The Hartree-von Neumann limit of many body dynamics

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Abstract

In the mean-field regime, we prove convergence (with explicit bounds) of the many-body von Neumann dynamics with bounded interactions to the Hartree-von Neumann dynamics.

1 Introduction

Derivation of macroscopic equations from microscopic ones is one of the main challenges of Mathematical Physics. This is usually a daunting task met with a very limited success. In the last few years a considerable progress was made on one such problem - derivation of the Hartree, Hartree-Fock and Gross-Pitaevskii equations in the mean-field and Gross-Pitaevskii regimes, respectively ([BEGMY, BGGM, FGS, FKS, FKP, AN, LSY, LS, ErY, ESY, ES, KS, KM, GM, KSS]). Though the work on the Gross-Pitaevskii limit is quite recent, the work on the mean-field one goes back to the papers [He, GV, S].

In this note we prove the convergence of solutions of the \( N \)-body von Neumann equation with product initial conditions to the \( N \)-fold product of solutions of the Hartree-von Neumann equation with the corresponding initial conditions and estimate the rate of this convergence. The regime we consider is the mean-field one, i.e. with the number of particles going to infinity, while the strength of interaction decreasing in the inverse proportion to the number of particles. In our analysis we follow closely the beautiful work [FGS]. One of the new elements of our approach is a Hamiltonian formulation of the Hartree-von Neumann equation. While this work has been written up there appeared e-prints [RS, ErS and GMM] giving, by different techniques, estimates of

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the rate of convergence in the case of the $N$–body Schrödinger and Hartree equations.

Let $\rho_{\otimes N} := \rho \otimes \ldots \otimes \rho$. We start with the time-dependent von Neumann equation for a system of $N$ bosons

$$\frac{ih\partial \rho_N}{\partial t} = [H_N, \rho_N], \quad \rho_N|_{t=0} = \rho_{\otimes N}^0,$$

with $\rho_N = \rho_N(t)$ acting on $L^2(\mathbb{R}^3)^{\otimes N}$ and $\rho_0$, a positive, trace-class operator on $L^2(\mathbb{R}^3)$ of trace 1. Here $H_N = H_N^0 + V_N$, with $H_N^0 = -\sum_{i=1}^N h_{x_i}$, $h_x \equiv h$ is a self-adjoint operator in a variable $x$, e.g. $h_x := \hbar^2 \Delta_x + W(x)$, and

$$V_N = \frac{g}{2} \sum_{i \neq j} v(x_i - x_j).$$

Since $\sum_{i \neq j} v(x_i - x_j) = \sum_{i \neq j} \frac{1}{2}(v(x_i - x_j) + v(x_j - x_i))$ we can assume without loss of generality that the two-body potential $v$ is even: $v(x) = v(-x)$. We consider the mean field regime: $N \to \infty$ and $g \to 0$ with $gN \to c$. By changing $v$, if necessary, we can assume that

$$g = \frac{1}{N}. \quad (3)$$

We will relate the von Neumann equation (1) to the Hartree-von Neumann equation

$$\frac{ih\partial \rho}{\partial t} = [h + (v \ast n_{\rho}), \rho], \quad \rho|_{t=0} = \rho_0,$$

with $\rho = \rho(x)$ is the same two-body potential as above and $n_{\rho}(x,t) := \rho(x;x,t)$, the probability or charge density, with $\rho(x;y,t)$ the integral kernel of $\rho$.

For $v \in L^\infty$ one can show easily that (4) is globally well-posed on the space of positive, trace-class operators and that the trace, $Tr \rho$, and the energy,

$$E(\rho) := Tr(h\rho) + \frac{1}{2} \int n_{\rho} \cdot v \ast n_{\rho}, \quad (5)$$

are conserved. Moreover, $\rho$ is non-negative, provided so is $\rho_0$. See Appendix A.

In Section 4 we show that (4) is a Hamiltonian system with the Hamiltonian (5) and the Poisson bracket

$$\{A(\rho), B(\rho)\} = -\frac{i}{\hbar} Tr(\partial_\rho A(\rho) \rho \partial_\rho B(\rho) - \partial_\rho B(\rho) \rho \partial_\rho A(\rho)),$$

where $A(\rho)$ and $B(\rho)$ are differentiable functionals of $\rho$ and the operator (Fréchet derivative) $\partial_\rho A(\rho)$ is defined by the equation $Tr(\partial_\rho A(\rho) \xi) = \partial_s A(\rho + s\xi)|_{s=0}$. This, as was mentioned above, plays an important role in our analysis.
Finaly, note that since the integral kernel of the operator $\rho_N|_{t=0}$ is symmetric with respect to permutations of particle coordinates, the same is true for the solution to (1).

To formulate the main result we need some notation and definitions. For any Banach space $X$, we denote the space of bounded linear operators from $X$ to itself by $B(X)$. Let $L^2_S(\mathbb{R}^3)$ be the subspace of $L^2(\mathbb{R}^3)$ consisting of the functions that are symmetric with respect to permutation of particle coordinates, and let

$$P^M_S \Psi(x_1, \ldots, x_M) := \frac{1}{M!} \sum_{\sigma \in S^M} \Psi(x_{\sigma(1)}, \ldots, x_{\sigma(M)}), \quad (7)$$

where $S^M$ denotes the permutation group of the set $\{1, 2, \ldots, M\}$, be the orthogonal projection onto the subspace $L^2_S(\mathbb{R}^3)$ of $L^2(\mathbb{R}^3)$.

We denote by $I^q$ the identity operator acting on $q$ coordinates.

**Definition 1.** Let $A_p := B(L^2_S(\mathbb{R}^3_p))$. For $p < N$, we define the maps $\phi^N_p : A_p \rightarrow A_N$ by

$$\phi^N_p(a) := P^N_S (a \otimes I^{N-p}) P^N_S. \quad (8)$$

Let $A_{N,p}$ be the image of $A_p$ under $\phi^N_p$. Its elements will be called quantum $p$-particle observables or simply $p$-particle observables. Note that $A_{N,1} \subset A_{N,2} \subset \ldots A_{N,N} = A_N$.

The following theorem relates the asymptotic behavior of (1) as $N \rightarrow \infty$ with (4).

**Theorem 1.1.** Assume that $v$ is bounded and even and that (3) holds. Let $\rho_N$ solve (1) with $\text{Tr}\rho_0 = 1$. Then for any $p$ and any $A = \phi^N_p(a) \in A_{N,p}$, and for $N \rightarrow \infty$,

$$\text{Tr}(A\rho_N) - \text{Tr}(A\rho^\otimes N) \rightarrow 0,$$

where $\rho$ solves (4). Moreover, we have the estimate

$$|\text{Tr}(A\rho_N) - \text{Tr}(A\rho^\otimes N)| \leq 2^t [t]^{p} N^{-\gamma(t)} \|a\|_{A_p}, \quad (9)$$

where $t = \frac{\hbar}{\|v\|_{\infty}}$, $[t]$ is the integer part of $\frac{t}{\tau}$ and $\gamma(t) := \frac{1}{4\|\frac{t}{\tau} + 1\|}$. \textit{Remark 1.} The $N$-bound in this theorem is rather poor, especially compared with estimates for the Schrödinger equation mentioned above. It is improved somewhat in [An], where an extension of this result to Coulomb-type potentials is also presented.

