of the phase-space empirical measure of the N-particle system governed by a system of coupled ordinary differential equations. This property, first established by Klimontovich (see [27] and references therein), is stated as Proposition 1.2 below. See also [33] for another approach, which avoids using the nice properties of this empirical measure, and applies to more general dynamics (involving jump or diffusion processes for instance).

In quantum mechanics, the analogous mean-field approximation goes back to the work of Hartree [23]. Rigorous derivations of the time-dependent Hartree equation from the quantum N-body problem have been obtained in the case of bounded potentials by Spohn [40] (for pure states, using the BBGKY hierarchy)—see also [3] for a discussion of the case of mixed states following Spohn's very concise argument. The case of singular potentials, including the Coulomb potential, is treated in [13] (see also [4]) in terms of the BBGKY hierarchy, in [28,37] by a simpler argument in the case of pure states, and in [7,11,39] with second quantization techniques (using in particular an important observation on coherent states due to Hepp [26] in the case of bounded potentials, and extended by Ginibre and Velo [15,16] for singular potentials). All these results assume that the value of the Planck constant is kept fixed while N tends to infinity. This is also true in the special case of the Fermi-Dirac statistics which involves a mean-field scaling of the interaction leading, after some appropriate rescaling of time, to an *effective* Planck constant $\hbar \sim N^{-1/3}$: see [5,34,38].

On the other hand, the system of Newton's equations governs the asymptotic behavior of the quantum N-body problem for all N kept fixed as $\hbar$ tends to zero. Equivalently, the asymptotic behavior of solutions of the von Neumann equation in the classical limit is described by the Liouville equation. Since the von Neumann equation governs the evolution of time-dependent density operators on some Hilbert space, while the Liouville equation describes the dynamics of a probability density in phase space, the classical limit can be formulated in terms of the Wigner function, associated to any quantum observable as recalled in Appendix B. There is a huge literature on this subject; see for instance [31] for a proof of the weak convergence of the Wigner function of a solution of the von Neumann equation to a positive measure, solution of the Liouville equation, in the limit as $\hbar \to 0$. This result holds true for all $C^{1,1}$ potentials and a very general class of initial data (without any explicit dependence in $\hbar$). Likewise, the Vlasov equation governs the asymptotic behavior of solutions of the Hartree equation (equation (3) below) for a very large class of potentials including the Coulomb case: see again [31] for a result formulated in terms of weak convergence of Wigner functions. For regular potentials, more precise information on the convergence of Wigner functions can be found in [1,2,6].

In other words, the mean-field limit has been established rigorously both for each fixed $\hbar > 0$ and for the vanishing $\hbar$ limit of the quantum N-particle dynamics independently. This suggests the problem of obtaining a uniform in $\hbar \in (0, 1]$ convergence rate estimate for the mean-field limit of the quantum N-particle dynamics. A positive answer to this question, valid without restriction on the initial data, would justify in particular using the Vlasov instead of the Hartree equation for large systems of heavy particles.

The first results in this direction are [36] (where the mean-field limit is established term by term in the semiclassical expansion) and [22] for WKB states along distinguished limits of the form $N \to +\infty$ with $\hbar \equiv \hbar(N) \to 0$. See also [14] for results in the case of very special interactions, not defined in terms of a potential.

If both the interaction potential and the initial data are analytic, the BBGKY approach leads to a uniform in $\hbar \in (0, 1]$ convergence rate estimate for the mean-field limit, of optimal order $O(1/N)$: see [21]. This $O(1/N)$ bound, obtained at the cost of stringent, physically unsatisfying regularity assumptions, is similar to the nonuniform in $\hbar$ convergence rate obtained in [11]—except the latter result holds for singular potentials including the Coulomb case.

A new approach to the uniformity problem has been proposed in [17,19]; it is based on a quantum analogue of the quadratic Monge–Kantorovich–Wasserstein distance, similar to the one used in [12]. This method provides an estimate of the convergence rate in the mean-field limit that is uniform as $\hbar \to 0$. This method can be combined with the usual BBGKY strategy, following carefully the dependence of the error estimate in terms of $\hbar$, to produce a uniform in $\hbar \in (0, 1]$ convergence rate of order $O((\ln \ln N)^{-1/2})$ for initial data of semiclassical type: see [21].

The main results of the present article are Theorem 1.1, and Theorem 3.3 together with Definition 2.2. Theorem 1.1 establishes the quantum mean-field limit with rate of convergence of order $\frac{1}{\sqrt{N}}$, uniformly in $\hbar \in (0, 1]$ and for all initial factorized data. By "all", we mean that any dependence in the Planck constant is allowed. In our main statement ((7) in Theorem 1.1), the Planck constant appears only in the Wigner functions in terms of which the convergence rate at time t for the mean-field limit is expressed, in a Sobolev type dual norm (1)–(2). Equivalently, according to formula (63), this corresponds to pairing the evolved density operators with semiclassical Weyl operators whose full symbol is any test function in the definition of the dual norm.

The proof of Theorem 1.1 requires defining a notion of empirical "measure" in quantum mechanics. The precise definition of this new (to the best of our knowledge) mathematical object can be found in Definition 2.2 of Sect. 3, and the equation governing its dynamics is derived in Theorem 3.3.

1.2. The uniform in $\hbar$ convergence rate for the mean-field limit. Before stating this convergence rate estimate, we need to introduce some notation used systematically in the present paper.

Denote by $\mathfrak{H} := L^2(\mathbf{R}^d)$ (the single-particle Hilbert space) and, for each $N \geq 1$, let $\mathfrak{H}_N := \mathfrak{H}^{\otimes N} \simeq L^2((\mathbf{R}^d)^N)$. Henceforth, $\mathcal{L}(\mathfrak{H})$ (resp. $\mathcal{L}^1(\mathfrak{H})$) designates the space of bounded (resp. trace-class) operators on $\mathfrak{H}$. For each permutation $\sigma \in \mathfrak{S}_N$ (the group of permutations of $\{1, \ldots, N\}$), let U_σ be the unitary operator on $\mathfrak{H}_N$ defined by the formula

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

We denote by $\mathcal{L}_s(\mathfrak{H}_N)$ (resp. $\mathcal{L}_s^1(\mathfrak{H}_N)$) the set of bounded (resp. trace-class) operators F_N on $\mathfrak{H}_N$ satisfying the condition

$$U_\sigma F_N U_\sigma^* = F_N\,, \qquad \text{for all } \sigma \in \mathfrak{S}_N.$$

We denote by $\mathcal{D}(\mathfrak{H})$ the set of density operators on $\mathfrak{H}$, i.e. operators R satisfying

$$R = R^* \geq 0\,, \qquad \operatorname{trace}_{\mathfrak{H}}(R) = 1.$$

Likewise, we denote by $\mathcal{D}_s(\mathfrak{H}_N)$ the set of symmetric N-particle densities on $\mathfrak{H}_N$, i.e. $\mathcal{D}_s(\mathfrak{H}_N) := \mathcal{D}(\mathfrak{H}_N) \cap \mathcal{L}_s(\mathfrak{H}_N)$.

Let $R_N \in \mathcal{D}_s(\mathfrak{H}_N)$; set $r_N \equiv r_N(x_1, \ldots, x_N; y_1, \ldots, y_N)$ to be the integral kernel of R_N. The first marginal of the quantum density R_N is the element $R_{N:1}$ of $\mathcal{D}(\mathfrak{H})$ whose integral kernel is

$$r_{N:1}(x, y) := \int_{(\mathbf{R}^d)^{N-1}} r_N(x, z_2, \ldots, z_N; y, z_2, \ldots, z_N)\, dz_2 \ldots dz_N.$$

For each integer $n \geq 0$, we denote by $C_b^{n,n}(\mathbf{R}^d \times \mathbf{R}^d)$ the set of complex-valued functions $f \equiv f(x,\xi)$ on $\mathbf{R}^d \times \mathbf{R}^d$ such that $\partial_x^\alpha \partial_\xi^\beta f$ exists, and is continuous and bounded on $\mathbf{R}^d \times \mathbf{R}^d$ for all $\alpha, \beta \in \mathbf{N}^d$ such that $\max(|\alpha|,|\beta|) \leq n$. This is a Banach space for the norm

$$\|f\|_{n,n,\infty} := \max_{\max(|\alpha|,|\beta|)\leq n} \|\partial_x^\alpha \partial_\xi^\beta f\|_{L^\infty(\mathbf{R}^d\times\mathbf{R}^d)}. \tag{1}$$

Finally, let $\|\cdot\|'_{n,n,\infty}$ be the norm of the topological dual of $C_b^{n,n}(\mathbf{R}^d \times \mathbf{R}^d)$. In other words, for each continuous linear functional L on $C_b^{n,n}(\mathbf{R}^d \times \mathbf{R}^d)$, one has

$$\|L\|'_{n,n,\infty} := \sup\{|\langle L, f\rangle| \text{ s.t. } \|f\|_{n,n,\infty} \leq 1\}. \tag{2}$$

Theorem 1.1. *Assume that $V \in C_0(\mathbf{R}^d)$ is an even, real-valued function whose Fourier transform $\hat{V}$ satisfies*

$$\mathbf{V} := \tfrac{1}{(2\pi)^d} \int_{\mathbf{R}^d} |\hat{V}(\omega)|(1+|\omega|)^{[d/2]+3}\, \mathrm{d}\omega < \infty.$$

Let $R^{in} \in \mathcal{D}(\mathfrak{H})$, and let $t \mapsto R(t)$ be the solution to the Cauchy problem for the Hartree equation

$$i\hbar\partial_t R(t) = [-\tfrac{1}{2}\hbar^2\Delta + V_{R(t)}, R(t)]\,, \qquad R(0) = R^{in}\,, \tag{3}$$

with mean-field potential

$$V_{R(t)}(x) := \int_{\mathbf{R}^d} V(x-z) r(t,z,z)\, \mathrm{d}z\,, \tag{4}$$

where $r \equiv r(t,x,y)$ is the integral kernel of $R(t)$.

For each $N \geq 2$, let $t \mapsto F_N(t)$ be the solution to the Cauchy problem for the von Neumann equation

$$i\hbar\partial_t F_N(t) = [\mathscr{H}_N, F_N(t)]\,, \qquad F_N(0) = F_N^{in}\,, \tag{5}$$

with initial data $F_N^{in} = (R^{in})^{\otimes N}$, where the N-body quantum Hamiltonian is

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

Then, for all $\hbar \in (0,1]$, all $N \geq 1$ and all $t \geq 0$, the Wigner transforms at scale $\hbar$ of $F_{N:1}(t)$ and $R(t)$ satisfy the bound

$$\|W_\hbar[F_{N:1}(t)] - W_\hbar[R(t)]\|'_{[d/2]+2,[d/2]+2,\infty} \leq \frac{\gamma_d + 1}{\sqrt{N}} \exp\left(\sqrt{d}\gamma_d t e^{t\max(1,\Gamma_2)}\mathbf{V}\right), \tag{7}$$

where

$$\Gamma_2 := \max_{1\leq j\leq d} \sum_{k=1}^d \tfrac{1}{(2\pi)^d} \int_{\mathbf{R}^d} |\hat{V}(\omega)||\omega_j||\omega_k|\, \mathrm{d}\omega\,,$$

while γ_d is a positive constant which depends only on the space dimension d.

The definition and the elementary properties of the Wigner transform are recalled in the Appendix. We recall that, in the classical limit, i.e. for $\hbar \to 0$, quantum densities propagated by the von Neumann equation will typically fail to converge to any limiting density operator. However, up to extracting subsequences $\hbar_n \to 0$, the corresponding sequence of Wigner transforms will have limit points in $\mathcal{S}'(\mathbf{R}^d \times \mathbf{R}^d)$, and the classical limit of quantum mechanics can be described in terms of the evolution of these limit points. See [31] for a presentation of this description of the classical limit (especially Theorems III.1 and IV.1 in [31]).

The $O(1/\sqrt{N})$ estimate in this result is on a par with the convergence rate obtained in [39]—except (7) is uniform in $\hbar \in (0, 1]$, unlike the bound in [39]. On the other hand, one should keep in mind that the regularity assumptions on the potential are more stringent in Theorem 1.1 than in [39], which can handle singular potentials, including the Coulomb case.

Notice that γ_d is the constant which appears in the Calderon–Vaillancourt theorem (Theorem B.1 in Appendix B).

Notice also the double exponential growth in time of the bound in Theorem 1.1, to be compared either with the simple exponential growth in the nonuniform in $\hbar$ convergence rate in [39], or in the uniform as $\hbar \to 0$ estimate in [17].

A last difference between the convergence rate obtained in [11,39] and the bound in Theorem 1.1 lies in the metric used to measure the difference between the Hartree solution and the first marginal of the N-body density operator: the estimate in [11,39] is expressed in terms of the trace norm, whereas (7) is formulated in terms of Wigner transforms, whose difference is measured in some dual Sobolev norm. In the classical limit, quantum particles are expected to be perfectly localized on phase-space curves, and Schatten norms (including the trace norm) are ill-suited to capturing this asymptotic behavior—see section 5 of [20] for a detailed discussion of this point.

Finally, the choice of initial data $F_N^{in} = (R^{in})^{\otimes N}$ in Theorem 1.1 is consistent with bosonic statistics, i.e. with the assumption that

$$U_\sigma F^{in} = F_N^{in} U_\sigma = F^{in} \qquad \text{for all } \sigma \in \mathfrak{S}_N \,,$$

if and only if R^{in} is of the form

$$R^{in} = |\psi^{in}\rangle\langle\psi^{in}| \,, \qquad \text{with } \psi^{in} \in L^2(\mathbf{R}^d) \text{ and } \|\psi^{in}\|_{L^2(\mathbf{R}^d)} = 1 \,,$$

(using Dirac's bra-ket notation) i.e. if and only if R^{in} is a rank-one orthogonal projection. In other words, the initial data in Theorem 1.1 is consistent with bosonic statistics if and only if it is a factorized pure state. Of course the mathematical result holds for the more general class of initial data considered in Theorem 1.1.

1.3. Empirical measure of N-particle systems in classical mechanics. As mentioned above, an important ingredient in the rigorous derivation of the Vlasov equation from the N-particle system of Newton's equations in classical mechanics (see [10,12]) is the following remarkable property of the empirical measure, which is briefly recalled below for the reader's convenience.

Consider the system of Newton's equations of motion for a system of N identical point particles of mass 1, with pairwise interaction given by a (real-valued) potential V/N assumed to be even and smooth (at least C^2) on $\mathbf{R}^d$, and such that V, ∇V and $\nabla^2 V$ are bounded on $\mathbf{R}^d$:

$$\begin{cases} \dot{x}_k = \xi_k \,, & x_k(0) = x_k^{in} \,, \\ \\ \dot{\xi}_k = -\dfrac{1}{N}\displaystyle\sum_{l=1}^{N} \nabla V(x_k - x_l) \,, & \xi_k(0) = \xi_k^{in} . \end{cases} \tag{8}$$

(The term corresponding to $l = k$ in the sum is equal to 0 since V is even). We denote by T_t^N the flow defined by the differential system (8).

Set $z_k := (x_k, \xi_k)$ and $Z_N := (z_1, \dots, z_N)$. To each N-tuple $Z_N \in (\mathbf{R}^d \times \mathbf{R}^d)^N$, one associates the empirical measure

$$\mu_{Z_N} := \frac{1}{N} \sum_{k=1}^{N} \delta_{z_k} . \tag{9}$$

One defines in this way a map

$$(\mathbf{R}^d \times \mathbf{R}^d)^N \ni Z_N \mapsto \mu_{Z_N} \in \mathcal{P}(\mathbf{R}^d \times \mathbf{R}^d)$$

(where $\mathcal{P}(X)$ designates the set of Borel probability measures on X). The system (8) takes the form

$$\dot{x}_k = \xi_k \,, \qquad \dot{\xi}_k = -\int_{\mathbf{R}^d \times \mathbf{R}^d} \nabla V(x_k - y) \mu_{Z_N}(\mathrm{d}y\,\mathrm{d}\eta) \,, \qquad 1 \le k \le N \,,$$

and this implies the following remarkable result.

Proposition 1.2. *For each $N \ge 1$, the map $t \mapsto \mu_{T_t^N Z_N}$ is continuous on $\mathbf{R}$ with values in $\mathcal{P}(\mathbf{R}^d \times \mathbf{R}^d)$ equipped with the weak topology, and is a weak solution (in the sense of distributions) to the Vlasov equation*

$$\partial_t f + \xi \cdot \nabla_x f - \operatorname{div}_\xi \big(f (\nabla_x V \star_{x,\xi} f) \big) = 0. \tag{10}$$

With Proposition 1.2, the derivation of the Vlasov equation (10) from Newton's equations (8) for N-particle systems is equivalent to the continuous dependence of weak solutions to (10) on the initial data for the weak topology of Borel probability measures on the single particle phase-space.