From now on we fix the particle number $N$ and sometimes drop the corresponding index from the notation. For instance, we write $P_S$ for $P^N_S$, $\phi_p$ for $\phi^N_p$, and $V$ for $V_N$.

The rest of the paper is devoted to a proof of Theorem 1.1. The paper is organized as follows. In Section 2 we derive a convenient equation for the map
\[ \Gamma_t(A) := e^{iH_N t} e^{-iH_0 t} A e^{iH_0 t} e^{-iH_N t}, \] which is connected to the l.h.s. of (9).

To this end we use a decomposition of the commutator with the many-body potential into the tree and loop operators, introduced in [FGS]. We use this equation in Section 3 in order to approximate \( \Gamma_t \) by an operator \( \Gamma^H_t \) whose expansion contains only tree operators. In Section 4 we discuss the Hamiltonian and Liouvillean formulations of the Hartree-von Neumann equation and the Dyson expansion for the latter. We also show that in certain (symbolic) representation the tree operators act as Poisson brackets. In Section 5 we prove the result of Theorem A.1 for small times and in Section 6 we use the group properties of the von Neumann and Hartree-von Neumann dynamics in order to extend the proof to all times.

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### 2 Map \( \Gamma_t \) and its equation

In this section we derive a convenient equation for the family of operators \( \Gamma_t \) acting on elements of \( \mathcal{A}_N \) and defined by

\[ \Gamma_t(A) := e^{iH_N t} e^{-iH_0 t} A e^{iH_0 t} e^{-iH_N t}. \] (10)

This family is related to the l.h.s. of (9) as \( Tr(A \rho_N) = Tr(\Gamma_t(A_t) \rho_0^{\otimes N}) \), where \( \rho_0, \rho_N \) are the same as in (11) and \( A_t \) denotes the free evolution of \( A \):

\[ A_t := e^{iH_0 t} A e^{-iH_0 t}. \] (11)

Writing \( \Gamma_r(A) \) as the integral of derivative, we obtain

\[ \Gamma_t(A) = A + \frac{i}{\hbar} \int_0^t \Gamma_r([V_r, A]) dr. \] (12)

A simple analysis shows that the solution of this equation is unique in \( C([0, \infty), B(\mathcal{A}_N)) \).

Now we decompose the commutator on the r.h.s. of (12) in a convenient way (cf. [FGS]). For any \( i, j \leq N, i \neq j \) denote by \( V_{ij} \) the multiplication operator by \( v(x_i - x_j) \).
Proposition 2.1. We have for \( a \in A_p \),

\[
\frac{i}{\hbar}[V_r, \phi_p(a)] = T_r(\phi_p(a)) + L_r(\phi_p(a)),
\]

where \( T_r(\phi_p(a)) = 0 \) for \( p \geq N \) and otherwise

\[
T_r(\phi_p(a)) = \frac{N - p}{N} \phi_{p+1}(X_{p,r}(a)),
\]

with \( X_{p,r} : A_p \to A_{p+1} \), defined by

\[
X_{p,r}(a) := pP^{p+1} \frac{i}{\hbar}[V_p^{p+1}, a \otimes I]P^{p+1}_S,
\]

for \( p < N \), and

\[
L_r(\phi_p(a)) = \phi_p(Y_{p,r}(a)), \quad \text{with } Y_{p,r}(a) = \frac{p(p-1)}{2N} (P^p_S \frac{i}{\hbar}[V_{r,p-1}^p, a]P^p_S).
\]

Proof. Recall the notation \( V_t = e^{-iH_0 t/\hbar} V e^{iH_0 t/\hbar} \). Using equations \( V_r = \frac{1}{N} \sum_{i<j} V_{r,ij} \) and \( (3) \), we obtain

\[
[V_r, A] = \frac{1}{N} \sum_{i<j} [V_{r,ij}, A],
\]

Since the operator \( V_r = \frac{1}{N} \sum_{i<j} V_{r,ij} \) is permutationally symmetric, we have from \( (5) \) that

\[
\frac{i}{\hbar}[V_r, A] = \frac{i}{\hbar} P_S[V_r, a \otimes I^{N-p}]P_S
\]

\[
= \frac{i}{\hbar} P_S \sum_{i<j}^{1,N} [V_{r,ij}, a \otimes I^{N-p}]P_S = T_r(A) + L_r(A),
\]

where

\[
T_r(A) = \frac{i}{N\hbar} P_S \left( \sum_{i=1}^{p} \sum_{j=p+1}^{N} [V_{r,ij}, a \otimes I^{N-p}] \right)P_S
\]

and

\[
L_r(A) = \frac{1}{N} P_S \left( \frac{i}{\hbar} \sum_{i<j}^{1,p} [V_{r,ij}, a \otimes I^{N-p}] \right)P_S.
\]

By symmetry we have

\[
T_r(A) = \frac{p(N-p)}{N} P_S \left( \frac{i}{\hbar} [V_{r,p+1}^p, a \otimes I^{N-p}] \right)P_S.
\]

Now, since \( P^{p+1}_S P_S = P_S P^{p+1}_S = P_S \), we have furthermore

\[
T_r(A) = \frac{N - p}{N} P_S (pP^{p+1}_S \left( \frac{i}{\hbar} [V_{r,p+1}^p, a \otimes I] \right)P^{p+1}_S \otimes I^{N-p-1})P_S
\]
\[
\frac{N-p}{N} \phi_{p+1}(pP_S^{p+1} \frac{i}{\hbar} [V_r^{p,p+1}, a \otimes I] P_S^{p+1}),
\]
which gives (14)-(15). Similarly, we find
\[
L_r(A) = \frac{p(p-1)}{2N} P_S(i \hbar [V_r^{p-1}, a] \otimes I^{N-p}) P_S.
\]
This, due to (8), gives (16).

**Remark 2.** In general, \( T_r(\phi_p(a)) \neq T_r(\phi_q(b)) \), even if \( \phi_p(a) = \phi_q(b) \). Thus, e.g. the expression \( T_rA \) should be understood as \( T_r\phi_p(a) \) with \( A = \phi_p(a) \). However, our abuse of notation will not cause a confusion.

\( T_r \) and \( L_r \) will be called the tree and loop operators, respectively (see [FGS]).