In view of the conceptual simplicity of the approach of the mean-field limit in classical mechanics based on the empirical measure (see [10,12,35]), it seems that a similar structure on the quantum N-body problem would be extremely helpful for the purpose of deriving the mean-field limit with a uniform convergence rate in the Planck constant $\hbar$.

A notion of empirical measure in quantum mechanics will be introduced in Definition 2.2 below. The equation governing its evolution—equation (34)—will be derived in Theorem 3.3. The Hartree equation can be viewed as a "special case" of equation (34). More precisely, Theorem 3.5 states that solutions to the Hartree equation can be identified with a special class of solutions to equation (34).

There is an obvious difficulty with the problem addressed in Theorems 3.3 and 3.5: indeed, the proof of Proposition 1.2 is based on the method of characteristics for solving transport equations such as (10). But there is no obvious analogue of particle trajectories or of the method of characteristics in quantum mechanics. This explains why the proofs of Theorems 3.3 and 3.5 require a quite involved algebraic setting. (See Appendix A for additional insight on this algebraic structure).

1.4. Outline of the paper. Sections 2 and 3 are focussed on the problem of defining a notion of quantum empirical measure and deriving the equation governing its evolution. The analogue of the empirical measure in quantum mechanics proposed here is $\mathcal{M}_N(t)$ introduced in Definition 2.2 (in Sect. 2). The equation governing the evolution of $\mathcal{M}_N(t)$ is (34), established in Theorem 3.3 (in Sect. 3).

Of critical importance in (34) is the contribution of the interaction term involving the potential V. This interaction term can be viewed as a twisted variant of the commutator $[V_{R(t)}, R(t)]$ that appears on the right hand side of (3), and is defined in formula (27) and in Proposition 3.2. In fact, equation (34) itself is a noncommutative variant of the time-dependent Hartree equation (3) (in terms of density operators).

More precisely, there exists a special class (defined in (36)) of solutions to the equation (34) satisfied by our quantum analogue of the empirical measure, for which this equation is exactly equivalent to the time-dependent Hartree equation (3): see Theorem 3.5.

The main application of this new notion of quantum empirical "measure" is Theorem 1.1, whose proof occupies Sect. 4.

Various fundamental notions and results on Weyl's quantization needed in this paper are recalled in Appendix B.

2. A Quantum Analogue of the Notion of Empirical Measure

2.1. Marginals of N-particle densities. First we recall the notion of k-particle marginal of a symmetric probability density f_N on $(\mathbf{R}^d \times \mathbf{R}^d)^N$, the N-particle (classical) phase-space.

For each $p \in [1, +\infty]$, we designate by $L^p_s((\mathbf{R}^d \times \mathbf{R}^d)^N)$ the set of functions $\phi \equiv \phi(x_1, \xi_1, \dots, x_N, \xi_N)$ such that $\phi \in L^p((\mathbf{R}^d \times \mathbf{R}^d)^N)$ and

$$\phi(x_{\sigma(1)}, \xi_{\sigma(1)}, \dots, x_{\sigma(N)}, \xi_{\sigma(N)}) = \phi(x_1, \xi_1, \dots, x_N, \xi_N) \quad \text{a.e. on } (\mathbf{R}^d \times \mathbf{R}^d)^N$$

for all $\sigma \in \mathfrak{S}_N$.

For each $N > 1$, let $f_N \equiv f_N(x_1, \xi_1, \dots, x_N, \xi_N)$ be a symmetric probability density on the N-particle phase-space $(\mathbf{R}^d \times \mathbf{R}^d)^N$. In other words,

$$f_N \in L^1_s((\mathbf{R}^d \times \mathbf{R}^d)^N), \qquad f_N \geq 0 \quad \text{a.e. on } (\mathbf{R}^d \times \mathbf{R}^d)^N,$$

and

$$\int_{(\mathbf{R}^d \times \mathbf{R}^d)^N} f_N(x_1, \xi_1, \dots, x_N, \xi_N)\, \mathrm{d}x_1\, \mathrm{d}\xi_1 \dots \mathrm{d}x_N\, \mathrm{d}\xi_N = 1.$$

The k-particle marginal of f_N is the symmetric probability density on the k-particle phase-space $(\mathbf{R}^d \times \mathbf{R}^d)^k$ defined by the formula

$$\begin{aligned} &f_{N:k}(x_1, \xi_1, \dots, x_k, \xi_k) \\ &\quad := \int_{(\mathbf{R}^d \times \mathbf{R}^d)^{N-k}} f_N(x_1, \xi_1, \dots, x_N, \xi_N)\, \mathrm{d}x_{k+1}\, \mathrm{d}\xi_{k+1} \dots \mathrm{d}x_N\, \mathrm{d}\xi_N. \end{aligned}$$

The analogous notion for symmetric, quantum N-particle density operators is defined as follows.

Definition 2.1. Let $N \geq 1$ and $F_N \in \mathcal{D}_s(\mathfrak{H}_N)$. For each $k = 1, \dots, N$, the k-particle marginal of F_N is the unique $F_{N:k} \in \mathcal{D}_s(\mathfrak{H}_k)$ such that

$$\operatorname{trace}_{\mathfrak{H}_k}(A_k F_{N:k}) = \operatorname{trace}_{\mathfrak{H}_N}((A_k \otimes I^{\otimes(N-k)}) F_N), \qquad \text{for all } A_k \in \mathcal{L}(\mathfrak{H}_k).$$

(In particular $F_{N:N} = F_N$.)

2.2. A quantum notion of empirical measure. Let f_N^{in} be a symmetric probability density on $(\mathbf{R}^d \times \mathbf{R}^d)^N$, and set

$$f_N(t, x_1, \xi_1, \ldots, x_N, \xi_N) := f^{in}(T_{-t}^N(x_1, \xi_1, \ldots, x_N, \xi_N)),$$

where T_t^N is the flow defined by the differential system (8).

Specializing formula (32) in [18] to $m = 1$ leads to the identity

$$f_{N:1}(t, x, \xi)\,\mathrm{d}x\,\mathrm{d}\xi = \int_{(\mathbf{R}^d\times\mathbf{R}^d)^N} \mu_{T_t^N Z_N}(\mathrm{d}x\,\mathrm{d}\xi) f_N^{in}(Z_N)\,\mathrm{d}Z_N, \tag{11}$$

which holds for each symmetric probability density f_N^{in} on $(\mathbf{R}^d \times \mathbf{R}^d)^N$. Equivalently, equation (11) can be recast as

$$\begin{aligned} &\int_{\mathbf{R}^d\times\mathbf{R}^d} \phi(x, \xi) f_{N:1}(t, x, \xi)\,\mathrm{d}x\,\mathrm{d}\xi \\ &= \int_{(\mathbf{R}^d\times\mathbf{R}^d)^N} \left(\int_{\mathbf{R}^d\times\mathbf{R}^d} \phi(x, \xi)\mu_{T_t^N Z_N}(\mathrm{d}x\,\mathrm{d}\xi)\right) f_N^{in}(Z_N)\,\mathrm{d}Z_N \end{aligned} \tag{12}$$

for each test function $\phi \in L^\infty(\mathbf{R}^d \times \mathbf{R}^d)$.

In other words, for each $t \in \mathbf{R}$, the time-dependent, measure-valued function

$$m_N(t; Z_N, \mathrm{d}x\,\mathrm{d}\xi) := \mu_{T_t^N Z_N}(\mathrm{d}x\,\mathrm{d}\xi) \tag{13}$$

is the integral kernel of the (unique) linear map

$$M_N(t) : L^\infty(\mathbf{R}^d \times \mathbf{R}^d) \to L_s^\infty((\mathbf{R}^d \times \mathbf{R}^d)^N) \tag{14}$$

such that

$$\int_{\mathbf{R}^d\times\mathbf{R}^d} (M_N(t)\phi)(Z_N) f_N^{in}(\mathrm{d}Z_N) := \int_{\mathbf{R}^d\times\mathbf{R}^d} \phi(x, \xi) f_{N:1}(t, x, \xi)\,\mathrm{d}x\,\mathrm{d}\xi \tag{15}$$

for each symmetric probability density on $(\mathbf{R}^d \times \mathbf{R}^d)^N$. That (15) holds for each symmetric probability density f_N^{in} on $(\mathbf{R}^d \times \mathbf{R}^d)^N$ implies indeed that

$$M_N(t)\phi := \Phi_N \circ T_t^N,$$

where

$$\Phi_N(Z_N) := \frac{1}{N}\sum_{j=1}^N \phi(x_j, \xi_j) = \int_{\mathbf{R}^d\times\mathbf{R}^d} \phi(x, \xi)\mu_{Z_N}(\mathrm{d}x\,\mathrm{d}\xi).$$

In quantum mechanics, the analogue of the differential system (8) is the N-body Schrödinger equation

$$i\hbar\partial_t \Psi_N = \mathscr{H}_N \Psi_N, \tag{16}$$

where $\Psi_N \equiv \Psi_N(t, x_1, \ldots, x_N) \in \mathbf{C}$ is the N-body wave function, and where $\mathscr{H}_N$ is the quantum N-body Hamiltonian defined in (6), which is recast as

$$\mathscr{H}_N := \sum_{k=1}^N -\tfrac{1}{2}\hbar^2\Delta_{x_k} + \frac{1}{N}\sum_{1\le k<l\le N} V_{kl}. \tag{17}$$

For each $k, l = 1, \ldots, N$, the notation V_{kl} in (17) designates the (multiplication) operator defined by

$$(V_{kl}\Psi_N)(x_1, \ldots, x_N) := V(x_k - x_l)\Psi_N(x_1, \ldots, x_N).$$

Since $V \in L^\infty(\mathbf{R}^d)$, the operator V_{kl} is bounded on $\mathfrak{H}_N$ for all $k, l = 1, \ldots, N$, and $\mathscr{H}_N$ defines a self-adjoint operator on $\mathfrak{H}_N$ with domain $H^2((\mathbf{R}^d)^N)$. The quantum analogue of the flow T_t^N is the unitary group $U_N(t) := e^{it\mathscr{H}_N/\hbar}$, and, since the function V is even, one easily checks that

$$F_N^{in} \in \mathcal{D}_s(\mathfrak{H}_N) \Rightarrow F_N(t) := U_N(t)^* F_N^{in} U_N(t) \in \mathcal{D}_s(\mathfrak{H}_N) \text{ for all } t \in \mathbf{R}. \tag{18}$$

Formula (15) suggests that the quantum analogue of the empirical measure

$$\mu_{T_t^N Z_N}(\mathrm{d}x\,\mathrm{d}\xi)$$

used in classical mechanics is the time-dependent linear map defined below.

For each $k = 1, \ldots, N$, we denote by J_k the linear map from $\mathcal{L}(\mathfrak{H})$ to $\mathcal{L}(\mathfrak{H}_N)$ defined by the formula

$$J_k A := \underbrace{I \otimes \ldots \otimes I}_{k-1 \text{ terms}} \otimes A \otimes \underbrace{I \otimes \ldots \otimes I}_{N-k \text{ terms}}.$$

Definition 2.2. For each $N \geq 1$, set

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

For all $t \in \mathbf{R}$, we define $\mathcal{M}_N(t) \in \mathcal{L}(\mathcal{L}(\mathfrak{H}), \mathcal{L}_s(\mathfrak{H}_N))$ by the formula

$$\mathcal{M}_N(t)A := U_N(t)(\mathcal{M}_N^{in}A)U_N(t)^*.$$

With this definition, one easily arrives at the quantum analogue of (12).

Lemma 2.3. *For each $F_N^{in} \in \mathcal{D}_s(\mathfrak{H}_N)$ and all $t \in \mathbf{R}$, set $F_N(t) := U_N(t)^* F_N^{in} U_N(t)$. Then one has*

$$\mathrm{trace}_{\mathfrak{H}}(AF_{N:1}(t)) = \mathrm{trace}_{\mathfrak{H}_N}((\mathcal{M}_N(t)A)F_N^{in}) \quad \textit{for all } A \in \mathcal{L}(\mathfrak{H}).$$

Proof. Since the density operator F_N^{in} is symmetric, applying (18) implies that $F_N(t) \in \mathcal{D}_s(\mathfrak{H}_N)$ for all $t \in \mathbf{R}$. Therefore

$$\mathrm{trace}_{\mathfrak{H}}(AF_{N:1}(t)) = \mathrm{trace}_{\mathfrak{H}_N}((J_1A)F_N(t)) = \mathrm{trace}_{\mathfrak{H}_N}((J_kA)F_N(t)) \tag{19}$$

for all $k = 1, \ldots, N$. Averaging both sides of (19) in k, we find that

$$\begin{aligned}\mathrm{trace}_{\mathfrak{H}}(AF_{N:1}(t)) &= \mathrm{trace}_{\mathfrak{H}_N}((\mathcal{M}_N^{in}A)F_N(t)) = \mathrm{trace}_{\mathfrak{H}_N}((\mathcal{M}_N^{in}A)U_N(t)^*F_N^{in}U_N(t)) \\ &= \mathrm{trace}_{\mathfrak{H}_N}(U_N(t)(\mathcal{M}_N^{in}A)U_N(t)^*F_N^{in}) = \mathrm{trace}_{\mathfrak{H}_N}((\mathcal{M}_N(t)A)F_N^{in}),\end{aligned}$$

which is the desired identity. □

3. An Evolution Equation for $\mathcal{M}_N(t)$

In the present section, we seek to establish a quantum analogue of Proposition 1.2 for the time dependent linear map $t \mapsto \mathcal{M}_N(t)$. At variance with the proof of Proposition 1.2, which is based on the method of characteristics for the transport equation, and of which there is no quantum analogue as mentioned above, our approach to this problem is based solely on the first equation in the BBGKY hierarchy.

3.1. The first BBGKY equation. The time dependent density $t \mapsto F_N(t)$ given in terms of the initial quantum density F_N^{in} by the formula

$$F_N(t) := U_N(t)^* F_N^{in} U_N(t)\,,$$

is the solution of the Cauchy problem for the von Neumann equation (5).

The BBGKY hierarchy is the sequence of differential equations for the marginals $F_{N:k}$ (for $k = 1, \dots, N$) deduced from (5). Because of the pairwise particle interaction, the equation for $F_{N:k}$ always involves $F_{N:k+1}$ and is never in closed form for $1 \leq k \leq N-1$.

Nevertheless, only the first equation in the BBGKY hierarchy is needed in the sequel. It is obtained as follows: let $A \in \mathcal{L}(\mathfrak{H})$ satisfy $[\Delta, A] \in \mathcal{L}(\mathfrak{H})$. Multiplying both sides of (5) by $J_1 A$ and taking the trace shows that

$$\begin{aligned} i\hbar\partial_t \operatorname{trace}_{\mathfrak{H}}(AF_{N:1}(t)) &= i\hbar\partial_t \operatorname{trace}_{\mathfrak{H}_N}((J_1 A)F_N(t)) \\ &= \operatorname{trace}_{\mathfrak{H}_N}((J_1 A)[\mathscr{H}_N, F_N(t)]) \\ &= -\operatorname{trace}_{\mathfrak{H}_N}([\mathscr{H}_N, J_1 A]F_N(t))\,, \end{aligned} \tag{20}$$

where the first equality above follows from the first identity in (19). Next one has

$$\begin{aligned} [\mathscr{H}_N, J_1 A] &= \sum_{k=1}^{N} \left[-\tfrac{1}{2}\hbar^2\Delta_{x_k}, J_1 A\right] + \frac{1}{N} \sum_{1\leq k<l\leq N} [V_{kl}, J_1 A] \\ &= J_1\left(\left[-\tfrac{1}{2}\hbar^2\Delta, A\right]\right) + \frac{1}{N}\sum_{l=2}^{N}[V_{1l}, J_1 A]. \end{aligned}$$

Using the first identity in (19) with $\left[-\frac{1}{2}\hbar^2\Delta, A\right]$ in the place of A shows that

$$\begin{aligned} \operatorname{trace}_{\mathfrak{H}_N}([\mathscr{H}_N, J_1 A]F_N(t)) &= \operatorname{trace}_{\mathfrak{H}}\left(\left[-\tfrac{1}{2}\hbar^2\Delta, A\right] F_{N:1}(t)\right) \\ &\quad + \frac{1}{N}\sum_{l=2}^{N} \operatorname{trace}_{\mathfrak{H}_N}([V_{1l}, J_1 A]F_N(t)). \end{aligned} \tag{21}$$

If σ is the transposition exchanging 2 and $l = 3, \dots, N$, then

$$U_\sigma[V_{1l}, J_1 A]U_\sigma^* = [V_{12}, J_1 A]\,,$$

and since $F_N(t)$ is symmetric, for each $l = 3, \dots, N$, one has

$$\begin{aligned} \operatorname{trace}_{\mathfrak{H}_N}([V_{1l}, J_1 A]F_N(t)) &= \operatorname{trace}_{\mathfrak{H}_N}(U_\sigma[V_{1l}, J_1 A]U_\sigma^* F_N(t)) \\ &= \operatorname{trace}_{\mathfrak{H}_N}([V_{12}, J_1 A]F_N(t)) \\ &= \operatorname{trace}_{\mathfrak{H}_N}\left(\left([V_{12}, A\otimes I]\otimes I^{\otimes(N-2)}\right) F_N(t)\right) \\ &= \operatorname{trace}_{\mathfrak{H}_2}([V_{12}, A\otimes I]F_{N:2}(t)). \end{aligned}$$

Hence

$$\frac{1}{N}\sum_{l=2}^{N}\mathrm{trace}_{\mathfrak{H}_N}([V_{1l},J_1A]F_N(t))=\frac{N-1}{N}\mathrm{trace}_{\mathfrak{H}_2}([V_{12},A\otimes I]F_{N:2}(t)). \quad (22)$$

Substituting the second term in the right hand side of (21) with the right hand side of (22) shows that (20) can be put in the form

$$\begin{aligned}&i\hbar\partial_t\,\mathrm{trace}_{\mathfrak{H}}(AF_{N:1}(t))+\mathrm{trace}_{\mathfrak{H}}\left(\left[-\tfrac{1}{2}\hbar^2\Delta,A\right]F_{N:1}(t)\right)\\&\quad=-\frac{N-1}{N}\mathrm{trace}_{\mathfrak{H}_2}([V_{12},A\otimes I]F_{N:2}(t))\,,\end{aligned} \quad (23)$$

for all $A\in\mathcal{L}(\mathfrak{H})$ such that $[\Delta,A]\in\mathcal{L}(\mathfrak{H})$, which is the first BBGKY equation.[1]

Using Lemma 2.3, we easily express the left-hand side of (23) in terms of $\mathcal{M}_N(t)$:

$$\begin{aligned}&i\hbar\partial_t\,\mathrm{trace}_{\mathfrak{H}}(AF_{N:1}(t))+\mathrm{trace}_{\mathfrak{H}}\left(\left[-\tfrac{1}{2}\hbar^2\Delta,A\right]F_{N:1}(t)\right)\\&\quad=i\hbar\partial_t\,\mathrm{trace}_{\mathfrak{H}_N}((\mathcal{M}_N(t)A)F_N^{in})+\mathrm{trace}_{\mathfrak{H}_N}\left(\left(\mathcal{M}_N(t)\left[-\tfrac{1}{2}\hbar^2\Delta,A\right]\right)F_N^{in}\right).\end{aligned}$$

For each $\Lambda\in\mathcal{L}(\mathcal{L}(\mathfrak{H}),\mathcal{L}_s(\mathfrak{H}_N))$ and each (possibly unbounded) operator D on $\mathfrak{H}$, we henceforth denote[2] by $\mathbf{ad}^*(D)\Lambda$ the linear map defined by

$$(\mathbf{ad}^*(D)\Lambda)A:=-\Lambda[D,A] \quad (24)$$

for all $A\in\mathcal{L}(\mathfrak{H})$ such that $[D,A]\in\mathcal{L}(\mathfrak{H})$. With this notation, (23) becomes

$$\begin{aligned}&\mathrm{trace}_{\mathfrak{H}_N}\left(\left(\left(i\hbar\partial_t\mathcal{M}_N(t)-\mathbf{ad}^*(-\tfrac{1}{2}\hbar^2\Delta)\mathcal{M}_N(t)\right)A\right)F_N^{in}\right)\\&\quad=-\frac{N-1}{N}\mathrm{trace}_{\mathfrak{H}_2}([V_{12},A\otimes I]F_{N:2}(t)).\end{aligned} \quad (25)$$

3.2. The interaction term. The present section is focussed on the problem of expressing the right hand side of (25) in terms of $\mathcal{M}_N(t)$, which is the most critical part of our analysis. Since the right hand side of (25) involves $F_{N:2}$ and cannot be expressed exclusively in terms of $F_{N:1}$, it is not a priori obvious that there is an equation in closed form governing the evolution of $\mathcal{M}_N(t)$.

First, we introduce some additional notation. For each $\omega\in\mathbf{R}^d$, we denote by $E_\omega\in\mathcal{L}(\mathfrak{H})$ the multiplication operator defined by the formula

$$E_\omega\psi(x):=e^{i\omega\cdot x}\psi(x).$$

The family of operators E_ω obviously satisfies

$$E_\omega^*=E_{-\omega}=E_\omega^{-1}.$$

For each $\Lambda\in\mathcal{L}(\mathcal{L}(\mathfrak{H}),\mathcal{L}_s(\mathfrak{H}_N))$ and each $B\in\mathcal{L}(\mathfrak{H})$, denote by $\Lambda(\bullet B)$ and $\Lambda(B\bullet)$ the elements of $\mathcal{L}(\mathcal{L}(\mathfrak{H}),\mathcal{L}_s(\mathfrak{H}_N))$ defined by

$$\Lambda(\bullet B):\ A\mapsto\Lambda(AB)\quad\text{and}\quad\Lambda(B\bullet):\ A\mapsto\Lambda(BA).$$

[1] More precisely, it is the weak formulation of the first BBGKY equation.

[2] By analogy with the notation for the co-adjoint representation of a Lie algebra.

Definition 3.1. For each integer $N \geq 2$, set

$$\begin{aligned}\mathcal{E}_N := \{(\Lambda_1, \Lambda_2) \in \mathcal{L}(\mathcal{L}(\mathfrak{H}), \mathcal{L}(\mathfrak{H}_N))^2 \text{ s.t. for all } F \in \mathcal{L}^1(\mathfrak{H}_N) \text{ the map} \\ \omega \mapsto \operatorname{trace}_{\mathfrak{H}_N}((\Lambda_1 E_\omega^*)(\Lambda_2 E_\omega) F) \text{ is continuous on } \mathbf{R}^d\}.\end{aligned} \tag{26}$$

For each $S \in \mathcal{S}'(\mathbf{R}^d)$ whose Fourier transform $\hat{S}$ is a bounded measure on $\mathbf{R}^d$, and for each $\Lambda_1, \Lambda_2 \in \mathcal{L}(\mathcal{L}(\mathfrak{H}), \mathcal{L}(\mathfrak{H}_N))$ such that

$$(\Lambda_1, \Lambda_2(\bullet A)) \text{ and } (\Lambda_2(A\bullet), \Lambda_1) \in \mathcal{E}_N \quad \text{for all } A \in \mathcal{L}(\mathfrak{H}),$$

let $\mathcal{C}[S, \Lambda_1, \Lambda_2]$ be the element of $\mathcal{L}(\mathcal{L}(\mathfrak{H}), \mathcal{L}(\mathfrak{H}_N))$ defined by the formula

$$\mathcal{C}[S, \Lambda_1, \Lambda_2]A := \int_{\mathbf{R}^d} \big((\Lambda_1 E_\omega^*)(\Lambda_2(E_\omega A)) - (\Lambda_2(A E_\omega))(\Lambda_1 E_\omega^*)\big)\, \hat{S}(\mathrm{d}\omega) \tag{27}$$

for all $A \in \mathcal{L}(\mathfrak{H})$. The linear map $\mathcal{C}[S, \Lambda_1, \Lambda_2]$ satisfies

$$\|\mathcal{C}[S, \Lambda_1, \Lambda_2]\| \leq 2\|\Lambda_1\|\|\Lambda_2\|\|\hat{S}\|_{TV}. \tag{28}$$

The integral defining $\mathcal{C}[S, \Lambda_1, \Lambda_2]A$ on the right hand side of (27) is to be understood in the ultraweak sense.[3] Indeed, for each $A \in \mathcal{L}(\mathfrak{H})$, the function

$$\mathbf{R}^d \ni \omega \mapsto (\Lambda_1 E_\omega^*)(\Lambda_2(E_\omega A)) - (\Lambda_2(A E_\omega))(\Lambda_1 E_\omega^*) \in \mathcal{L}(\mathfrak{H}_N)$$

is ultraweakly continuous since $(\Lambda_1, \Lambda_2(\bullet A))$ and $(\Lambda_2(A\bullet), \Lambda_1) \in \mathcal{E}_N$. Moreover

$$\|(\Lambda_1 E_\omega^*)(\Lambda_2(E_\omega A)) - (\Lambda_2(A E_\omega))(\Lambda_1 E_\omega^*)\| \leq 2\|\Lambda_1\|\|\Lambda_2\|\|A\|.$$

Hence, the integral on the right hand side of (27) is well defined in the ultraweak sense, and satisfies

$$\|\mathcal{C}[S, \Lambda_1, \Lambda_2]A\| \leq 2\|\Lambda_1\|\|\Lambda_2\|\|A\| \int_{\mathbf{R}^d} |\hat{S}|(\mathrm{d}\omega) = 2\|\Lambda_1\|\|\Lambda_2\|\|A\|\|\hat{S}\|_{TV}$$

for all $A \in \mathcal{L}(\mathfrak{H})$, which implies (28).

The main result in this section is the following proposition.

---

[3] Let $\mathfrak{H}$ be a separable Hilbert space. The ultraweak topology is the topology defined on $\mathcal{L}(\mathfrak{H})$ by the family of seminorms $A \mapsto |\operatorname{trace}_{\mathfrak{H}}(AF)|$ as F runs through $\mathcal{L}^1(\mathfrak{H})$. Let m be a bounded, complex-valued Borel measure on $\mathbf{R}^d$, and let $f : \mathbf{R}^d \to \mathcal{L}(\mathfrak{H})$ be ultraweakly continuous and such that

$$\sup_{\omega \in \mathbf{R}^d} \|f(\omega)\| < \infty.$$

Then the linear functional

$$\mathcal{L}^1(\mathfrak{H}) \ni F \mapsto \langle L_{f,m}, F\rangle := \int_{\mathbf{R}^d} \operatorname{trace}_{\mathfrak{H}}(f(\omega)F) m(\mathrm{d}\omega) \in \mathbf{C}$$

is continuous with norm

$$\|L_{f,m}\| \leq \sup_{\omega \in \mathbf{R}^d} \|f(\omega)\| \|m\|_{TV}.$$

Hence there exists a unique $\Phi_m \in \mathcal{L}(\mathfrak{H})$ such that $\langle L_{f,m}, F\rangle = \operatorname{trace}_{\mathfrak{H}}(\Phi_m F)$. The operator Φ_m is the ultraweak integral of fm, denoted

$$\int_{\mathbf{R}^d} f(\omega) m(\mathrm{d}\omega) := \Phi_m.$$

Proposition 3.2. *Let V be an even, real-valued element of $\mathcal{S}'(\mathbf{R}^d)$ whose Fourier transform $\hat{V}$ is a bounded measure. Let F_N be the solution to the Cauchy problem for the von Neumann equation (5) with initial condition F_N^{in}. Then, for each $t \in \mathbf{R}$, each integer $N > 1$ and each $A \in \mathcal{L}(\mathfrak{H})$, one has*

$$\frac{N-1}{N}\operatorname{trace}_{\mathfrak{H}_2}([V_{12}, A \otimes I]F_{N:2}(t)) = \operatorname{trace}_{\mathfrak{H}_N}\left((\mathcal{C}[V, \mathcal{M}_N(t), \mathcal{M}_N(t)]A)F_N^{in}\right),$$

where $\mathcal{C}[V, \mathcal{M}_N(t), \mathcal{M}_N(t)]A$ is the element of $\mathcal{L}_s(\mathfrak{H}_N)$ defined in (27).

Proof. Observe first that, for each $G \in \mathcal{L}^1(\mathfrak{H}_2)$, one has

$$\operatorname{trace}_{\mathfrak{H}_2}(V_{12}G) = \tfrac{1}{(2\pi)^d}\int_{\mathbf{R}^d}\operatorname{trace}_{\mathfrak{H}_2}(E_\omega \otimes E_\omega^* G)\hat{V}(\mathrm{d}\omega). \tag{29}$$

Indeed, for all $\phi_1, \phi_2, \psi_1, \psi_2 \in \mathfrak{H}$, applying the formula for the Fourier transform of a convolution product and Plancherel's equality shows that

$$\begin{aligned}\langle\psi_1 \otimes \psi_2|V_{12}|\phi_1 \otimes \phi_2\rangle &= \langle\overline{\phi_1}\psi_1|V \star (\overline{\psi_2}\phi_2)\rangle\\ &= \tfrac{1}{(2\pi)^d}\int_{\mathbf{R}^d}\overline{\mathcal{F}(\bar{\phi}_1\psi_1)(\omega)}\mathcal{F}(\bar{\psi}_2\phi_2)(\omega)\hat{V}(\mathrm{d}\omega)\\ &= \tfrac{1}{(2\pi)^d}\int_{\mathbf{R}^d}\langle\psi_1 \otimes \psi_2|E_\omega \otimes E_\omega^*|\phi_1 \otimes \phi_2\rangle\hat{V}(\mathrm{d}\omega),\end{aligned}$$

which proves (29) for $G = |\phi_1 \otimes \phi_2\rangle\langle\psi_1 \otimes \psi_2|$. The general case follows by a straightforward density argument involving dominated convergence.

Setting successively $G = (A \otimes I)F_{N:2}(t)$ and $G = F_{N:2}(t)(A \otimes I)$ in (29) shows that

$$\begin{aligned}&\tfrac{N-1}{N}\operatorname{trace}_{\mathfrak{H}_2}([V_{12}, A \otimes I]F_{N:2}(t))\\ &\quad= \tfrac{N-1}{N}\int_{\mathbf{R}^d}\operatorname{trace}_{\mathfrak{H}_2}(([E_\omega, A] \otimes E_\omega^*)F_{N:2}(t))\tfrac{\hat{V}(\mathrm{d}\omega)}{(2\pi)^d}\\ &\quad= \tfrac{N-1}{N}\int_{\mathbf{R}^d}\operatorname{trace}_{\mathfrak{H}_N}(((J_2E_\omega^*)J_1(E_\omega A) - J_1(AE_\omega)(J_2E_\omega^*))F_N(t))\tfrac{\hat{V}(\mathrm{d}\omega)}{(2\pi)^d},\end{aligned} \tag{30}$$

where the second equality follows from Definition 2.1 with $k = 2$ and the obvious identity

$$k \neq l \implies [J_kS, J_lT] = 0 \text{ for all } S, T \in \mathcal{L}(\mathfrak{H}). \tag{31}$$

By symmetry of $F_N(t)$,

$$\begin{aligned}&\tfrac{N-1}{N}\int_{\mathbf{R}^d}\operatorname{trace}_{\mathfrak{H}_N}(((J_2E_\omega^*)J_1(E_\omega A) - J_1(AE_\omega)(J_2E_\omega^*))F_N(t))\tfrac{\hat{V}(\mathrm{d}\omega)}{(2\pi)^d}\\ &\quad= \tfrac{1}{N^2}\sum_{1\le k\neq l\le N}\int_{\mathbf{R}^d}\operatorname{trace}_{\mathfrak{H}_N}(((J_lE_\omega^*)J_k(E_\omega A) - J_k(AE_\omega)(J_lE_\omega^*))F_N(t))\tfrac{\hat{V}(\mathrm{d}\omega)}{(2\pi)^d}\\ &\quad= \tfrac{1}{N^2}\sum_{1\le k,l\le N}\int_{\mathbf{R}^d}\operatorname{trace}_{\mathfrak{H}_N}(((J_lE_\omega^*)J_k(E_\omega A) - J_k(AE_\omega)(J_lE_\omega^*))F_N(t))\tfrac{\hat{V}(\mathrm{d}\omega)}{(2\pi)^d}\\ &\quad= \int_{\mathbf{R}^d}\operatorname{trace}_{\mathfrak{H}_N}(((\mathcal{M}_N^{in}E_\omega^*)\mathcal{M}_N^{in}(E_\omega A) - \mathcal{M}_N^{in}(AE_\omega)(\mathcal{M}_N^{in}E_\omega^*))F_N(t))\tfrac{\hat{V}(\mathrm{d}\omega)}{(2\pi)^d},\end{aligned} \tag{32}$$

since, for each $k = 1, \dots, N$ and for all $\omega \in \mathbf{R}^d$,

$$(J_k E_\omega^*) J_k(E_\omega A) = J_k(E_\omega^* E_\omega A) = J_k A = J_k(A E_\omega E_\omega^*) = J_k(A E_\omega)(J_k E_\omega^*).$$