Observe that the equation (14) implies that
\[
A \in A_{N,p} \implies T_r(A) \in A_{N,p+1}
\]
and equation (16) implies that
\[
A \in A_{N,p} \implies L_r(A) \in A_{N,p}.
\]

Combining equations (12) and (13) from above we obtain the following equation for \( \Gamma_t \)
\[
\Gamma_t(A) = A + \int_0^t \Gamma_r(T_r(A))dr + \int_0^t \Gamma_r(L_r(A)))dr.
\]
Introducing the notation \( \Gamma \equiv (\Gamma_t, t \geq 0) \) we rewrite this equation in a more compact way
\[
\Gamma = I + KG + R(\Gamma)
\]
where
\[
(KG)_t := \int_0^t G_s T_s ds
\]
and
\[
R(\Gamma)_t = \int_0^t \Gamma_s L_s ds.
\]
Equation (24) defines the operator \( K : G \to KG \) acting on the families \( G = \{G_t \in B(A_N), t \geq 0\} \). Clearly, \( K \) is a bounded operator on \( C([0, T], B(A_N)), \forall T \geq 0 \).

**Proposition 2.2.** Let \( K \) be the operator defined in equation (24). Then \( I - K \) is invertible and
\[
\forall A \in A_{N,p}, \ (I - K)^{-1} GA = \sum_{n=1}^{N-p} K^n GA.
\]
Proof. Let \( A \in A_{N,p} \). The definition of the operator \( K \) implies that

\[
(K^n G)_t A = \int_{\Delta^t_n} d^n t G_{t_1} T_{t_2} ... T_{t_1} A, \tag{27}
\]

where \( \int_{\Delta^t_n} d^n t = \int_0^t dt_1 \int_0^{t_1} dt_2 ... \int_0^{t_{n-1}} dt_n \). (Here \( \Delta^t_n \) is the \( n \)-symplex \( 0 \leq t_n \leq t_{n-1} \leq ... \leq t_1 \).)

Equations (20) and \( T_r(A) = 0 \ \forall A \in A_{N,N} \) imply

\[
T_{r_n} T_{r_{n-1}} ... T_{r_1} A = 0, \quad \forall A \in A_{N,p}, \quad n > N - p. \tag{28}
\]

Hence, by (28), \( (K^n G)_t A = 0 \) for \( n > N - p \). This gives

\[
\sum_{n=1}^{\infty} K^n GA = \sum_{n=1}^{N-p} K^n GA. \tag{29}
\]

On the other hand, \( (I - K) \sum_{n=1}^{\infty} K^n GA = GA \) and \( \sum_{n=1}^{\infty} K^n (I - K)GA = GA \), which completes the proof. \( \square \)

3 Approximation of \( \Gamma \)

Let \( \Gamma^{(H)} := \sum_{n=0}^{\infty} K^n I \), which, due to (29), is a finite series on \( A_{N,p} \). Equivalently, we write

\[
\Gamma^{(H)}_t := \sum_{n=0}^{\infty} \int_{\Delta^t_n} d^n t T_{t_2} ... T_{t_1}. \tag{30}
\]

Proposition 3.1. For \( t \leq \tau := \frac{\hbar}{8\|v\|_\infty} \), we have

\[
\| (\Gamma_t - \Gamma^{(H)}_t) \phi_p \|_{A_p \rightarrow A_N} \leq 2(2-p) \frac{p t}{N \tau}. \tag{31}
\]

Proof. Using Proposition 2.2 and equation (23) we obtain that

\[
\Gamma - \Gamma^{(H)} = (I - K)^{-1} R(\Gamma) = \sum_{n=0}^{\infty} K^n R(\Gamma). \tag{32}
\]

Using equations (25) and (27), we find that

\[
(K^n R(\Gamma))_t = \int_{\Delta^t_{n+1}} d^{n+1} t \Gamma_{t_{n+1}} L_{t_{n+1}} T_{t_2} ... T_{t_1}. \tag{33}
\]

Using equation (14) and (16), we obtain that

\[
L_{t_{n+1}} T_{t_2} ... T_{t_1} \phi_p(a) = \phi_{p+n}(\frac{(N - p)!}{(N - p - n)! N^n} \sum_{n_{t_1},...t_{n}} X_{p+n, t_1} X_{p+n-1, t_2} ... X_{p, t_1} (a)). \tag{34}
\]
Using equations (15), $\|P_S^M\| = 1$ and $\|V_{ij}\|_{B(L^2(\mathbb{R}^d))} = \|v\|_\infty$, we derive the estimate on the tree and loop operators

$$\|X_{p,t}(a)\|_{A_{p+1}} \leq \frac{2\|v\|_\infty p}{h} \|a\|_{A_p},$$  

(34)

$$\|Y_{p,t}(a)\|_{A_p} \leq \frac{\|v\|_\infty p(p-1)}{N} \|a\|_{A_p}.$$  

(35)

Equations (34), (35), (3) and $\|\phi_p(a)\|_{A_{N,p}} \leq \|a\|_{A_p}$ (since $\|P_S\| = 1$) imply that

$$\|L_{t_{n+1}} T_{t_n} \ldots T_{t_1} \phi_p\|_{A_{p} \to A_{N,p+n}} \leq \left(\frac{2\|v\|_\infty}{h}\right)^n \frac{(N-p)!}{(N-p-n)!N^n} \frac{(p+n)!}{(p-1)!} \frac{p+n-1}{2N} \|a\|_{A_p},$$  

(36)

which together with the fact that $\|\Gamma_t\|_{A_{N,p} \to A_N} = 1$ and the equality

$$\int_{\Delta_h} dt \equiv \int_0^t dt_1 \int_0^{t_1} dt_2 \ldots \int_0^{t_{n-1}} dt_n = \frac{t^n}{n!},$$  

(37)

implies that

$$\|((K^n R(\Gamma))_t \phi_p\|_{A_{N,p} \to A_N} \leq \frac{1}{2} \left(\frac{t}{4\tau}\right)^{n+1} \frac{(N-p)!}{(N-p-n)!N^n} \frac{(p+n)!}{(p-1)!} \frac{p+n-1}{N}.$$  

(38)

Furthermore, using the inequalities

$$\frac{(p+n)!}{(p-1)!(n+1)!} \leq 2^{p+n},$$  

(39)

and

$$\frac{(N-p)!}{(N-p-n)!N^n} \leq 1,$$  

(40)

we simplify (38) as

$$\|((K^n R(\Gamma))_t \phi_p\|_{A_{N,p} \to A_N} \leq 2^{p-2} \left(\frac{t}{2\tau}\right)^{n+1} \frac{p+n-1}{N}.$$  

(41)

To conclude our calculations we use the following equality:

$$\sum_{n=0}^\infty 2^{-n} (p+n-1) = 2p.$$  

(42)

To derive (42), let $A = \sum_{n=0}^\infty 2^{-n} (p+n-1)$. Then $\frac{A}{2} = \sum_{n=0}^\infty 2^{-n-1} (p+n-1) = \sum_{n=1}^\infty 2^{-n} (p+n-2)$, and therefore subtracting the latter equation from the former, we obtain that $\frac{A}{2} = (p-1) + \sum_{n=1}^\infty 2^{-n} = p$, which gives immediately equation (42). Equation (42) yields for $t \leq \tau$ that

$$\sum_{n=0}^{N-p-1} \|((K^n R(\Gamma))_t \phi_p\|_{A_{N,p} \to A_N} \leq 2^{p-2} \frac{p}{N} \frac{t}{\tau}.$$  