By cyclicity of the trace,

$$\begin{aligned}
&\operatorname{trace}_{\mathfrak{H}_N}(((\mathcal{M}_N^{in} E_\omega^*)\mathcal{M}_N^{in}(E_\omega A) - \mathcal{M}_N^{in}(AE_\omega)(\mathcal{M}_N^{in} E_\omega^*)) F_N(t)) \\
&\quad = \operatorname{trace}_{\mathfrak{H}_N}(((\mathcal{M}_N^{in} E_\omega^*)\mathcal{M}_N^{in}(E_\omega A) - \mathcal{M}_N^{in}(AE_\omega)(\mathcal{M}_N^{in} E_\omega^*)) U_N(t)^* F_N^{in} U_N(t)) \\
&\quad = \operatorname{trace}_{\mathfrak{H}_N}(U_N(t)((\mathcal{M}_N^{in} E_\omega^*)\mathcal{M}_N^{in}(E_\omega A) - \mathcal{M}_N^{in}(AE_\omega)(\mathcal{M}_N^{in} E_\omega^*)) U_N(t)^* F_N^{in}) \\
&\quad = \operatorname{trace}_{\mathfrak{H}_N}(((\mathcal{M}_N(t) E_\omega^*)\mathcal{M}_N(t)(E_\omega A) - \mathcal{M}_N(t)(AE_\omega)(\mathcal{M}_N(t) E_\omega^*)) F_N^{in}),
\end{aligned} \tag{33}$$

since

$$\begin{aligned}
U_N(t)(\mathcal{M}_N^{in} S)(\mathcal{M}_N^{in} T) U_N(t)^* &= U_N(t)(\mathcal{M}_N^{in} S) U_N(t)^* U_N(t)(\mathcal{M}_N^{in} T) U_N(t)^* \\
&= (\mathcal{M}_N(t) S)(\mathcal{M}_N(t) T)
\end{aligned}$$

for all $S, T \in \mathcal{L}(\mathfrak{H})$ according to Definition 2.2. Putting together (30), (32), and (33) shows that

$$\begin{aligned}
&\tfrac{N-1}{N} \operatorname{trace}_{\mathfrak{H}_2}([V_{12}, A \otimes I] F_{N:2}(t)) \\
&\quad = \int_{\mathbf{R}^d} \operatorname{trace}_{\mathfrak{H}_N}(((\mathcal{M}_N(t) E_\omega^*)\mathcal{M}_N(t)(E_\omega A) - \mathcal{M}_N(t)(AE_\omega)(\mathcal{M}_N(t) E_\omega^*)) F_N^{in}) \tfrac{\hat{V}(d\omega)}{(2\pi)^d} \\
&\quad = \operatorname{trace}_{\mathfrak{H}_N}((\mathcal{C}[V, \mathcal{M}_N(t), \mathcal{M}_N(t)] A) F_N^{in})
\end{aligned}$$

as expected. □

3.3. Writing an equation for $\mathcal{M}_N(t)$. With (25) and Proposition 3.2, we see that $\mathcal{M}_N(t)$ satisfies

$$\begin{aligned}
\operatorname{trace}_{\mathfrak{H}_N} \left(\left(\left(i\hbar\partial_t \mathcal{M}_N(t) - \mathbf{ad}^*(-\tfrac{1}{2}\hbar^2\Delta)\mathcal{M}_N(t) \right) A \right) F_N^{in} \right) \\
= -\operatorname{trace}_{\mathfrak{H}_N} \left((\mathcal{C}[V, \mathcal{M}_N(t), \mathcal{M}_N(t)] A)\, F_N^{in} \right)
\end{aligned}$$

for all $A \in \mathcal{L}(\mathfrak{H})$ such that $[\Delta, A] \in \mathcal{L}(\mathfrak{H})$, and all $F_N^{in} \in \mathcal{L}_s(\mathfrak{H}_N)$.

Our first main result in this paper is the following theorem.

Theorem 3.3. *Let $V \in C_b(\mathbf{R}^d)$ be an even, real-valued function whose Fourier transform $\hat{V}$ is a bounded measure. Let*

$$U_N(t) = e^{it\mathscr{H}_N/\hbar}, \quad \text{with } \mathscr{H}_N := \sum_{k=1}^{N} -\tfrac{1}{2}\hbar^2 \Delta_{x_k} + \frac{1}{N} \sum_{1 \le k < l \le N} V(x_k - x_l),$$

and let $\mathcal{M}_N(t)$ be the element of $\mathcal{L}(\mathcal{L}(\mathfrak{H}), \mathcal{L}_s(\mathfrak{H}_N))$ in Definition 2.2. Then

$$i\hbar\partial_t \mathcal{M}_N(t) = \mathbf{ad}^*(-\tfrac{1}{2}\hbar^2\Delta)\mathcal{M}_N(t) - \mathcal{C}[V, \mathcal{M}_N(t), \mathcal{M}_N(t)]. \tag{34}$$

Remark. Unfortunately the terms

$$\mathbf{ad}^*(-\tfrac{1}{2}\hbar^2\Delta)\mathcal{M}_N(t) \quad \text{and} \quad \mathcal{C}[V, \mathcal{M}_N(t), \mathcal{M}_N(t)]$$

on the right hand side of (34) seem to be of a very different nature. This is in sharp contrast with the Hartree equation, where the kinetic energy $-\frac{1}{2}\hbar^2\Delta$ and the interaction potential energy $V_{R(t)}$ defined in (4) appear together on an equal footing in right hand side of (3). However, both terms appearing on the right hand side of (34) can be formally assembled in a single expression which is reminiscent of the commutator appearing on the right hand side of (3). See Appendix A for a complete discussion of this point.

Proof. Setting

$$S_N := i\hbar\partial_t(\mathcal{M}_N(t)A) - \Big(\mathbf{ad}^*(-\tfrac{1}{2}\hbar^2\Delta)\mathcal{M}_N(t)\Big)A + \mathcal{C}[V, \mathcal{M}_N(t), \mathcal{M}_N(t)]A\,,$$

one has

$$S_N \in \mathcal{L}_s(\mathfrak{H}_N) \quad \text{and } \operatorname{trace}_{\mathfrak{H}_N}(S_N F_N^{in}) = 0$$

for all $F_N^{in} \in \mathcal{D}_s(\mathfrak{H}_N)$.

Lemma 3.4. *Any $G_N \in \mathcal{L}_s^1(\mathfrak{H}_N)$ can be decomposed as*

$$G_N = \sum_{k=1}^{4} \lambda_k G_N^k\,, \quad \textit{with } G_N^k \in \mathcal{D}_s(\mathfrak{H}_N) \textit{ and } \lambda_k \in \mathbf{C}. \tag{35}$$

Therefore

$$\operatorname{trace}_{\mathfrak{H}_N}(S_N G_N) = 0 \quad \text{for all } G_N \in \mathcal{L}_s^1(\mathfrak{H}_N).$$

Pick G_N of the form

$$G_N := S_N^*|\Psi_N\rangle\langle\Psi_N|\,,$$

where

$$\Psi_N \in \mathfrak{H}_N\,, \quad \text{such that } \|\Psi_N\|_{\mathfrak{H}_N} = 1\,, \quad \text{and } U_\sigma\Psi_N = \Psi_N \text{ for all } \sigma \in \mathfrak{S}_N.$$

Thus

$$0 = \operatorname{trace}_{\mathfrak{H}_N}(S_N G_N) = \langle\Psi_N|S_N S_N^*|\Psi_N\rangle = \|S_N^*\Psi_N\|_{\mathfrak{H}_N}^2\,,$$

i.e.

$$S_N^*\Psi_N = 0 \quad \text{for all } \Psi_N \in \mathfrak{H}_N \text{ such that } U_\sigma\Psi_N = \Psi_N \text{ for all } \sigma \in \mathfrak{S}_N.$$

For each $\Phi_N \in \mathfrak{H}_N$, one has

$$S_N^*\Phi_N = S_N^*\tilde{\Phi}_N\,, \qquad \text{with } \tilde{\Phi}_N = \frac{1}{N!}\sum_{\tau\in\mathfrak{S}_N} U_\tau\Phi_N.$$

By construction, $U_\sigma\tilde{\Phi}_N = \tilde{\Phi}_N$ for all $\sigma \in \mathfrak{S}_N$, so that $S_N^*\Phi_N = 0$ for all $\Phi_N \in \mathfrak{H}_N$. Hence $S_N^* = 0$, or equivalently $S_N = 0$. Since this holds for all $A \in \mathcal{L}(\mathfrak{H})$ such that $[\Delta, A] \in \mathfrak{H}$, we conclude that (34) holds. $\square$

Proof of the lemma. Indeed, write

$$G_N = \Re(G_N) + i\Im(G_N)\,, \quad \text{with} \begin{cases} \Re(G_N) := \frac{1}{2}(G_N + G_N^*)\,, \\ \Im(G_N) := \frac{1}{2i}(G_N - G_N^*). \end{cases}$$

One has

$$\Re(G_N) = \Re(G_N)^* \text{ and } \Im(G_N) = \Im(G_N)^* \in \mathcal{L}^1_s(\mathfrak{H}_N)\,,$$

so that $\Re(G_N)$ and $\Im(G_N)$ have spectral decompositions of the form

$$\Re(G_N) = \sum_{n\geq 0} \alpha_n \mathbf{p}_n\,, \quad \Im(G_N) = \sum_{n\geq 0} \beta_n \mathbf{q}_n\,,$$

where

$$\begin{cases} \mathbf{p}_n^2 = \mathbf{p}_n = \mathbf{p}_n^* = U_\sigma \mathbf{p}_n U_\sigma^*\,, \\ \mathbf{q}_n^2 = \mathbf{q}_n = \mathbf{q}_n^* = U_\sigma \mathbf{q}_n U_\sigma^*\,, \end{cases} \quad \text{and } m \neq n \Rightarrow \begin{cases} \operatorname{trace}_{\mathfrak{H}_N}(\mathbf{p}_n \mathbf{p}_m) = 0\,, \\ \operatorname{trace}_{\mathfrak{H}_N}(\mathbf{q}_n \mathbf{q}_m) = 0\,, \end{cases}$$

for all $m, n \geq 0$ and $\sigma \in \mathfrak{S}_N$, and

$$\sum_{n\geq 0} |\alpha_n| \operatorname{trace}_{\mathfrak{H}_N}(\mathbf{p}_n) < \infty\,, \quad \sum_{n\geq 0} |\beta_n| \operatorname{trace}_{\mathfrak{H}_N}(\mathbf{q}_n) < \infty.$$

The decomposition (35) is obtained with

$$\lambda_1 G_N^1 = \sum_{n\geq 0} \alpha_n^+ \mathbf{p}_n\,, \qquad \lambda_2 G_N^2 = -\sum_{n\geq 0} \alpha_n^- \mathbf{p}_n\,,$$
$$\lambda_3 G_N^3 = \sum_{n\geq 0} i\beta_n^+ \mathbf{q}_n\,, \qquad \lambda_4 G_N^4 = -\sum_{n\geq 0} i\beta_n^- \mathbf{q}_n\,,$$

setting

$$\lambda_1 = \sum_{n\geq 0} \alpha_n^+ \operatorname{trace}_{\mathfrak{H}_N}(\mathbf{p}_n)\,, \qquad \lambda_2 = -\sum_{n\geq 0} \alpha_n^- \operatorname{trace}_{\mathfrak{H}_N}(\mathbf{p}_n)\,,$$
$$\lambda_3 = i\sum_{n\geq 0} \beta_n^+ \operatorname{trace}_{\mathfrak{H}_N}(\mathbf{p}_n)\,, \qquad \lambda_4 = -i\sum_{n\geq 0} \beta_n^- \operatorname{trace}_{\mathfrak{H}_N}(\mathbf{p}_n).$$

Of course, if one of the numbers λ_j for $j = 1, \ldots, 4$ is equal to zero, the corresponding density G_N^j can be chosen arbitrarily in $\mathcal{D}_s(\mathfrak{H}_N)$. □

3.4. Hartree's equation is a special case of equation (34). In order to complete the analogy between Proposition 1.2 and Theorem 3.3, we now explain the connection between Hartree's equation (the quantum analogue of Vlasov's equation (10)) and the evolution equation (34) satisfied by $t \mapsto \mathcal{M}_N(t)$.

In the classical case, $t \mapsto \mu_{T_t^N Z_N}(\mathrm{d}x\,\mathrm{d}\xi) := m(t,\,\mathrm{d}x\,\mathrm{d}\xi; Z_N)$ is a measured-valued function of t, parametrized by Z_N. This measured-valued function of time m is a solution of the Vlasov equation (10) for all $Z_N \in (\mathbf{R}^d \times \mathbf{R}^d)^N$: the partial derivatives in (10) act on the variables t, x, ξ in m, and not on Z_N. Any classical solution $f \equiv f(t,x,\xi)$ of the Vlasov equation can be viewed as special case of m of the form $m(t,\,\mathrm{d}x\,\mathrm{d}\xi; Z_N) = f(t,x,\xi)\,\mathrm{d}x\,\mathrm{d}\xi$; most importantly, such an m is constant in Z_N.

The quantum analogue of such an m is a time-dependent element $t \mapsto \mathscr{R}(t)$ of $\mathcal{L}(\mathcal{L}(\mathfrak{H}), \mathcal{L}_s(\mathfrak{H}_N))$ of the form

$$\mathscr{R}(t) :\ A \mapsto \operatorname{trace}_{\mathfrak{H}}(R(t)A) I_{\mathfrak{H}_N}\,, \tag{36}$$

assuming that $R(t) \in \mathcal{D}(\mathfrak{H})$ for all $t \in \mathbf{R}$.

Theorem 3.5. *The time-dependent element $t \mapsto \mathscr{R}(t)$ of $\mathcal{L}(\mathcal{L}(\mathfrak{H}), \mathcal{L}_s(\mathfrak{H}_N))$ defined by* (36) *is a solution to the evolution equation* (34) *if and only if $t \mapsto R(t)$ is a solution to the Hartree equation*

$$i\hbar\partial_t R(t) = [-\tfrac{1}{2}\hbar^2\Delta + V_{R(t)}, R(t)]. \tag{37}$$

Here $V_{R(t)} \in \mathcal{L}(\mathfrak{H})$ designates the operator defined by

$$(V_{R(t)}\phi)(x) := \phi(x)\int_{\mathbf{R}^d} V(x-z) r(t,z,z)\,\mathrm{d}z\,,$$

denoting by $r(t,x,y)$ the integral kernel of the trace-class operator $R(t)$.

The key observation in the proof of Theorem 3.5 is summarized in the next lemma.

Lemma 3.6. *Let $R \in \mathcal{D}(\mathfrak{H})$ and define $\mathscr{R} \in \mathcal{L}(\mathcal{L}(\mathfrak{H}), \mathcal{L}_s(\mathfrak{H}_N))$ by the formula*

$$\mathscr{R}A := \operatorname{trace}_{\mathfrak{H}}(RA) I_{\mathfrak{H}_N}\,, \qquad \textit{for all } A \in \mathcal{L}(\mathfrak{H}).$$

Then, for each $\Lambda \in \mathcal{L}(\mathcal{L}^1(\mathfrak{H}_N), \mathcal{L}^1(\mathfrak{H}))$ and each $A \in \mathcal{L}(\mathfrak{H})$, one has

$$(\mathscr{R}, \Lambda^*(\bullet A)) \textit{ and } (\Lambda^*(A\bullet), \mathscr{R}) \in \mathcal{E}_N$$

(where $\Lambda^* \in \mathcal{L}(\mathcal{L}(\mathfrak{H}), \mathcal{L}(\mathfrak{H}_N))$ is the adjoint of Λ), and

$$\mathcal{C}[V, \mathscr{R}, \Lambda^*] = -\,\mathbf{ad}^*(V_R)\Lambda^*$$

for all even, real-valued $V \in C_b(\mathbf{R}^d)$ whose Fourier transform $\hat{V}$ is a bounded measure.