(43)

This together with (32) and (29) proves equation (31) for $t \leq \tau$. $\Box$
4 Classical Field Theory for the Hartree-von Neumann Equation

In this section we develop Hamiltonian and Liouvillian representations for the Hartree equation viewed as a classical field theory. We begin with key definitions. Let $\mathbb{I}_1$ denote the space of all positive, trace class operators on $L^2(\mathbb{R}^3)$. For any operator $a \in \mathcal{A}_p$ we define the $p$-particle classical field observable $A^p : \mathbb{I}_1 \to \mathbb{C}$ by the equation

$$A^p(\rho) := Tr(\rho \otimes^p).$$

We equip the space of these functionals with the norm

$$||A^c|| := \sup_{\rho \in \mathbb{I}_1, Tr\rho = 1} |A^c(\rho)|.$$

The last two equations imply that

$$||A^c|| \leq ||a||_{\mathcal{A}_p}. \tag{46}$$

For a functional $A^c(\rho)$ we define the operator (Fréchet derivative) $\partial_\rho A^c(\rho)$ by the equation $Tr(\partial_\rho A^c(\rho) \xi) = \partial_\rho A^c(\rho + s\xi)|_{s=0}$. On the space of classical field observables we define the Poisson bracket by

$$\{A^c(\rho), B^c(\rho)\} = -\frac{i}{\hbar} Tr(\partial_\rho A^c(\rho) \rho \partial_\rho B^c(\rho) - \partial_\rho B^c(\rho) \rho \partial_\rho A^c(\rho)). \tag{47}$$

The Jacobi identity is proven in Appendix B. Note that if $A^c$ is a $p$-particle classical field observable, and $B^c$ is a $q$-particle classical field observable, then $\{A^c, B^c\}$ is a $p + q - 1$-particle classical field observable.

Furthermore, we observe that

$$\{A^c(\rho), B^c(\rho)\}|_{\rho = P_\psi} = \frac{i}{\hbar} \int (\partial_{\psi(x)} A^c(\psi(x)) B^c(\psi(x)) - \partial_{\psi(x)} A^c(\psi(x)) \partial_{\psi(x)} B^c(\psi(x)) \psi(x)) dx, \tag{48}$$

where $P_\psi$ is the rank-one projection on the vector $\psi$ and $A^c(\psi, \overline{\psi}) := A^c(P_\psi)$. The r.h.s. is the standard Poisson bracket for the Hartree equation (see [FGS]). Indeed, $\partial_\rho A^c(\rho)$ and $\partial_\rho B^c(\rho)$ are operators on $L^2(\mathbb{R}^3)$ (1-particle observables) and therefore

$$Tr((\partial_\rho B^c(\rho) P_\psi(\partial_\rho A^c))(P_\psi)) = \langle (\partial_\rho A^c)(P_\psi)^* \psi, (\partial_\rho B^c)(P_\psi) \psi \rangle.$$

Since, as it is easy to see, $(\partial_\rho B^c(\rho) P_\psi) \psi = \partial_{\psi(x)} B^c(\psi(x))$ and $(\partial_\rho A^c)(P_\psi)^* \psi = \partial_{\psi(x)} A^c(\psi(x))$, this gives $Tr((\partial_\rho B^c(\rho) P_\psi(\partial_\rho A^c))(P_\psi)) = \int \partial_{\psi(x)} A^c \partial_{\psi(x)} B^c$, which implies the desired relation.

Introduce the classical Hamiltonian functional

$$H^c(\rho) := H_{0,c}^c(\rho) + V^c(\rho),$$
where (extending (44) to the unbounded 1-particle observable \( h \))

\[
H^{0,c}(\rho) := \text{Tr}(h\rho), \quad \text{and} \quad V^{c}(\rho) := \frac{1}{2}\text{Tr}(v\rho \otimes v).
\]

(49)

Note that the Hartree-von Neumann equation (44) is equivalent to the equation

\[
\partial_t \rho = \{ H^c(\rho), \rho \},
\]

(50)

which motivates the above definition of the Poisson bracket.

**Remark 3.** The last equation holds in the weak sense that for all \( a \in A_1 \),

\[
\partial_t \text{Tr}(a \rho) = \text{Tr}(a \{ H^c, \rho \}).
\]

(51)

Using the linearity of the Poisson brackets in the second factor, we obtain

\[
\text{Tr}(a \{ H^c, \rho \}) = \{ H^c, \text{Tr}(a \rho) \}.
\]

(52)

Thus equation (50) is equivalent to the equation

\[
\partial_t \text{Tr}(a \rho) = \{ H^c, \text{Tr}(a \rho) \},
\]

(53)

or \( \partial_t a^c(\rho) = \{ H^c(\rho), a^c(\rho) \} \) for all 1 particle observables \( a \).

To show (50) we use the definition of the Poisson bracket and the relation

\[
\text{Tr}(\partial_\rho \rho \xi) = \xi,
\]

which follows from the definition of \( \partial_\rho A^c(\rho) \) above to obtain

\[
\{ H^c, \rho \} = -\frac{i}{\hbar} (\partial_\rho H^c(\rho) \rho - \rho \partial_\rho H^c(\rho)).
\]

(54)

Next, computing \( \partial_\rho H^c(\rho) \), we conclude that \( \{ H^c, \rho \} \) is equal to the r.h.s. of (4).

Let \( \Phi_t \) be the flow given by the Hartree-von Neumann initial value problem (44), i.e. \( \Phi_t(\rho_0) := \rho_t \) where \( \rho_t \) is the solution of (44) at time \( t \). We denote by \( \Phi^0_t \) the flow of (44) for \( v = 0 \) (the free flow). We define the Hartree-von Neumann evolution on the space of \( p \)-particle classical field observables by

\[
U_t(A^c(\rho)) := A^c(\Phi_t(\rho)),
\]

(55)

and the free Hartree-von Neumann evolution by \( U^0_t(A^c(\rho)) := A^c(\Phi^0_t(\rho)) \). In a standard way we derive the following equation

\[
\partial_t U_t(A^c(\rho)) = U_t(\{ H_{cl}^c, A^c \}(\rho))
\]

(56)

(and similarly for \( U^0_t(A^c(\rho)) \)).

Let \( V_t^c \) denote the free evolution, \( U^0_t(V^c) \), of the 2-particle classical observable \( V^c \). A simple computation gives that

\[
V_t^c(\rho) := \frac{1}{2}\text{Tr}(v_t \rho \otimes v_t),
\]

(57)

where \( v_t \) is the operator \( \psi(x_1, x_2) \rightarrow e^{\frac{i}{\hbar} (h_{x_1} + h_{x_2})t} \psi(x_1 - x_2) e^{-\frac{i}{\hbar} (h_{x_1} + h_{x_2})t} \psi(x_1, x_2) \).

In what follows we denote the action of Poisson bracket as

\[
P_V A^c := \{ V, A^c \}.
\]

(58)
Proposition 4.1. We have the following expansion:

\[ U_t(A^c) = \sum_{n=0}^{\infty} A_{t,n}^c, \quad (59) \]

where \( A_{t,0}^c = A_t^c := U_t^0(A^c) \) and, for \( n \geq 1 \),

\[ A_{t,n}^c = \int_{\Delta_t^n} d^n t \; P_{V_{t_n}} \cdots P_{V_{t_1}} A_t^c, \quad (60) \]

with the following the estimates

\[ ||A_{t,n}^c|| \leq \left( \frac{t}{2\tau} \right)^n 2^{p-1} ||a||_{A_p}, \quad (61) \]

(in particular, for \( t \leq \tau \) the series converges in the norm \( (65) \)).

Proof. Define \( \tilde{A}_t^c := U_t^0(U_t(A^c)) \). By a standard argument we have that \( \partial_t \tilde{A}_t^c = P_{V_{t,1}} \tilde{A}_t^c \). Integrating this equation, we obtain immediately that

\[ \tilde{A}_t^c = A^c + \int_0^t dt_1 P_{V_{t,1}} \tilde{A}_{t_1}^c. \quad (62) \]

Iterating this equation and applying \( U_t^0 \) to the result we obtain \( (59) \), with \( A_{t,0}^c := U_t^0(A^c) \) and \( A_{t,n}^c := \int_0^t dt_1 \int_0^{t_1} dt_2 \int_0^{t_n} dt_n U_t^0(P_{V_{t_n}} \cdots P_{V_{t_1}} A^c), \; n \geq 1 \), which after a change of variables of integration gives \( (60) \).

It remains to prove \( (61) \), which shows that the series \( (59) \) converges and which we are going to prove next. Recall the notation \( \rho^\otimes N = \rho \otimes \cdots \otimes \rho \), the \( N \)-fold tensor product.

Lemma 4.2. Let \( X_{n,t} \) be the operator defined in equation \( (15) \). Then

\[ Tr(X_{p,t})(a)\rho^{\otimes (p+1)} = P_{V_t} a(\rho). \quad (63) \]

Proof. The proof follows from the relation \( \partial_p A^c(\rho) = p Tr_{p-1}(a p^{p-1} \otimes I) \), where \( Tr_{p-1} \) is the partial trace over the first \( p-1 \) coordinates, and a simple computation. \( \square \)

Iterating \( (63) \) we obtain equation

\[ \quad (64) \quad Tr(X_{p+n-1,t_n} \cdots X_{p,t_1})(a)\rho^{\otimes (p+n)} = P_{V_{t_n}} \cdots P_{V_{t_1}} a(\rho). \]

Next, using equation \( (64) \) we obtain that

\[ \|X_{p+n-1,t_n} \cdots X_{p,t_1}(a)\|_{A_{p+n}} \leq \left( \frac{2\|v\|_{\infty}}{h} \right)^n (p+n-1)! \frac{(p-1)!}{(p-1)!} \|a\|_{A_p}, \quad (65) \]

The last two equations together with \( (45) \), the formula \( A_t = \phi_p(a_t) \), where \( a_t = e^{-\frac{ih}{\hbar} t} a e^{-\frac{ih}{\hbar} t} \), and the isometry of the free evolution, \( a_t \), imply

\[ \|P_{V_{t_n}} \cdots P_{V_{t_1}} A_t^c\| \leq \frac{(p+n-1)!}{(p-1)!} \left( \frac{2\|v\|_{\infty}}{h} \right)^n \|a\|_{A_p}. \quad (66) \]

Equations \( (67) \), \( (69) \), \( (66) \), \( (68) \) and the definition \( \tau := \frac{\hbar}{8\|v\|_{\infty}} \) give \( (61) \), which completes the proof of the proposition. \( \square \)
5 Hartree von Neumann approximation for \( t \leq \tau \)

In this section we estimate the difference between the quantum \( N \)-body average \( Tr(A(t)\rho^{\otimes N}) \), where \( A(t) := e^{-iHt/\hbar} Ae^{-iHt/\hbar} \), and the classical evolution \( U_t(A^c(\rho)) \), where \( \rho \) satisfies \( Tr\rho = 1 \).

**Proposition 5.1.** For all \( A \in \mathcal{A}_{N,p} \) and for all \( t \leq \tau \) we have that

\[
|Tr(A(t)\rho^{\otimes N}) - U_t(A^c(\rho))| \leq 2^{p+1}\frac{1}{N} t \|a\|_{\mathcal{A}_p}.
\]

**Proof.** The proof of this proposition uses the following auxiliary lemma:

**Lemma 5.2.** For any \( p \)-particle observable \( A \) and any \( n \leq N - p \) we have that

\[
(T_t \cdots T_1 (A_t))^c = \frac{(N - p)!}{(N - p - n)! N^n} P_{V_{t_1}} \cdots P_{V_{t_n}} A_t^c.
\]

**Proof.** Let \( A = \phi_p(a) \) with \( a \in \mathcal{A}_p \). Then \( A_t = \phi_p(a_t) \), where, recall, \( a_t = e^{iHt/\hbar} ae^{-iHt/\hbar} \). Now, using the facts that

\[
T_t \cdots T_1 \phi_p(a) = \frac{(N - p)!}{(N - p - n)! N^n} \phi_{p+n}(X_{p+n-1,t_n}X_{p+n-2,t_{n-1}} \cdots X_{p,t_1}(a)),
\]

which follows from equation (14), that \( P_S \rho^{\otimes N} = \rho^{\otimes N} \) and that \( Tr(\phi_p(a)\rho^{\otimes N}) = Tr(a\rho^{\otimes p}) \), we find

\[
(T_t \cdots T_1 (A_t))^c(\rho) = \frac{(N - p)!}{(N - p - n)! N^n} Tr(X_{p+n-1,t_n} \cdots X_{p,t_1}(a_t)\rho^{\otimes p+n}).
\]

Now, equation (68) follows from the last equation and equations (61), (44) and \( A_t = \phi_p(a_t) \).