Proof of the lemma. For all $G \in \mathcal{L}^1(\mathfrak{H}_N)$, one has

$$\begin{aligned}\operatorname{trace}_{\mathfrak{H}_N}((\mathscr{R}E_\omega^*)(\Lambda^*(E_\omega A))G) &= \operatorname{trace}_{\mathfrak{H}}(RE_\omega^*)\operatorname{trace}_{\mathfrak{H}_N}((\Lambda^*(E_\omega A))G)\\ &= \operatorname{trace}_{\mathfrak{H}}(RE_\omega^*)\operatorname{trace}_{\mathfrak{H}}(E_\omega A(\Lambda G))\end{aligned}$$

and likewise

$$\operatorname{trace}_{\mathfrak{H}_N}((\Lambda^*(AE_\omega))(\mathscr{R}E_\omega^*)G) = \operatorname{trace}_{\mathfrak{H}}(RE_\omega^*)\operatorname{trace}_{\mathfrak{H}}(E_\omega(\Lambda G)A).$$

Hence both functions

$$\omega \mapsto \operatorname{trace}_{\mathfrak{H}_N}((\mathscr{R}E_\omega^*)(\Lambda^*(E_\omega A))G) \text{ and } \omega \mapsto \operatorname{trace}_{\mathfrak{H}_N}((\Lambda^*(AE_\omega))(\mathscr{R}E_\omega^*)G)$$

are continuous on $\mathbf{R}$, so that

$$(\mathscr{R}, \Lambda^*(\bullet A)) \text{ and } (\Lambda^*(A\bullet), \mathscr{R}) \in \mathcal{E}_N.$$

Since the potential V is even, the bounded measure $\hat{V}$ is invariant under the transformation $\omega \mapsto -\omega$, and therefore

$$\begin{aligned}
&\mathcal{C}[V, \mathscr{R}, \Lambda^*]A \\
&= \tfrac{1}{(2\pi)^d} \int_{\mathbf{R}^d} \left(\operatorname{trace}(RE_\omega^*)\Lambda^*(E_\omega A) - \Lambda^*(AE_\omega) \operatorname{trace}(RE_\omega^*)\right) \hat{V}(\mathrm{d}\omega) \\
&= \tfrac{1}{(2\pi)^d} \int_{\mathbf{R}^d} \hat{V}(\omega) \operatorname{trace}(RE_\omega^*)\Lambda^*([E_\omega, A]) \,\mathrm{d}\omega \\
&= \Lambda^* \left[\tfrac{1}{(2\pi)^d} \int_{\mathbf{R}^d} \hat{V}(\omega) \operatorname{trace}(RE_\omega^*) E_\omega \,\mathrm{d}\omega, A \right].
\end{aligned}$$

Since

$$\operatorname{trace}(RE_\omega^*) = \hat{\rho}(\omega), \quad \text{where } \rho(x) := r(x, x)$$

(where $r \equiv r(x, y)$ is the integral kernel of the trace-class operator R), one has

$$\tfrac{1}{(2\pi)^d} \int_{\mathbf{R}^d} \hat{V}(\omega) \operatorname{trace}(RE_\omega^*) E_\omega \,\mathrm{d}\omega = \tfrac{1}{(2\pi)^d} \int_{\mathbf{R}^d} \hat{V}(\omega)\hat{\rho}(\omega) E_\omega \,\mathrm{d}\omega = V \star \rho = V_R.$$

Therefore

$$\mathcal{C}[V, \mathscr{R}, \Lambda^*]A = \Lambda^* [V_R, A] = -(\mathbf{ad}^*(V_R)\Lambda^*)A.$$

□

Proof of the theorem. First observe that $\mathscr{R}(t)$ is the adjoint of the linear map

$$\mathcal{L}^1(\mathfrak{H}_N) \ni G \mapsto (\operatorname{trace}_{\mathfrak{H}_N}(G))R(t) \in \mathcal{L}^1(\mathfrak{H}),$$

which is obviously continuous, since

$$\|(\operatorname{trace}_{\mathfrak{H}_N}(G))R(t)\|_{\mathcal{L}^1(\mathfrak{H})} \le \|G\|_{\mathcal{L}^1(\mathfrak{H}_N)} \|R(t)\|_{\mathcal{L}^1(\mathfrak{H})} = \|G\|_{\mathcal{L}^1(\mathfrak{H}_N)}.$$

By Lemma 3.6

$$\mathcal{C}[V, \mathscr{R}(t), \mathscr{R}(t)] = -\,\mathbf{ad}^*(V_{R(t)})\mathscr{R}(t)$$

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

$$\begin{aligned}
\mathcal{C}[V, \mathscr{R}(t), \mathscr{R}(t)]A &= (-\,\mathbf{ad}^*(V_{R(t)})\mathscr{R}(t))A = \mathscr{R}(t)[V_{R(t)}, A] \\
&= \operatorname{trace}_{\mathfrak{H}}(R(t)[V_{R(t)}, A])I_{\mathfrak{H}_N} = -\operatorname{trace}_{\mathfrak{H}}([V_{R(t)}, R(t)]A)I_{\mathfrak{H}_N}.
\end{aligned}$$

On the other hand, for each $A \in \mathcal{L}(\mathfrak{H})$ such that $[\Delta, A] \in \mathcal{L}(\mathfrak{H})$, one has

$$\begin{aligned}(\mathbf{ad}^*(-\tfrac{1}{2}\hbar^2\Delta)\mathscr{R}(t))A &= -\mathscr{R}(t)[-\tfrac{1}{2}\hbar^2\Delta, A] \\ &= -\operatorname{trace}_{\mathfrak{H}}(R(t)[-\tfrac{1}{2}\hbar^2\Delta, A])I_{\mathfrak{H}_N} \\ &= \operatorname{trace}_{\mathfrak{H}}([-\tfrac{1}{2}\hbar^2\Delta, R(t)]A)I_{\mathfrak{H}_N}.\end{aligned}$$

In other words

$$\begin{aligned}&\left(i\hbar\partial_t\mathscr{R}(t) - \mathbf{ad}^*(-\tfrac{1}{2}\hbar^2\Delta)\mathscr{R}(t) + \mathcal{C}[V, \mathscr{R}(t), \mathscr{R}(t)]\right)A \\ &\quad = \operatorname{trace}_{\mathfrak{H}}\left((i\hbar\partial_t R(t) - [-\tfrac{1}{2}\hbar^2\Delta + V_{R(t)}, R(t)])A\right)I_{\mathfrak{H}_N}\end{aligned}$$

for each $A \in \mathcal{L}(\mathfrak{H})$ such that $[\Delta, A] \in \mathcal{L}(\mathfrak{H})$.

Thus, $\mathscr{R}(t)$ is a solution to the evolution equation (34) if and only if $R(t)$ is a solution to the Hartree equation (37). □

4. Uniformity in $\hbar$ of the Mean-Field Limit: Proof of Theorem 1.1

The proof of Theorem 1.1 is quite involved, and will be split in several steps.
Step 1. Set $\mathscr{R}(t)A := \operatorname{trace}_{\mathfrak{H}}(R(t)A)I_{\mathfrak{H}_N}$ for all $A \in \mathcal{L}(\mathfrak{H})$. By Theorems 3.3 and 3.5, one has

$$\begin{aligned}i\hbar\partial_t(\mathcal{M}_N(t) - \mathscr{R}(t)) = \mathbf{ad}^*\left(-\tfrac{1}{2}\hbar^2\Delta\right)(\mathcal{M}_N(t) - \mathscr{R}(t)) \\ + \mathcal{C}[V, \mathscr{R}(t), \mathscr{R}(t)] - \mathcal{C}[V, \mathcal{M}_N(t), \mathcal{M}_N(t)].\end{aligned}$$

Formula (27) shows that $(\Lambda_1, \Lambda_2) \mapsto \mathcal{C}[V, \Lambda_1, \Lambda_2]$ is **C**-bilinear on its domain of definition. More precisely, let $\Lambda_1, \Lambda_2, \Lambda'_1, \Lambda'_2 \in \mathcal{L}(\mathcal{L}(\mathfrak{H}), \mathcal{L}(\mathfrak{H}_N))$ satisfy

$$(\widetilde{\Lambda}_1, \widetilde{\Lambda}_2(\bullet A)) \text{ and } (\widetilde{\Lambda}_2(A\bullet), \widetilde{\Lambda}_1) \in \mathcal{E}_N \quad \text{with } \widetilde{\Lambda}_j = \Lambda_j \text{ or } \Lambda'_j, \quad j = 1, 2$$

for all $A \in \mathcal{L}(\mathfrak{H})$. Then, for all $\lambda_1, \lambda_2, \lambda'_1, \lambda'_2 \in \mathbf{C}$, one has

$$((\lambda_1\Lambda_1 + \lambda'_1\Lambda'_1), (\lambda_2\Lambda_2 + \lambda'_2\Lambda'_2)(\bullet A)) \text{ and } ((\lambda_2\Lambda_2 + \lambda'_2\Lambda'_2)(A\bullet), (\lambda_1\Lambda_1 + \lambda'_1\Lambda'_1)) \in \mathcal{E}_N$$

and

$$\begin{aligned}\mathcal{C}[V, \lambda_1\Lambda_1 + \lambda'_1\Lambda'_1, \lambda_2\Lambda_2 + \lambda'_2\Lambda'_2] = \lambda_1\lambda_2\mathcal{C}[V, \Lambda_1, \Lambda_2] + \lambda'_1\lambda_2\mathcal{C}[V, \Lambda'_1, \Lambda_2] \\ + \lambda_1\lambda'_2\mathcal{C}[V, \Lambda_1, \Lambda'_2] + \lambda'_1\lambda'_2\mathcal{C}[V, \Lambda'_1, \Lambda'_2].\end{aligned}$$

Hence

$$\begin{aligned}\mathcal{C}[V, \mathscr{R}(t), \mathscr{R}(t)] - \mathcal{C}[V, \mathcal{M}_N(t), \mathcal{M}_N(t)] = \mathcal{C}[V, \mathscr{R}(t), \mathscr{R}(t) - \mathcal{M}_N(t)] \\ - \mathcal{C}[V, \mathcal{M}_N(t) - \mathscr{R}(t), \mathcal{M}_N(t)].\end{aligned}$$

On the other hand, Lemma 2.3 shows that $\mathcal{M}_N(t)$ is the adjoint of the continuous linear map

$$\mathcal{L}^1_s(\mathfrak{H}_N) \ni G \mapsto G_{:1} \in \mathcal{L}^1(\mathfrak{H}),$$

where $G_{:1}$ is the unique element of $\mathcal{L}^1(\mathfrak{H})$ such that

$$\operatorname{trace}_{\mathfrak{H}}(GA) = \operatorname{trace}_{\mathfrak{H}_N}(G(J_1A)), \quad \text{for all } A \in \mathcal{L}(\mathfrak{H}).$$

Therefore, one has

$$\mathcal{C}[V, \mathscr{R}(t), \mathscr{R}(t) - \mathcal{M}_N(t)] = \mathbf{ad}^*(V_{R(t)})(\mathcal{M}_N(t) - \mathscr{R}(t))$$

by Lemma 3.6, and hence

$$\begin{aligned} i\hbar\partial_t(\mathcal{M}_N(t) - \mathscr{R}(t)) =& \, \mathbf{ad}^*\left(-\tfrac{1}{2}\hbar^2\Delta + V_{R(t)}\right)(\mathcal{M}_N(t) - \mathscr{R}(t)) \\ & - \mathcal{C}[V, \mathcal{M}_N(t) - \mathscr{R}(t), \mathcal{M}_N(t)]. \end{aligned} \tag{38}$$

Step 2. Let $A^{in} \in \mathcal{L}(\mathfrak{H})$, and let $t \mapsto A(t)$ be the solution to the Cauchy problem

$$\begin{cases} i\hbar\partial_t A(t) = [-\tfrac{1}{2}\hbar^2\Delta + V_{R(t)}, A(t)]\,, \\ A(0) = A^{in}. \end{cases}$$

Thus

$$\begin{aligned} i\hbar\partial_t((\mathcal{M}_N(t) - \mathscr{R}(t))(A(t))) =& \, (\mathcal{M}_N(t) - \mathscr{R}(t))(i\hbar\partial_t A(t)) \\ & + \left(\mathbf{ad}^*\left(-\tfrac{1}{2}\hbar^2\Delta + V_{R(t)}\right)(\mathcal{M}_N(t) - \mathscr{R}(t))\right)A(t) \\ & - \mathcal{C}[V, \mathcal{M}_N(t) - \mathscr{R}(t), \mathcal{M}_N(t)]A(t) \\ =& \, (\mathcal{M}_N(t) - \mathscr{R}(t))(i\hbar\partial_t A(t) - [-\tfrac{1}{2}\hbar^2\Delta + V_{R(t)}, A(t)]) \\ & - \mathcal{C}[V, \mathcal{M}_N(t) - \mathscr{R}(t), \mathcal{M}_N(t)]A(t) \\ =& -\mathcal{C}[V, \mathcal{M}_N(t) - \mathscr{R}(t), \mathcal{M}_N(t)]A(t). \end{aligned}$$

Hence

$$\begin{aligned} (\mathcal{M}_N(t) - \mathscr{R}(t))(A(t)) =& \, (\mathcal{M}_N(0) - \mathscr{R}(0))(A(0)) \\ & - \frac{i}{\hbar}\int_0^t \mathcal{C}[V, \mathcal{M}_N(s) - \mathscr{R}(s), \mathcal{M}_N(s)]A(s)\,\mathrm{d}s. \end{aligned}$$

Step 3. Let $W(t)$ be a unitary operator on $\mathfrak{H}_N$ such that

$$\begin{aligned} & \|(\mathcal{M}_N(t) - \mathscr{R}(t))(A(t))F_N^{in}\|_{\mathcal{L}^1(\mathfrak{H}_N)} \\ & = \mathrm{trace}_{\mathfrak{H}_N}((\mathcal{M}_N(t) - \mathscr{R}(t))(A(t))F_N^{in}W(t))\,; \end{aligned}$$

then

$$\begin{aligned} & \|(\mathcal{M}_N(t) - \mathscr{R}(t))(A(t))F_N^{in}\|_{\mathcal{L}^1(\mathfrak{H}_N)} \\ & = \mathrm{trace}_{\mathfrak{H}_N}((\mathcal{M}_N(0) - \mathscr{R}(0))(A(0))F_N^{in}W(t)) \\ & \quad - \frac{i}{\hbar}\int_0^t \mathrm{trace}_{\mathfrak{H}_N}((\mathcal{C}[V, \mathcal{M}_N(s) - \mathscr{R}(s), \mathcal{M}_N(s)]A(s))F_N^{in}W(t))\,\mathrm{d}s \\ & \le \|(\mathcal{M}_N(0) - \mathscr{R}(0))(A(0))F_N^{in}\|_{\mathcal{L}^1(\mathfrak{H}_N)} \\ & \quad + \frac{1}{\hbar}\int_0^t |\,\mathrm{trace}_{\mathfrak{H}_N}((\mathcal{C}[V, \mathcal{M}_N(s) - \mathscr{R}(s), \mathcal{M}_N(s)]A(s))F_N^{in}W(t))|\,\mathrm{d}s. \end{aligned} \tag{39}$$

Returning to the formula (27), we see that

$$\begin{aligned}
&|\operatorname{trace}_{\mathfrak{H}_N}((\mathcal{C}[V, \mathcal{M}_N(s) - \mathscr{R}(s), \mathcal{M}_N(s)]A(s))F_N^{in}W(t))| \\
&= \tfrac{1}{(2\pi)^d}\left|\int_{\mathbf{R}^d} \operatorname{trace}_{\mathfrak{H}_N}((\mathcal{C}[E_\omega, \mathcal{M}_N(s) - \mathscr{R}(s), \mathcal{M}_N(s)]A(s))F_N^{in}W(t))\hat{V}(\mathrm{d}\omega)\right| \\
&\le \tfrac{1}{(2\pi)^d}\int_{\mathbf{R}^d} |\operatorname{trace}_{\mathfrak{H}_N}((\mathcal{C}[E_\omega, \mathcal{M}_N(s) - \mathscr{R}(s), \mathcal{M}_N(s)]A(s))F_N^{in}W(t))||\hat{V}|(\mathrm{d}\omega).
\end{aligned} \tag{40}$$

Observe that

$$\begin{aligned}
\mathcal{C}[E_\omega, \mathcal{M}_N(s)-\mathscr{R}(s), \mathcal{M}_N(s)]A(s) &= ((\mathcal{M}_N(s)-\mathscr{R}(s))E_\omega^*)(\mathcal{M}_N(s)(E_\omega A(s))) \\
&\quad -(\mathcal{M}_N(s)(A(s)E_\omega))((\mathcal{M}_N(s)-\mathscr{R}(s))E_\omega^*) \\
&= (\mathcal{M}_N(s)[E_\omega, A(s)])((\mathcal{M}_N(s) - \mathscr{R}(s))E_\omega^*) \\
&\quad + [\mathcal{M}_N(s)E_\omega^*, \mathcal{M}_N(s)(E_\omega A(s))] \\
&= (\mathcal{M}_N(s)[E_\omega, A(s)])((\mathcal{M}_N(s) - \mathscr{R}(s))E_\omega^*) \\
&\quad + \frac{1}{N}\mathcal{M}_N(s)[E_\omega^*, E_\omega A(s)].
\end{aligned}$$

The last equality follows from the following simple computation: because of (31)

$$[\mathcal{M}_N^{in}S, \mathcal{M}_N^{in}T] = \frac{1}{N}\mathcal{M}_N^{in}[S, T]$$

for all $S, T \in \mathcal{L}(\mathfrak{H})$ and each $N \ge 1$, so that, for each $t \in \mathbf{R}$

$$\begin{aligned}
[\mathcal{M}_N(t)S, \mathcal{M}_N(t)T] &= [U_N(t)(\mathcal{M}_N^{in}S)U_N(t)^*, U_N(t)(\mathcal{M}_N^{in}T)U_N(t)^*] \\
&= U_N(t)[\mathcal{M}_N^{in}S, \mathcal{M}_N^{in}T]U_N(t)^* = \frac{1}{N}\mathcal{M}_N(t)[S, T],
\end{aligned}$$

according to Definition 2.2.