Now, equations (68) and (50) imply that for any \( n \leq N - p \)

\[
\int_{\Delta_t^n} d\rho (T_{r_n} \cdots T_{r_1} (A_t))^c = \frac{(N - p)!}{(N - p - n)! N^n} A_{t,n}^c.
\]

This, together with (28), (30), (44) and (59), yields that

\[
Tr(\Gamma_t^H(A_t)\rho^{\otimes N}) - U_t(A^c(\rho))
\]

\[
= - \sum_{n=1}^{N-p} \left( 1 - \frac{(N - p)!}{(N - p - n)! N^n} \right) A_{t,n}(\rho) - \sum_{n=N-p+1}^{\infty} A_{t,n}(\rho),
\]

which together with (12), \( Tr\rho = 1 \) and (61) gives for \( t \leq \tau \)

\[
|Tr(\Gamma_t^H(A_t)\rho^{\otimes N}) - U_t(A^c(\rho))| \leq \frac{t}{\tau} S_{p,N} \|a\|_{\mathcal{A}_p},
\]

\[
|Tr(A(t)\rho^{\otimes N}) - U_t(A^c(\rho))| \leq 2^{p+1}\frac{1}{N} t \|a\|_{\mathcal{A}_p},
\]

where $S_{p,N} := \left[ \sum_{n=1}^{N-p} \left( 1 - \frac{(N-p)!}{(N-p-n)!N^n} \right) \frac{1}{2^n} + \sum_{n=N-p+1}^{\infty} \frac{1}{2^n} \right] 2^{p-1}$. We transform

$$S_{p,N} := \left( 1 - \sum_{n=1}^{N-p} \frac{(N-p)!}{(N-p-n)!N^n} \frac{1}{2^n} \right) 2^{p-1}. \quad (73)$$

The following inequality is proven in Appendix C:

$$1 - \sum_{n=1}^{N-p} \frac{(N-p)!}{(N-p-n)!N^n} \frac{1}{2^n} \leq \frac{2(p+1)}{N}. \quad (74)$$

Equations (73) and (74) imply that $S_{p,N} \leq 2^{p+1}$, which together with (72) and (31) implies that for $t \leq \tau$

$$|Tr(\Gamma_t(A_t)\rho^\otimes N) - U_t(A^c(\rho))| \leq \left[ \frac{p}{N} 2^{p-2} + 2^{p+1} \right] \|a\|_{A_p}. \quad (75)$$

Recall the notation $A(t) = e^{i\frac{Ht}{\hbar}}Ae^{-i\frac{Ht}{\hbar}}$. Due to the equations (10) and (11), we have that $A(t) = \Gamma_t(A_t)$. This, together with (75), implies Proposition 5.1 \hfill \Box

## 6 Hartree approximation for arbitrary $t$

Now we prove our main result, Theorem A.1. In what follows $A = \phi_p(a)$ is a $p$-particle observable and $\alpha_t(A) = A(t) = e^{i\frac{Ht}{\hbar}}Ae^{-i\frac{Ht}{\hbar}}$. We proceed by induction. Equations (67) and $A(t) = \alpha_t(A)$ imply that

$$|Tr(\alpha_t(A)\rho^\otimes N) - U_t(A^c(\rho))| \leq \frac{2^{p+1}(p+1)}{N} \|a\|_{A_p}. \quad (76)$$

Let $L_k = \frac{L_0}{(k-1)!}$ so that $L_k = kL_{k+1}$. We assume that for any $A = \phi_p(a) \in A_{N,p}$ and for some $k \geq 1$

$$|Tr(\alpha_{k\tau}(A)\rho^\otimes N) - U_{k\tau}(A^c)| \leq R_{p,k} \|a\|_{A_p}, \quad (77)$$

where

$$R_{p,k} = 2^k \left( 2\sum_{r=1}^{k} rL_r \frac{p}{N} + 2^{-L_k} \right). \quad (78)$$

and prove it for $k + 1$. For $k = 1$, (74) follows from (76), since $L_1 \geq 3$ and $p \geq 1$.

We begin with some preliminary inequalities. Let $A = \phi_p(a)$ and

$$A_n(t) := \int_{\Delta_t^n} d^n t \ T_{t_n}...T_{t_1} A_t. \quad (79)$$

Since $A_t = \phi_p(a_t)$, where $a_t = e^{i\frac{H_0t}{\hbar}}a e^{-i\frac{H_0t}{\hbar}}$ is a $p$-observable, we have by (69) that $A_n(t) := \phi_{p+n}(a_n(t))$ with

$$a_n(t) = \frac{(N-p)!}{(N-p-n)!N^n} \int_{\Delta_t^n} d^n t \ X_{p+n-1,t_n}X_{p+n-2,t_{n-1}}...X_{p,t_1} a_t. \quad (80)$$
which, together with (34), (37), (39) and (40) and the definition $\tau := \frac{\hbar}{8\|v\|_\infty}$, gives
\[
\|A_{n}(t)\|_{A_{N,p+n}} \leq \|a_{n}(t)\|_{A_{p+n}}
\]
\[
\leq \frac{(p + n - 1)!}{(p - 1)!n!} (N - p)! \sum_{n=0}^{\infty} \frac{t}{\tau} \|a\|_{A_p} \tag{81}
\]
\[
\leq 2^{p-1-n} \sum_{n=0}^{\infty} \frac{(N - p)!}{(N - p - n)!N^n} \left( \frac{t}{\tau} \right)^n \|a\|_{A_p} \tag{82}
\]
\[
\leq 2^{p-1-n} \left( \frac{t}{\tau} \right)^n \|a\|_{A_p}. \tag{83}
\]

Using that $\alpha_{\tau}(A) = \Gamma_{\tau}(A_{\tau})$ and using (30) with (31) and (83), we obtain for $L \leq N - p$ that
\[
\|\alpha_{\tau}(A) - \sum_{n=0}^{L-1} A_{n}(\tau)\|_{A_N} \leq 2^p \left( \frac{p}{4N} + 2^{-L} \right) \|a\|_{A_p}. \tag{84}
\]

Next, we claim that for $L \leq N - p$
\[
|U_{\tau}(A^c) - \sum_{n=0}^{L-1} A_{n}(\tau)^c| \leq 2^p \left( \frac{p + 1}{N} + 2^{-L} \right) \|a\|_{A_p}. \tag{85}
\]

Indeed, by (59), (70) and (79) we have that for $L \leq N - p$
\[
U_{\tau}(A^c) - \sum_{n=0}^{L-1} A_{n}(\tau)^c = \sum_{n=0}^{L-1} \left( 1 - \frac{(N - p)!}{(N - p - n)!N^n} A_{\tau,n}^c \right) + \sum_{n=L}^{\infty} A_{\tau,n}^c, \tag{86}
\]
where $A_0(\tau) = A_{\tau}$. This and equation (61) imply
\[
|U_{\tau}(A^c) - \sum_{n=0}^{L-1} A_{n}(\tau)^c| \leq S_{p,N,L} \|a\|_{A_p}, \tag{87}
\]
where $S_{p,N,L} := \sum_{n=0}^{L-1} \left( 1 - \frac{(N - p)!}{(N - p - n)!N^n} \right) 2^{p-1-n} + \sum_{n=L}^{\infty} 2^{p-n-1}$. Proceeding as in Eqns (73) and (74), we obtain $S_{p,N,L} \leq \frac{p+1}{N} 2^p + 2^{p-L}$. This inequality together with (87) gives (85).