Hence

$$\begin{aligned}
&|\operatorname{trace}_{\mathfrak{H}_N}((\mathcal{C}[E_\omega, \mathcal{M}_N(s) - \mathscr{R}(s), \mathcal{M}_N(s)]A(s))F_N^{in}W(t))| \\
&\quad \le \|W(t)(\mathcal{M}_N(s)[E_\omega, A(s)])\|\|((\mathcal{M}_N(s) - \mathscr{R}(s))E_\omega^*)F_N^{in}\|_{\mathcal{L}^1(\mathfrak{H}_N)} \\
&\quad + \frac{1}{N}\|W(t)(\mathcal{M}_N(s)[E_\omega^*, E_\omega A(s)])\|\|F_N^{in}\|_{\mathcal{L}^1(\mathfrak{H}_N)}.
\end{aligned} \tag{41}$$

By construction

$$\begin{aligned}
\|\mathcal{M}_N(t)A\| &= \|U_N(t)(\mathcal{M}_N^{in}A)U_N(t)^*\| \\
&= \|\mathcal{M}_N^{in}A\| \le \frac{1}{N}\sum_{k=1}^N \|J_k^*A\| = \|A\|.
\end{aligned}$$

Since $W(t)$ is unitary, the inequality above implies that

$$\|W(t)(\mathcal{M}_N(s)[E_\omega, A(s)])\| \le \|[E_\omega, A(s)]\|,$$

and

$$\|W(t)(\mathcal{M}_N(s)[E_\omega^*, E_\omega A(s)])\| \leq \|[E_\omega^*, E_\omega A(s)]\| = \|[E_\omega^*, A(s)]\|$$

because $[E_\omega^*, E_\omega A(s)] = E_\omega[E_\omega^*, A(s)]$ and E_ω is unitary.

Since $F_N^{in} \in \mathcal{D}_s(\mathfrak{H}_N)$, we conclude from the two previous inequalities and (41) that

$$\begin{aligned} &|\operatorname{trace}_{\mathfrak{H}_N}((\mathcal{C}[E_\omega, \mathcal{M}_N(s) - \mathscr{R}(s), \mathcal{M}_N(s)]A(s))F_N^{in}W(t))| \\ &\quad \leq \|[E_\omega, A(s)]\| \|((\mathcal{M}_N(s) - \mathscr{R}(s))E_\omega^*)F_N^{in}\|_{\mathcal{L}^1(\mathfrak{H}_N)} + \frac{1}{N}\|[E_\omega^*, A(s)]\|. \end{aligned} \tag{42}$$

Step 4. As mentioned above, for each integer $n \geq 0$, we designate by $C_b^{n,n}(\mathbf{R}^d \times \mathbf{R}^d)$ the set of complex-valued functions $f \equiv f(x, \xi)$ defined on $\mathbf{R}^d \times \mathbf{R}^d$ such that $\partial_x^\alpha \partial_\xi^\beta f$ exists, is continuous and bounded on $\mathbf{R}^d \times \mathbf{R}^d$ for all $\alpha, \beta \in \mathbf{N}^d$ satisfying $\max(|\alpha|, |\beta|) \leq n$. This is a Banach space for the norm

$$\|f\|_{n,n,\infty} = \max_{\max(|\alpha|,|\beta|)\leq n} \|\partial_x^\alpha \partial_\xi^\beta f\|_{L^\infty(\mathbf{R}^d \times \mathbf{R}^d)}.$$

Denote by $\mathcal{B}^n$ the closed unit ball of $C_b^{n,n}(\mathbf{R}^d \times \mathbf{R}^d)$ centered at the origin, i.e.

$$\mathcal{B}^n := \{a \in C_b^{n,n}(\mathbf{R}^d \times \mathbf{R}^d) \text{ s.t. } \|a\|_{n,n,\infty} \leq 1\}.$$

Pick $T > 0$; for each $t \in \mathbf{R}$, define

$$d_N^T(t) := \sup_{B \in \mathcal{W}[T]} \|((\mathcal{M}_N(t) - \mathscr{R}(t))(S(t,0)BS(0,t)))F_N^{in}\|_{\mathcal{L}^1(\mathfrak{H}_N)}, \tag{43}$$

where

$$\mathcal{W}[T] := \bigcup_{0\leq\tau\leq T} \mathcal{V}[\tau], \quad \text{with } \mathcal{V}[\tau] := \left\{S(0,\tau)\mathrm{OP}_\hbar^W[a]S(\tau,0) \,:\, a \in \mathcal{B}^{[d/2]+2}\right\},$$

denoting by $t \mapsto S(t, s)$ the operator-valued solution to the Cauchy problem

$$i\hbar\partial_t S(t,s) = (-\tfrac{1}{2}\hbar^2\Delta + V_{R(t)})S(t,s), \qquad S(s,s) = I_{\mathfrak{H}}. \tag{44}$$

Since E_ω^* is the Weyl operator with symbol $(x, \xi) \mapsto e^{-i\omega\cdot x}$, one has obviously

$$\max(1, |\omega|)^{-[d/2]-2} E_\omega^* \in \mathcal{V}[0] = \mathcal{W}[0].$$

Hence

$$\begin{aligned} &\|((\mathcal{M}_N(s) - \mathscr{R}(s))E_\omega^*)F_N^{in}\|_{\mathcal{L}^1(\mathfrak{H}_N)} \\ &\quad \leq \max(1, |\omega|)^{[d/2]+2} \sup_{a\in\mathcal{B}^{[d/2]+2}} \|((\mathcal{M}_N(s) - \mathscr{R}(s))\mathrm{OP}_\hbar^W[a])F_N^{in}\|_{\mathcal{L}^1(\mathfrak{H}_N)} \\ &\quad = \max(1, |\omega|)^{[d/2]+2} \sup_{B\in\mathcal{V}[s]} \|((\mathcal{M}_N(s) - \mathscr{R}(s))(S(s,0)BS(0,s)))F_N^{in}\|_{\mathcal{L}^1(\mathfrak{H}_N)} \\ &\quad \leq \max(1, |\omega|)^{[d/2]+2} d_N^T(s). \end{aligned}$$

Therefore, inequality (42) becomes

$$\begin{aligned}&\frac{1}{\hbar}|\operatorname{trace}_{\mathfrak{H}_N}((\mathcal{C}[E_\omega,\mathcal{M}_N(s)-\mathscr{R}(s),\mathcal{M}_N(s)]A(s))F_N^{in}W(t))|\\&\quad\le\frac{1}{\hbar}\|[E_\omega,A(s)]\|\max(1,|\omega|)^{[d/2]+2}d_N^T(s)+\frac{1}{N\hbar}\|[E_\omega^*,A(s)]\|.\end{aligned}\tag{45}$$

We are left with the task of estimating

$$\frac{\|[E_\omega,A(s)]\|}{\hbar}\quad\text{for all } A(s)=S(s,0)A^{in}S(0,s)\text{ with } A^{in}\in\mathcal{W}[T].$$

In other words, $A(s)$ is of the form

$$S(s,\tau)\mathrm{OP}_\hbar^W[a]S(\tau,s)\quad\text{with } a\in\mathcal{B}^{[d/2]+2},\ \text{and } 0\le\tau\le T.$$

The key estimate for all such operators is provided by the following lemma.

Lemma 4.1. *Under the assumptions of Theorem 1.1, there exists a positive constant $\gamma_d>0$ such that, for all $A^{in}\in\mathcal{W}[T]$, all $\omega\in\mathbf{R}^d$ and all $s\in[0,T]$, the operator $A(s)=S(s,0)A^{in}S(0,s)$ satisfies*

$$\frac{\|[E_\omega,A(s)]\|}{\hbar}\le\sqrt{d}\gamma_d|\omega|e^{T\max(1,\Gamma_2)},$$

where

$$\Gamma_2:=\max_{1\le j\le d}\sum_{k=1}^d\tfrac{1}{(2\pi)^d}\int_{\mathbf{R}^d}|\hat{V}(\xi)||\xi_j||\xi_k|\,\mathrm{d}\xi.$$

We shall take Lemma 4.1 for granted, finish the proof of Theorem 1.1, and postpone the proof of Lemma 4.1 until the end of the present section.

Inserting the bound provided by Lemma 4.1 shows that for all $s,t\in[0,T]$ and all $A^{in}\in\mathcal{W}[T]$, one has

$$\begin{aligned}&\frac{1}{\hbar}|\operatorname{trace}_{\mathfrak{H}_N}((\mathcal{C}[E_\omega,\mathcal{M}_N(s)-\mathscr{R}(s),\mathcal{M}_N(s)]A(s))F_N^{in}W(t))|\\&\quad\le\sqrt{d}\gamma_d e^{T\max(1,\Gamma_2)}|\omega|\left(\max(1,|\omega|)^{[d/2]+2}d_N^T(s)+\frac{1}{N}\right).\end{aligned}\tag{46}$$

Step 5. Now we use the inequality (46) to bound the right hand side of the integral inequality (39). One finds that, for each $t\in[0,T]$ and each $A^{in}\in\mathcal{W}[T]$,

$$\begin{aligned}\|(\mathcal{M}_N(t)-\mathscr{R}(t))(A(t))F_N^{in}\|_{\mathcal{L}^1(\mathfrak{H}_N)}&\le\|((\mathcal{M}_N(0)-\mathscr{R}(0))A^{in})F_N^{in}\|_{\mathcal{L}^1(\mathfrak{H}_N)}\\&+\sqrt{d}\gamma_d e^{T\max(1,\Gamma_2)}\int_0^t\int_{\mathbf{R}^d}\left(\max(1,|\omega|)^{[d/2]+2}d_N^T(s)+\tfrac{1}{N}\right)|\omega||\hat{V}(\omega)|\tfrac{\mathrm{d}\omega\,\mathrm{d}s}{(2\pi)^d}\\&\le d_N^T(0)+d\gamma_d e^{T\max(1,\Gamma_2)}\mathbf{V}\int_0^t\left(d_N^T(s)+\frac{1}{N}\right)\mathrm{d}s,\end{aligned}\tag{47}$$

where we recall that

$$\mathbf{V}:=\tfrac{1}{(2\pi)^d}\int_{\mathbf{R}^d}|\hat{V}(\omega)|(1+|\omega|)^{[d/2]+3}\,\mathrm{d}\omega<\infty,$$

since

$$\|((\mathcal{M}_N(0)-\mathscr{R}(0))A^{in})F_N^{in}\|_{\mathcal{L}^1(\mathfrak{H}_N)} \le d_N^T(0).$$

Observing that $A(t)=S(t,0)A^{in}S(0,t)$ with $t\in[0,T]$, and maximizing the left hand side of the inequality (47) as A^{in} runs through $\mathcal{W}[T]$, one finds that

$$d_N^T(t) \le d_N^T(0) + \sqrt{d}\gamma_d e^{T\max(1,\Gamma_2)\mathbf{V}} \int_0^t \left(d_N^T(s)+\frac{1}{N}\right) \mathrm{d}s \tag{48}$$

for all $t\in[0,T]$. Applying Gronwall's lemma to the integral inequality (48) shows that

$$d_N^T(T)+\frac{1}{N} \le \left(d_N^T(0)+\frac{1}{N}\right)\exp\left(\sqrt{d}\gamma_d T e^{T\max(1,\Gamma_2)}\mathbf{V}\right). \tag{49}$$

Step 6. Next, observe that

$$\begin{aligned} d_N^T(T) &\ge \sup_{B\in\mathcal{V}[T]} \|((\mathcal{M}_N(T)-\mathscr{R}(T))(S(T,0)BS(0,T)))F_N^{in}\|_{\mathcal{L}^1(\mathfrak{H}_N)} \\ &= \sup_{B\in\mathcal{V}[0]} |\operatorname{trace}_{\mathfrak{H}_N}(((\mathcal{M}_N(T)-\mathscr{R}(T))B)F_N^{in})| \\ &= \sup_{B\in\mathcal{V}[0]} |\operatorname{trace}_{\mathfrak{H}}((F_{N:1}(T)-R(T))B)|. \end{aligned}$$

On the other hand

$$\begin{aligned} &\operatorname{trace}_{\mathfrak{H}}((F_{N:1}(T)-R(T))\mathrm{OP}_\hbar^W[a]) \\ &= \iint_{\mathbf{R}^d\times\mathbf{R}^d} (W_\hbar[F_{N:1}(T)]-W_\hbar[R(T)])(x,\xi)a(x,\xi)\,\mathrm{d}x\,\mathrm{d}\xi\,, \end{aligned}$$

according to formula (63) in Appendix B. Hence

$$\begin{aligned} d_N^T(T) &\ge \sup_{a\in\mathcal{B}^{[d/2]+2}} \left|\iint_{\mathbf{R}^d\times\mathbf{R}^d} (W_\hbar[F_{N:1}(T)]-W_\hbar[R(T)])(x,\xi)a(x,\xi)\,\mathrm{d}x\,\mathrm{d}\xi\right| \\ &= \|W_\hbar[F_{N:1}(T)]-W_\hbar[R(T)]\|'_{[d/2]+2,[d/2]+2,\infty}\,. \end{aligned} \tag{50}$$

Step 7. Next we seek an upper bound for $d_N^T(0)$, to be inserted on the right hand side of (49). By the Calderon–Vaillancourt theorem (see Theorem B.1 in Appendix B), one has

$$\mathcal{V}[0]\subset \overline{B(0,\gamma_d)}_{\mathcal{L}(\mathfrak{H})}.$$

Hence

$$\begin{aligned} d_N^T(0) &:= \sup_{B\in\mathcal{V}[0]} \|((\mathcal{M}_N(0)-\mathscr{R}(t))B)F_N^{in}\|_{\mathcal{L}^1(\mathfrak{H}_N)} \\ &\le \sup_{\|B\|\le\gamma_d} \|((\mathcal{M}_N(0)-\mathscr{R}(t))B)F_N^{in}\|_{\mathcal{L}^1(\mathfrak{H}_N)} \\ &\le \gamma_d \sup_{\|B\|\le 1} \left\|((\mathcal{M}_N(0)-\mathscr{R}(0))B)\sqrt{F_N^{in}}\sqrt{F_N^{in}}\right\|_{\mathcal{L}^1(\mathfrak{H}_N)} \\ &\le \gamma_d \sup_{\|B\|\le 1} \left\|((\mathcal{M}_N(0)-\mathscr{R}(0))B)\sqrt{F_N^{in}}\right\|_{\mathcal{L}^2(\mathfrak{H}_N)}\,, \end{aligned} \tag{51}$$

by the Cauchy-Schwarz inequality, since $\|\sqrt{F_N^{in}}\|_{\mathcal{L}^2(\mathfrak{H}_N)} = 1$, so that one is left with the task of computing

$$\left\|((\mathcal{M}_N(0) - \mathscr{R}(0))B)\sqrt{F_N^{in}}\right\|_{\mathcal{L}^2(\mathfrak{H}_N)}.$$

One expands

$$\begin{aligned}
&\left\|((\mathcal{M}_N(0) - \mathscr{R}(0))B)\sqrt{F_N^{in}}\right\|^2_{\mathcal{L}^2(\mathfrak{H}_N)} \\
&= \mathrm{trace}_{\mathfrak{H}_N}\left(\sqrt{F_N^{in}}((\mathcal{M}_N(0) - \mathscr{R}(0))B)^*((\mathcal{M}_N(0) - \mathscr{R}(0))B)\sqrt{F_N^{in}}\right) \\
&= \mathrm{trace}_{\mathfrak{H}_N}(((\mathcal{M}_N(0) - \mathscr{R}(0))B)^*((\mathcal{M}_N(0) - \mathscr{R}(0))B)F_N^{in}) \\
&= \mathrm{trace}_{\mathfrak{H}_N}((\mathcal{M}_N(0)B)^*(\mathcal{M}_N(0)B)F_N^{in}) - \mathrm{trace}_{\mathfrak{H}_N}((\mathcal{M}_N(0)B)^*(\mathscr{R}(0)B)F_N^{in}) \\
&\quad - \mathrm{trace}_{\mathfrak{H}_N}((\mathscr{R}(0)B)^*(\mathcal{M}_N(0)B)F_N^{in}) + \mathrm{trace}_{\mathfrak{H}_N}((\mathscr{R}(0)B)^*(\mathscr{R}(0)B)F_N^{in}).
\end{aligned}$$

One has

$$\begin{aligned}
\mathrm{trace}_{\mathfrak{H}_N}((\mathscr{R}(0)B)^*(\mathscr{R}(0)B)F_N^{in}) &= |\,\mathrm{trace}_{\mathfrak{H}}(R(0)B)|^2\,\mathrm{trace}_{\mathfrak{H}_N}(F_N^{in}) \\
&= |\,\mathrm{trace}_{\mathfrak{H}}(R(0)B)|^2,
\end{aligned}$$

and

$$\begin{aligned}
\mathrm{trace}_{\mathfrak{H}_N}((\mathscr{R}(0)B)^*(\mathcal{M}_N(0)B)F_N^{in}) &= \overline{\mathrm{trace}_{\mathfrak{H}}((R(0)B)}\,\mathrm{trace}_{\mathfrak{H}_N}((\mathcal{M}_N(0)B)F_N^{in}) \\
&= \overline{\mathrm{trace}_{\mathfrak{H}}(R(0)B)}\,\mathrm{trace}_{\mathfrak{H}}(BF_{N:1}^{in}).
\end{aligned}$$

Then

$$\begin{aligned}
&\mathrm{trace}_{\mathfrak{H}_N}((\mathcal{M}_N(0)(B))^*\mathscr{R}(0)(B)F_N^{in}) = \mathrm{trace}_{\mathfrak{H}_N}(F_N^{in}(\mathcal{M}_N(0)(B))^*\mathscr{R}(0)(B)) \\
&= \overline{\mathrm{trace}_{\mathfrak{H}_N}((F_N^{in}(\mathcal{M}_N(0)(B))^*\mathscr{R}(0)(B))^*)} = \overline{\mathrm{trace}_{\mathfrak{H}_N}(\mathscr{R}(0)(B)^*\mathcal{M}_N(0)(B)F_N^{in})} \\
&= \mathrm{trace}_{\mathfrak{H}}(R(0)B)\overline{\mathrm{trace}_{\mathfrak{H}}(BF_{N:1}^{in})}.
\end{aligned}$$

It remains to compute

$$\begin{aligned}
&\mathrm{trace}_{\mathfrak{H}_N}((\mathcal{M}_N(0)B)^*(\mathcal{M}_N(0)B)F_N^{in}) \\
&= \frac{1}{N^2}\sum_{1\le k\ne l\le N}\mathrm{trace}_{\mathfrak{H}_N}\,\mathrm{trace}_{\mathfrak{H}_N}((J_kB^*)(J_lB)F_N^{in}) \\
&\quad + \frac{1}{N^2}\sum_{k=1}^{N}\mathrm{trace}_{\mathfrak{H}_N}((J_kB)^*(J_kB)F_N^{in}) \\
&= \frac{N-1}{N}\,\mathrm{trace}_{\mathfrak{H}_2}((B^*\otimes B)F_{N:2}^{in}) + \frac{1}{N}\,\mathrm{trace}_{\mathfrak{H}}(B^*BF_{N:1}^{in}).
\end{aligned}$$

Summarizing, we have found that

$$\begin{aligned}&\left\|(\mathcal{M}_N(0)-\mathscr{R}(0))(B)\sqrt{F_N^{in}}\right\|^2_{\mathcal{L}^2(\mathfrak{H}_N)}\\&=\frac{N-1}{N}\operatorname{trace}_{\mathfrak{H}_2}((B^*\otimes B)F^{in}_{N:2})+\frac{1}{N}\operatorname{trace}_{\mathfrak{H}}(B^*BF^{in}_{N:1})\\&\quad-2\Re\left(\overline{\operatorname{trace}_{\mathfrak{H}}(R(0)B)}\operatorname{trace}_{\mathfrak{H}}(BF^{in}_{N:1})\right)+|\operatorname{trace}_{\mathfrak{H}}(R(0)B)|^2.\end{aligned}$$

One can rearrange this term as

$$\begin{aligned}&\left\|((\mathcal{M}_N(0)-\mathscr{R}(0))B)\sqrt{F_N^{in}}\right\|^2_{\mathcal{L}^2(\mathfrak{H}_N)}\\&=\frac{N-1}{N}\operatorname{trace}_{\mathfrak{H}_2}((B^*\otimes B)(F^{in}_{N:2}-F^{in}_{N:1}\otimes F^{in}_{N:1}))\\&\quad+\frac{1}{N}(\operatorname{trace}_{\mathfrak{H}}(B^*BF^{in}_{N:1})-|\operatorname{trace}_{\mathfrak{H}}(BF^{in}_{N:1})|^2)\\&\quad+|\operatorname{trace}_{\mathfrak{H}}(B(F^{in}_{N:1}-R(0)))|^2.\end{aligned}$$

Hence

$$\begin{aligned}&\sup_{\|B\|\le 1}\left\|((\mathcal{M}_N(0)-\mathscr{R}(0))B)\sqrt{F_N^{in}}\right\|^2_{\mathcal{L}^2(\mathfrak{H}_N)}\\&\le\frac{N-1}{N}\|F^{in}_{N:2}-F^{in}_{N:1}\otimes F^{in}_{N:1}\|_{\mathcal{L}^1(\mathfrak{H}_2)}+\|F^{in}_{N:1}-R(0)\|^2_{\mathcal{L}^1(\mathfrak{H})}+\frac{1}{N}.\end{aligned}\tag{52}$$

Since we have assumed in Theorem 1.1 that $F_N^{in}=(R^{in})^{\otimes N}$, one has

$$F^{in}_{N:1}=R^{in}=R(0)\quad\text{and}\quad F^{in}_{N:2}=(R^{in})^{\otimes 2}=F^{in}_{N:1}\otimes F^{in}_{N:1}.$$

Therefore, we conclude from (51) and (52) that

$$d_N^T(0)\le\frac{\gamma_d}{\sqrt{N}}.\tag{53}$$

Inserting the bounds (53) and (50) in (49), we conclude that

$$\begin{aligned}&\|W_\hbar[F_{N:1}(T)]-W_\hbar[R(T)]\|'_{[d/2]+2,[d/2]+2,\infty}\le\frac{\gamma_d}{\sqrt{N}}\exp\left(\sqrt{d}\gamma_dTe^{T\max(1,\Gamma_2)}\mathbf{V}\right)\\&+\frac{1}{N}\left(\exp\left(\sqrt{d}\gamma_dTe^{T\max(1,\Gamma_2)}\mathbf{V}\right)-1\right),\end{aligned}$$

which obviously implies (7).

Remark. By comparison with the proofs of Theorem 2.4 in [17], a striking feature of the present proof is that it uses a different distance for each time t at which we seek to compare the Hartree solution $R(t)$ and the first marginal $F_{N:1}(t)$ of the N-particle density. Specifically, for each $T>0$, the distance $d_N^T(T)$ is used to estimate the difference, $W_\hbar[F_{N:1}(T)]-W_\hbar[R(T)]$. On the contrary, in [17], the convergence rate for all time intervals is estimated in terms of a single pseudo-distance constructed by analogy with the quadratic Monge-Kantorovich (or Wasserstein) distance used in optimal transport.

Proof of Lemma 4.1.[4]

Let S be the solution to the Cauchy problem (44). Then

$$i\hbar\partial_t A(t) = [-\tfrac{1}{2}\hbar^2\Delta + V_{R(t)}, A(t)], \qquad A(0) = A^{in} \iff A(t) = S(t,0)A^{in}S(0,t).$$

Picking $A^{in} \in \mathcal{W}[T]$ implies that A^{in} is of the form $A^{in} = S(0,\tau)\mathrm{OP}_\hbar^W[a]S(\tau,0)$ with $a \in \mathcal{B}^{[d/2]+2}$.

For each $j = 1, \ldots, d$, one has

$$\begin{aligned} i\hbar\partial_t[x_j, A(t)] &= [x_j, [-\tfrac{1}{2}\hbar^2\Delta + V_{R(t)}, A(t)]] \\ &= [-\tfrac{1}{2}\hbar^2\Delta + V_{R(t)}, [x_j, A(t)]] + \hbar^2[\partial_{x_j}, A(t)], \end{aligned}$$

so that, by Duhamel's formula,

$$[x_j, A(t)] = S(t,\tau)[x_j, \mathrm{OP}_\hbar^W[a]]S(\tau,t) - i\int_\tau^t S(t,s)[\hbar\partial_{x_j}, A(s)]S(s,t)\,\mathrm{d}s.$$

Since $S(t,s)$ is unitary and $S(s,t) = S(t,s)^*$, one has

$$\|[x_j, A(t)]\| \le \|[x_j, \mathrm{OP}_\hbar^W[a]]\| + \left|\int_\tau^t \|[\hbar\partial_{x_j}, A(s)]\|\,\mathrm{d}s\right|. \tag{54}$$

Likewise

$$\begin{aligned} i\hbar\partial_t[-i\hbar\partial_{x_j}, A(t)] &= [-i\hbar\partial_{x_j}, [-\tfrac{1}{2}\hbar^2\Delta + V_{R(t)}, A(t)]] \\ &= [-\tfrac{1}{2}\hbar^2\Delta + V_{R(t)}, [-i\hbar\partial_{x_j}, A(t)]] - i\hbar[\partial_j V_{R(t)}, A(t)]. \end{aligned}$$

Since

$$-i\hbar[\partial_j V_{R(t)}, A(t)] = \frac{\hbar}{(2\pi)^d}\int_{\mathbf{R}^d} \omega_j \hat{V}(\omega)\,\mathrm{trace}(R(t)E_\omega^*)[E_\omega, A(t)]\,\mathrm{d}\omega,$$

Duhamel's formula implies that

$$\begin{aligned} [-i\hbar\partial_{x_j}, A(t)] &= S(t,\tau)[-i\hbar\partial_{x_j}, \mathrm{OP}_\hbar^W[a]]S(\tau,t) \\ &- \frac{i}{(2\pi)^d}\int_{\mathbf{R}^d} \omega_j\hat{V}(\omega)\left(\int_\tau^t S(t,s)\,\mathrm{trace}(R(s)E_\omega^*)[E_\omega, A(t)]S(s,t)\,\mathrm{d}s\right)\mathrm{d}\omega. \end{aligned}$$

Since $R(s) = R(s)^* \ge 0$ and $\mathrm{trace}(R(s)) = 1$, one has $|\mathrm{trace}(R(s)E_\omega^*)| \le 1$ and therefore, arguing as in the proof of (54)

$$\begin{aligned} \|[-i\hbar\partial_{x_j}, A(t)]\| &\le \|[-i\hbar\partial_{x_j}, \mathrm{OP}_\hbar^W[a]]\| \\ &+ \frac{1}{(2\pi)^d}\int_{\mathbf{R}^d} |\omega_j||\hat{V}(\omega)|\left|\int_\tau^t \|[E_\omega, A(s)]\|\,\mathrm{d}s\right|\mathrm{d}\omega. \end{aligned}$$

[4] We thank one of the referees for suggesting the present proof of Lemma 4.1 based on the computations in Appendix B of [5] or Appendix C of [6]. This proof requires less regularity on the interaction potential V, and is much simpler than our original argument, which followed instead the analysis in [9].

On the other hand

$$[E_\omega, A(s)] = \left(\int_0^1 \frac{d}{d\lambda}\left(E_{\lambda\omega}A(s)E_{\lambda\omega}^*\right) \mathrm{d}\lambda\right) E_\omega$$
$$= \left(\int_0^1 E_{\lambda\omega}[i\omega\cdot x, A(s)]E_{\lambda\omega}^* \,\mathrm{d}\lambda\right) E_\omega\,,$$

so that

$$\|[E_\omega, A(t)]\| \le \sum_{k=1}^{d} |\omega_k| \|[x_k, A(t)]\|. \tag{55}$$

Thus

$$\|[-i\hbar\partial_{x_j}, A(t)]\| \le \|[-i\hbar\partial_{x_j}, \mathrm{OP}_\hbar^W[a]]\| + \tfrac{1}{(2\pi)^d}\sum_{k=1}^{d}\int_{\mathbf{R}^d} |\omega_j||\omega_k||\hat V(\omega)| \left|\int_\tau^t \|[x_k, A(s)]\|\,\mathrm{d}s\right| \mathrm{d}\omega. \tag{56}$$

Set

$$\mathcal{N}(t) := \max_{1\le j\le d}(\|[x_j, A(t)]\| + \|[-i\hbar\partial_{x_j}, A(t)]\|)\,,$$

and

$$\Gamma_2 := \max_{1\le j\le d}\sum_{k=1}^{d}\tfrac{1}{(2\pi)^d}\int_{\mathbf{R}^d} |\omega_j||\omega_k||\hat V(\omega)|\,\mathrm{d}\omega.$$

Then

$$\mathcal{N}(t) \le \mathcal{N}(\tau) + \max(1, \Gamma_2)\left|\int_\tau^t \mathcal{N}(s)\,\mathrm{d}s\right|\,,$$

and Gronwall's lemma implies that

$$\mathcal{N}(t) \le \mathcal{N}(\tau)e^{|t-\tau|\max(1,\Gamma_2)} \qquad t\in[0,T].$$

The argument leading to this bound is similar to Appendix C in [6].

Then, by (55) and the Cauchy-Schwarz inequality,

$$\frac{1}{\hbar}\|[E_\omega, A(t)]\| \le \frac{\sqrt{d}}{\hbar}|\omega|\mathcal{N}(t) \le \frac{\sqrt{d}}{\hbar}|\omega|\mathcal{N}(\tau)e^{|t-\tau|\max(1,\Gamma_2)}$$
$$\le \frac{\sqrt{d}}{\hbar}|\omega|\mathcal{N}(\tau)e^{T\max(1,\Gamma_2)}$$

since $t, \tau\in[0,T]$. We have assumed that $A^{in} = S(0,\tau)\mathrm{OP}_\hbar^W[a]S(\tau,0)$, so that one has $A(\tau) = \mathrm{OP}_\hbar^W[a]$. Hence

$$\mathcal{N}(\tau) := \max_{1\le j\le d}(\|[x_j, \mathrm{OP}_\hbar^W[a]]\| + \|[-i\hbar\partial_{x_j}, \mathrm{OP}_\hbar^W[a]]\|) \le \gamma_d\hbar$$

by the Calderon–Vaillancourt theorem (Theorem B.1 in Appendix B), since

$$[x_j, \mathrm{OP}_\hbar^W[a]] = i\hbar\mathrm{OP}_\hbar^W[\partial_{\xi_j}a]\,, \quad [-i\hbar\partial_{x_j}, \mathrm{OP}_\hbar^W[a]] = -i\hbar\mathrm{OP}_\hbar^W[\partial_{x_j}a]$$

and $a\in\mathcal{B}^{[d/2]+2}$. $\square$

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Appendix A. A Unified Setting for the Terms $\mathbf{ad}^*(-\frac{1}{2}\hbar^2\Delta)\mathcal{M}_N(t)$ and $\mathcal{C}[V, \mathcal{M}_N(t), \mathcal{M}_N(t)]$

According to Lemma 3.6,

$$\mathbf{ad}^*(-\tfrac{1}{2}\hbar^2\Delta)\mathscr{R}_N(t) - \mathcal{C}[V, \mathscr{R}_N(t), \mathscr{R}_N(t)] = \mathbf{ad}^*(-\tfrac{1}{2}\hbar^2\Delta + V_{R(t)})\mathscr{R}_N(t)\,,$$

when $\mathscr{R}_N(t)$ is of the form (36).