Now we prove (77) for $k+1$ (assuming it for $k$). In what follows we use the notation $\langle \cdot \rangle = Tr(\cdot \rho^{N})$. Let $s = k\tau$. We have by (84) and the linearity and unitarity of $\alpha_s$ that for $L_{k+1} \leq N - p$
\[
|\langle \alpha_s(\alpha_{\tau}(A)) \rangle - \langle \alpha_s(\sum_{n=0}^{L_{k+1}-1} A_{n}(\tau))\rangle| \leq 2^p \left( \frac{p}{4N} + 2^{-L_{k+1}} \right) \|a\|_{A_p}. \tag{88}
\]

Next, using this inequality, using that $A_{n}(\tau)$ are $(p + n)$-particle observables (which follows from equation (80)) and using (77) and (83), we obtain
\[
|\langle \alpha_s(\alpha_{\tau}(A)) \rangle - U_s(\sum_{n=0}^{L_{k+1}-1} A_{n}(\tau)^c)|\]
\[
\sum_{n=0}^{L_{k+1}-1} R_{p+n,k} 2^{-1-n} \leq 2^p \left( \sum_{n=0}^{L_{k+1}-1} R_{p+n,k} 2^{-1-n} + \frac{P}{4N} + 2^{-L_{k+1}} \right) \|a\|_{A_p}. \tag{88}
\]

Equations \((85), \tag{85}\) and \(\langle \alpha_{\tau+s}(A) \rangle = \langle \alpha_s(\alpha_{\tau}(A)) \rangle\) imply
\[
|\langle \alpha_{\tau+s}(A) \rangle - U_s(U_{\tau}(A^c))| \leq T_{p,N} \|a\|_{A_p}, \tag{89}
\]
where
\[
T_{p,N} := 2^p \left( \sum_{n=0}^{L_{k+1}-1} R_{p+n,k} 2^{-1-n} + 2^{-L_{k+1}+1} + \frac{P+1}{N} \right).
\]

We claim that
\[
T_{p,N} \leq R_{p,k+1}. \tag{90}
\]
Indeed,
\[
\sum_{n=0}^{L_{k+1}-1} R_{p+n,k} 2^{-1-n} = \sum_{n=0}^{L_{k+1}-1} 2^{(k+1)p+(k-1)n-1} \left( 2^{\sum_{r=1}^{k} rL_r \frac{p+n}{N} + 2^{-L_k}} \right)
\]
\[
\leq \sum_{n=0}^{L_{k+1}-1} 2^{(k+1)p+(k-1)n-1} \left( 2^{\sum_{r=1}^{k} rL_r \frac{p+L_{k+1}}{N} + 2^{-L_k}} \right)
\]
\[
\leq 2^{(k+1)p+(k-1)L_{k+1}-1} \left( 2^{\sum_{r=1}^{k} rL_r \frac{p+L_{k+1}}{N} + 2^{-L_k}} \right).
\]

Since \(L_k = kL_{k+1}\), we find
\[
\sum_{n=0}^{L_{k+1}-1} R_{p+n,k} 2^{-1-n} \leq 2^{(k+1)p-1} \left( 2^{\sum_{r=1}^{k+1} rL_r - 2L_{k+1} \frac{p+L_{k+1}}{N} + 2^{-L_{k+1}}} \right)
\]
\[
\leq 2^{(k+1)p-1} \left( 2^{\sum_{r=1}^{k+1} rL_r - L_{k+1} \frac{p}{N} + 2^{-L_{k+1}}} \right).
\]

This inequality, the definition of \(T_{p,N}\) and elementary bounds imply the estimate \((90)\), provided \(k \geq 2\).

Since \(s = k\tau\) and since \(U_s(U_{\tau}(A^c)) = U_{s+\tau}(A^c)\), \(\text{Eqs } (89) \tag{89}\) and \(\tag{90}\) imply equation \((77)\) with \(k \rightarrow k+1\). Thus \((77)\) is shown by induction. Take \(k-1\) to be the integer part of \(\frac{t}{\tau}\), i.e. \(k-1 = \lfloor \frac{t}{\tau} \rfloor\), and let \(\tau' := t/k\). Then \(\tau' \leq \tau\) and we proceed as above but with \(\tau\) replaced by \(\tau'\) to prove \((77)\) with \(\tau\) replaced by \(\tau'\). Next, using that \(\sum_{r=1}^{k} rL_r = \sum_{r=1}^{k} \frac{L_0}{(p-1)^r} \leq 2eL_0\) and taking \(L_0 = \frac{\log N}{4\epsilon}\) in \((77)\) we arrive at
\[
|\text{Tr}(\alpha_t(A)\rho^\otimes N) - U_t(A^c(\rho))| \leq 2^{\lfloor \frac{t}{\tau} \rfloor+1} p \left( \frac{pn^{-1/2} + N^{1/2}}{4\epsilon^{1/2}} \right) \|a\|_{A_p}. \tag{91}
\]

Now, by the definition of \(\alpha_t(A)\) and \(\rho_N\) we have that \(\text{Tr}(\alpha_t(A)\rho^\otimes N) = \text{Tr}(A\rho_N)\), and therefore \((91)\) implies \((9)\). Theorem \((A.1)\) is proven.
A Appendix: Hartree-von Neumann equation (4)

In this section we sketch proofs of some of key properties of the Hartree-von Neumann equation (4). For works on the related Hartree-Fock equation see \[ \text{BDE} \text{ C} \text{ CG}. \] Let \( \mathbb{I} \) denote the space of all positive, trace class operators on \( L^2(\mathbb{R}^3) \).

**Theorem A.1.** Assume that \( v \) is bounded. Then the Hartree-von Neumann equation (4) is globally well-posed on \( \mathbb{I} \) and the trace and the energy are conserved.

**Sketch of Proof.** We will display the \( t \)--dependence as a subindex. Let \( \mathbb{I} \) denote the space of all trace class operators on \( L^2(\mathbb{R}^3) \). Using the Duhamel formula we rewrite (4) as the fixed-point problem \( \rho = F(\rho) \) on \( C([0,T],\mathbb{I}) \). Here \( T \) will be chosen later and

\[
F(\rho)_t := \sigma_t(\rho_0) + i \int_0^t \sigma_{t-s}(v * _{\rho_s})\rho_s)ds. \tag{92}
\]

where \( \sigma_t(\gamma) = e^{\frac{it}{\hbar} \gamma} e^{-\frac{it}{\hbar}} \). Denote the trace norm by \( \| \cdot \|_1 \) and let \( \| \rho \|_T := \sup_{0 \leq s \leq T} \| \rho_s \|_1 \) be the norm on the space \( C([0,T],\mathbb{I}) \). Recall that \( \| f \|_\infty \) denotes the \( L^\infty \)-norm of a function \( f \). Let \( v_x(y) := v(x-y) \). Using that \( |(v * \rho_s)(x)| = |Tr(v_x \rho_s)| \leq \| v \|_\infty \| \rho_s \|_1 \), we obtain

\[
\| \sigma_{t-s}(v * _{\rho_s})\rho_s)\|_1 \leq \| v * _{\rho_s} \|_\infty \| \rho_s \|_1 \leq \| v \|_\infty \| \rho_s \|_2^2. \tag{93}
\]

This estimate shows that \( F \) maps any ball in \( C([0,T],\mathbb{I}) \) of radius \( R \geq 2 \) into itself, provided \( T \leq 1/\| v \|_\infty R^2 \). Similarly, one shows that \( F \) is a contraction on such a ball, if \( T \leq 1/2\| v \|_\infty R \). Hence our fixed point equation in any \( B_R, \ R \geq 2, \) has a unique solution for \( T = 1/2\| v \|_\infty R^2 \). This solution solves also the original initial value problem (4).