This suggests to look for a common structure in both terms $\mathbf{ad}^*(-\frac{1}{2}\hbar^2\Delta)\mathcal{M}_N(t)$ and $\mathcal{C}[V, \mathcal{M}_N(t), \mathcal{M}_N(t)]$, although $\mathcal{M}_N(t)$ is not in the form (36). This can be achieved, at least at the formal level, by the following remark.

All the tensor products appearing in the discussion below designate tensor products of $\mathbf{C}$- vector spaces. Observe that $\mathcal{L}(\mathcal{L}(\mathfrak{H}), \mathcal{L}(\mathfrak{H}_N))$ is a $\mathcal{L}(\mathfrak{H})^{op} \otimes \mathcal{L}(\mathfrak{H}_N)$-bimodule, where $\mathcal{L}(\mathfrak{H})^{op}$ is the opposite of the algebra $\mathcal{L}(\mathfrak{H})$—in other words, the product in $\mathcal{L}(\mathfrak{H})^{op}$ is

$$\mathcal{L}(\mathfrak{H}) \otimes \mathcal{L}(\mathfrak{H}) \ni A \otimes B \mapsto BA \in \mathcal{L}(\mathfrak{H}).$$

The product in the algebra $\mathcal{L}(\mathfrak{H})^{op} \otimes \mathcal{L}(\mathfrak{H}_N)$ is defined by the formula

$$(P \otimes Q_N)(P' \otimes Q'_N) := (P'P) \otimes (Q_N Q'_N)\,, \qquad P, P' \in \mathcal{L}(\mathfrak{H})\,, \quad Q_N, Q'_N \in \mathcal{L}(\mathfrak{H}_N).$$

The left scalar multiplication in the $\mathcal{L}(\mathfrak{H})^{op} \otimes \mathcal{L}(\mathfrak{H}_N)$-bimodule $\mathcal{L}(\mathcal{L}(\mathfrak{H}), \mathcal{L}(\mathfrak{H}_N))$ is defined as follows. Let $\Lambda \in \mathcal{L}(\mathcal{L}(\mathfrak{H}), \mathcal{L}(\mathfrak{H}_N))$, let $P \in \mathcal{L}(\mathfrak{H})$ and $Q_N \in \mathcal{L}(\mathfrak{H}_N)$, then

$$(P \otimes Q_N) \cdot \Lambda : \mathcal{L}(\mathfrak{H}) \ni A \mapsto Q_N \Lambda(PA) \in \mathcal{L}(\mathfrak{H}_N).$$

That this is a left action of $\mathcal{L}(\mathfrak{H})^{op} \otimes \mathcal{L}(\mathfrak{H}_N)$ on $\mathcal{L}(\mathcal{L}(\mathfrak{H}), \mathcal{L}(\mathfrak{H}_N))$ is seen with the following elementary computation

$$\begin{aligned}((P' \otimes Q'_N) \cdot ((P \otimes Q_N) \cdot \Lambda))A &= Q'_N((P \otimes Q_N) \cdot \Lambda)(P'A) \\ &= (Q'_N Q_N)\Lambda(PP'A) \\ &= (((PP') \otimes (Q'_N Q_N))\Lambda)A\,,\end{aligned}$$

for all P, P' and $A \in \mathcal{L}(\mathfrak{H})$ and $Q_N, Q'_N \in \mathcal{L}(\mathfrak{H}_N)$. Likewise, one easily checks that the right scalar multiplication in the $\mathcal{L}(\mathfrak{H})^{op} \otimes \mathcal{L}(\mathfrak{H}_N)$-bimodule $\mathcal{L}(\mathcal{L}(\mathfrak{H}), \mathcal{L}(\mathfrak{H}_N))$, defined by the formula

$$\Lambda \cdot (P \otimes Q_N) : \mathcal{L}(\mathfrak{H}) \ni A \mapsto \Lambda(AP)Q_N \in \mathcal{L}(\mathfrak{H}_N)$$

is indeed a right action.

In this setting, one has

$$\Lambda \cdot (P \otimes Q_N) - (P \otimes Q_N) \cdot \Lambda = \mathbf{b}_1(\Lambda \otimes (P \otimes Q_N))\,, \tag{57}$$

where

$$\mathbf{b}_1 : \mathcal{L}(\mathcal{L}(\mathfrak{H}), \mathcal{L}(\mathfrak{H}_N)) \otimes (\mathcal{L}(\mathfrak{H})^{op} \otimes \mathcal{L}(\mathfrak{H}_N)) \to \mathcal{L}(\mathcal{L}(\mathfrak{H}), \mathcal{L}(\mathfrak{H}_N))$$

is the Hochschild boundary map in degree one, defined on the space of Hochschild 1-chains

$$C_1(\mathcal{L}(\mathcal{L}(\mathfrak{H}), \mathcal{L}(\mathfrak{H}_N)); \mathcal{L}(\mathfrak{H})^{op} \otimes \mathcal{L}(\mathfrak{H}_N)) := \mathcal{L}(\mathcal{L}(\mathfrak{H}), \mathcal{L}(\mathfrak{H}_N)) \otimes (\mathcal{L}(\mathfrak{H})^{op} \otimes \mathcal{L}(\mathfrak{H}_N))$$

with values in the space of Hochschild 0-chains

$$C_0(\mathcal{L}(\mathcal{L}(\mathfrak{H}), \mathcal{L}(\mathfrak{H}_N)); \mathcal{L}(\mathfrak{H})^{op} \otimes \mathcal{L}(\mathfrak{H}_N)) := \mathcal{L}(\mathcal{L}(\mathfrak{H}), \mathcal{L}(\mathfrak{H}_N)).$$

(See for instance section 1.1 in [32] for a quick presentation of Hochschild homology.) Hence

$$\begin{aligned} \mathcal{C}[E_\omega, \mathcal{M}_N, \mathcal{M}_N] &= (\mathcal{M}_N E_\omega^*)\mathcal{M}_N(E_\omega A) - (\mathcal{M}_N(AE_\omega))(\mathcal{M}_N E_\omega^*) \\ &= -\mathbf{b}_1(\mathcal{M}_N \otimes (E_\omega \otimes (\mathcal{M}_N E_\omega^*))). \end{aligned} \tag{58}$$

In the special case where $Q_N = I_{\mathfrak{H}_N}$, the identity (57) takes the form

$$\mathbf{b}_1(\Lambda \otimes (P \otimes I_{\mathfrak{H}_N}) = \mathbf{ad}^*(P)\Lambda\,, \tag{59}$$

and this is the key observation leading to Lemma 3.6.

Since the Hochschild boundary map $\mathbf{b}_1$ is linear, one can think of the operator $\mathcal{C}[V, \mathcal{M}_N, \mathcal{M}_N]$ as

$$\mathcal{C}[V, \mathcal{M}_N, \mathcal{M}_N] = -\mathbf{b}_1\left(\mathcal{M}_N \otimes \int_{\mathbf{R}^d} E_\omega \otimes (\mathcal{M}_N E_\omega^*)\hat{V}(\,\mathrm{d}\omega)\right). \tag{60}$$

With the previous identity, equation (34) takes the form

$$i\hbar\partial_t \mathcal{M}_N(t) = \mathbf{b}_1(\mathcal{M}_N(t) \otimes \mathscr{H}[\mathcal{M}_N(t)]) \tag{61}$$

where $\mathscr{H}[\mathcal{M}_N(t)]$ is the N-body quantum Hamiltonian viewed as the element of $\mathcal{L}(\mathfrak{H})^{op} \otimes \mathcal{L}(\mathfrak{H}_N)$ defined by the formula

$$\mathscr{H}[\mathcal{M}_N(t)] := -\tfrac{1}{2}\hbar^2\Delta \otimes I_{\mathfrak{H}_N} + \int_{\mathbf{R}^d} E_\omega \otimes (\mathcal{M}_N E_\omega^*)\hat{V}(\,\mathrm{d}\omega). \tag{62}$$

While the discussion in the previous paragraphs is mathematically rigorous, writing (34) as (61) is purely formal for two reasons. First, Δ is an unbounded operator on $\mathfrak{H}$, so that one cannot think of $\mathcal{M}_N(t) \otimes (-\frac{1}{2}\hbar^2\Delta \otimes I_{\mathfrak{H}_N})$ as a Hochschild 1-chain, i.e. an element of $C_1(\mathcal{L}(\mathcal{L}(\mathfrak{H}), \mathcal{L}(\mathfrak{H}_N)); \mathcal{L}(\mathfrak{H})^{op} \otimes \mathcal{L}(\mathfrak{H}_N))$. The term

$$\int_{\mathbf{R}^d} E_\omega \otimes (\mathcal{M}_N E_\omega^*)\hat{V}(\,\mathrm{d}\omega)$$

is even more annoying. Unless $\hat{V}$ is a finite linear combination of Dirac measures, this integral does not define an element of $\mathcal{L}(\mathfrak{H})^{op} \otimes \mathcal{L}(\mathfrak{H}_N)$. At best, this integral could be thought of as an element of some completion of $\mathcal{L}(\mathfrak{H})^{op} \otimes \mathcal{L}(\mathfrak{H}_N)$, the choice of which might not be completely obvious. (For instance, using cross norms to define the topology on the algebra $\mathcal{L}(\mathfrak{H})^{op} \otimes \mathcal{L}(\mathfrak{H}_N)$ might lead to serious difficulties since the map $\mathbf{R} \ni \omega \mapsto E_\omega \in \mathcal{L}(\mathfrak{H})$ is not continuous for the norm topology. Likewise, one should probably avoid thinking of the integral above as a Bochner integral since $\mathcal{L}(\mathfrak{H})$

and $\mathcal{L}(\mathfrak{H}_N)$ are not separable.) In view of these difficulties, we shall not go further in this direction, and stick to our Definition 3.1 of the interaction term $\mathcal{C}[V, \mathcal{M}_N, \mathcal{M}_N]$. Nevertheless, it might be useful to keep in mind the form (61) of the governing equation (34) for $\mathcal{M}_N$, together with the formal expression of the interaction term as in (60)–(62).

Of course, if $\mathcal{M}_N(t)$ is of the form $\mathscr{R}(t)$ given by (36), then

$$\int_{\mathbf{R}^d} E_\omega \otimes (\mathcal{M}_N E_\omega^*)\hat{V}(\mathrm{d}\omega) = \left(\int_{\mathbf{R}^d} E_\omega \operatorname{trace}_{\mathfrak{H}}(R(t)E_\omega^*)\hat{V}(\mathrm{d}\omega)\right) \otimes I_{\mathfrak{H}_N} \\ = V_{R(t)} \otimes I_{\mathfrak{H}_N} ,$$

so that

$$\mathscr{H}[\mathscr{R}(t)] = (-\tfrac{1}{2}\hbar^2\Delta + V_{R(t)}) \otimes I_{\mathfrak{H}_N} .$$

Then, according to (59),

$$\mathbf{b}_1(\mathscr{R}(t) \otimes \mathscr{H}[\mathscr{R}(t)]) = \mathbf{ad}^*(-\tfrac{1}{2}\hbar^2\Delta + V_{R(t)})\mathscr{R}(t) ,$$

so that equation (61) for $\mathscr{R}$ given by (36) takes the form

$$i\hbar\partial_t\mathscr{R}(t) = \mathbf{b}_1(\mathscr{R}(t) \otimes \mathscr{H}[\mathscr{R}(t)]) = \mathbf{ad}^*(-\tfrac{1}{2}\hbar^2\Delta + V_{R(t)})\mathscr{R}(t) ,$$

which is clearly equivalent to (3) for $R(t)$.

Appendix B. Wigner Transformation, Weyl Quantization and the Calderon–Vaillancourt Theorem

We first recall the notion of Wigner transform [41]. For each $K \in \mathcal{L}(\mathfrak{H})$ with integral kernel $k \equiv k(x, y) \in \mathbf{C}$ such that $k \in \mathcal{S}(\mathbf{R}^d \times \mathbf{R}^d)$, the Wigner transform at scale $\hbar$ of K is the element of $\mathcal{S}(\mathbf{R}^d \times \mathbf{R}^d)$ defined by the formula

$$W_\hbar[K](x, \xi) := \tfrac{1}{(2\pi)^d} \int_{\mathbf{R}^d} k(x + \tfrac{1}{2}\hbar y, x - \tfrac{1}{2}\hbar y)e^{-i\xi\cdot y}\,\mathrm{d}y.$$

By Plancherel's theorem, for each pair of operators $K_1, K_2 \in \mathcal{L}(\mathfrak{H})$ with integral kernels $k_1, k_2 \in \mathcal{S}(\mathbf{R}^d \times \mathbf{R}^d)$, one has

$$\iint_{\mathbf{R}^d\times\mathbf{R}^d} \overline{W_\hbar[K_1](x, \xi)}W_\hbar[K_2](x, \xi)\,\mathrm{d}x\,\mathrm{d}\xi \\ = \frac{1}{(2\pi\hbar)^d}\iint_{\mathbf{R}^d\times\mathbf{R}^d} \overline{k_1(x, y)}k_2(x, y)\,\mathrm{d}x\,\mathrm{d}y = \frac{1}{(2\pi\hbar)^d}\operatorname{trace}_{\mathfrak{H}}(K_1^*K_2).$$

Therefore, the linear map $K \mapsto (2\pi\hbar)^{d/2}W_\hbar[K]$ extends as an unitary isomorphism from $\mathcal{L}^2(\mathfrak{H})$ to $L^2(\mathbf{R}^d \times \mathbf{R}^d)$. Observe that

$$W_\hbar[K^*](x, \xi) = \overline{W_\hbar[K](x, \xi)}, \qquad \text{for a.e. } (x, \xi) \in \mathbf{R}^d \times \mathbf{R}^d.$$

We next recall the semiclassical Weyl quantization. For each $a \in \mathcal{S}(\mathbf{R}_x^d \times \mathbf{R}_\xi^d)$ with polynomial growth as $|x| + |\xi| \to +\infty$, the expression

$$(\mathrm{OP}_\hbar^W[a]\psi)(x) = \tfrac{1}{(2\pi)^d}\iint_{\mathbf{R}^d\times\mathbf{R}^d} a\left(\frac{x+y}{2}, \hbar\xi\right)e^{i\xi\cdot(x-y)}\psi(y)\,\mathrm{d}\xi\,\mathrm{d}y$$

defines a linear map from $\mathcal{S}(\mathbf{R}^d)$ to itself. Observe that

$$\int_{\mathbf{R}^d} \overline{\phi(x)}(\mathrm{OP}_\hbar^W[a]\psi)(x)\,\mathrm{d}x = \iint_{\mathbf{R}^d\times\mathbf{R}^d} \overline{W_\hbar[|\phi\rangle\langle\psi|](x,\xi)}a(x,\xi)\,\mathrm{d}x\,\mathrm{d}\xi.$$

This formula extends to density operators more general than $|\phi\rangle\langle\psi|$, viz.

$$\mathrm{trace}_{L^2(\mathbf{R}^d)}(R\,\mathrm{OP}_\hbar^W[a]) = \iint_{\mathbf{R}^d\times\mathbf{R}^d} W_\hbar[R](x,\xi)a(x,\xi)\,\mathrm{d}x\,\mathrm{d}\xi \tag{63}$$

for all $R \in \mathcal{D}(\mathfrak{H})$.

This defines the operator $\mathrm{OP}_\hbar^W[a]$ by duality as a linear map from $\mathcal{S}(\mathbf{R}^d)$ to $\mathcal{S}'(\mathbf{R}^d)$ for all $a \in \mathcal{S}'(\mathbf{R}^d \times \mathbf{R}^d)$. Observe that

$$\mathrm{OP}_\hbar^W[a]^* = \mathrm{OP}_\hbar^W[\overline{a}].$$

Finally, we mention the following variant of the Calderon–Vaillancourt theorem due to Boulkhemair [8]—see also formula (54) on p. 236 in [9].

Theorem B.1 (Calderon–Vaillancourt). *For each integer $d \geq 1$, there exists a constant $\gamma_d > 0$ with the following property.*

Let $a \in \mathcal{S}'(\mathbf{R}_x^d \times \mathbf{R}_\xi^d)$ satisfy the condition

$$|\alpha|, |\beta| \leq [d/2]+1 \implies \partial_x^\alpha \partial_\xi^\beta a \in L^\infty(\mathbf{R}_x^d \times \mathbf{R}_\xi^d).$$

Then, for all $\hbar \in (0,1)$, one has

$$\|\mathrm{OP}_\hbar^W[a]\|_{\mathcal{L}(L^2(\mathbf{R}^d))} \leq \gamma_d \max_{|\alpha|,|\beta|\leq[d/2]+1} \|\partial_x^\alpha \partial_\xi^\beta a\|_{L^\infty(\mathbf{R}^d\times\mathbf{R}^d)}.$$

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