Since \( \rho_t \) and \( \rho_t^* \) satisfy the same equation (4) with the same initial condition \( \rho_0 = \rho_0^* \), we conclude by uniqueness that \( \rho_t = \rho_t^* \). Since the trace of a commutator vanishes, one has that the trace of \( \rho_t \) is independent of \( t \).

We show that the eigenvalues of \( \rho_t \) are independent of \( t \). We denote by \( \lambda_i \) and \( \phi_i \) the eigenvalues and the corresponding eigenfunctions of \( \rho_t \) and compute

\[
\partial_t \lambda_k = \partial_t(\phi_k, \rho_t \phi_k) = \phi_k, \rho_t \phi_k) = \phi_k, \frac{1}{\hbar} [h_p, \rho_t] \phi_k + \phi_k, \rho_t \phi_k. \tag{94}
\]

Since \( \rho \) is self-adjoint, \( \rho_t \phi_k = \lambda_k \phi_k \) and \( \phi_k, [h_p, \rho_t] \phi_k = 0 \), this gives

\[
\partial_t \lambda_k = \lambda_k \phi_k, \partial_t \phi_k + \phi_k, \partial_t \phi_k = \lambda_k \partial_t \phi_k = 0. \tag{95}
\]

Since the eigenvalues of \( \rho_t \) are independent of \( t \) and since \( \rho_0 \) is non-negative, \( \rho_t \) is non-negative as well. Hence \( \| \rho_t \|_1 = Tr \rho_t \) and is independent of \( t \). Therefore the local well-posedness of (4) can be extended to the global one.

The conservation of energy is proven in a standard way. \( \square \)
B Appendix: Jacobi identity for (47)

Lemma B.1. The Poisson bracket defined in (47) satisfies the Jacobi identity:

\[ \{\{A, B\}, C\} + \{\{C, A\}, B\} + \{\{B, C\}, A\} = 0. \]  \hfill (96)

Proof. In what follows we omit the argument \( \rho \) and the superindex \( c \). Denote \( A' = \partial_\rho A \). Recall the definition, \( \{A, B\} = -\frac{i}{\hbar} \text{Tr} (A' \rho B' - B' \rho A') \). We have

\[ \{A, B\} = \frac{i}{\hbar} \text{Tr}(A', B'|\rho). \]  \hfill (97)

We further denote \( A'' = \partial^2_\rho A \). We think about \( A'' \) as an operator on a two-particle space, or a two-particle operator. If we let \( K_1 = K \otimes I \) and \( K_2 = I \otimes K \), then we have (omitting from now on the factor \( \frac{i}{\hbar} \))

\[ \{A, B\}' = \text{Tr}_2(\{A'', B_2\}' + [A_2', B''_2]|\rho_2) + [A', B'], \]  \hfill (98)

where \( \text{Tr}_2 \) denotes the partial trace with respect to the second coordinate. The last two relations give

\[ \{\{A, B\}, C\} = \text{Tr}_1(\{\{A, B\}', C''_1|\rho\} = \text{Tr}_1(\{\{A', B_2\}'_2 + [A_2', B''_2]|\rho_2, C''_1|\rho_1\} + \text{Tr}_1(\{A', B', C'|\rho\}). \]  \hfill (99)

Let \( \text{Tr}^{\otimes 2} \) denote the trace over the two-particle space. We have furthermore

\[ \text{Tr}_1(\{\text{Tr}_2(\{A'', B_2\}'_2 + [A_2', B''_2]|\rho_2, C''_1|\rho_1\}) = \text{Tr}^{\otimes 2}(A'', B_2' + [A_2', B''_2]|\rho_1 \rho_2) \]

\[ = \text{Tr}^{\otimes 2}(A'', B_2'|\rho_1 \rho_2, C''_1|\rho_1 \rho_2). \]

and similarly for the second term on the r.h.s. of (98). Let \( R := \rho \otimes \rho \) and denote \( \text{Tr}^{\otimes 2}(K \rho \otimes \rho) = \text{Tr}_R(K) \). Then we have,

\[ \{\{A, B\}, C\} = \text{Tr}_R(\{A'', B_1'\} + [A''_2, B''_1], C''_1) + \text{Tr}_R(\{A', B', C'|\rho\}). \]

Since the commutator of operators satisfies the Jacobi identity, the last equation implies that

\[ \{\{A, B\}, C\} + \{\{C, A\}, B\} + \{\{B, C\}, A\} = \text{Tr}_R(\{A'', B_1'\} + [A''_2, B''_1], C''_1) + \{A', B', C'|\rho\} = 0. \]  \hfill (100)
C Appendix. Proof of Eqn (74)

Lemma C.1.

\[ 1 - \sum_{n=1}^{N-p} \frac{(N-p)!}{(N-p-n)!N^n} \frac{1}{2^n} \leq \frac{2(p+1)}{N}. \]  (101)

Proof. We derive this inequality from the following lemma:

Lemma C.2.

\[ 1 - \sum_{n=1}^{N-p} \frac{(N-p)!}{(N-p-n)!N^n} \left( \frac{1}{2} \right)^n = \sum_{n=0}^{N-p} \frac{(N-p)!}{(N-p-n)!N^n} \frac{p+n}{N} \left( \frac{1}{2} \right)^n \]  (102)

Proof. Let

\[ B = \sum_{n=1}^{N-p} \frac{(N-p)!}{(N-p-n)!N^n} \left( \frac{1}{2} \right)^n \]  (103)

Then,

\[ 2B = \sum_{n=1}^{N-p} \frac{(N-p)!}{(N-p-n)!N^n} \left( \frac{1}{2} \right)^{n-1} = \sum_{n=0}^{N-p-1} \frac{(N-p)!}{(N-p-n-1)!N^{n+1}} \left( \frac{1}{2} \right)^n \]  (104)

Subtracting equation (103) from (104), we obtain that

\[ B = \frac{N-p}{N} \left( \frac{1}{2} \right)^{N-p} - \sum_{n=1}^{N-p-1} \frac{(N-p)!}{(N-p-n)!N^n} \left( \frac{1}{2} \right)^n \]

\[ = 1 - \frac{p}{N} \left( \frac{1}{2} \right)^{N-p} - \sum_{n=1}^{N-p-1} \frac{(N-p)!}{(N-p-n)!N^n} \frac{p+n}{N} \left( \frac{1}{2} \right)^n \]

\[ = 1 - \sum_{n=0}^{N-p} \frac{(N-p)!}{(N-p-n)!N^n} \frac{p+n}{N} \left( \frac{1}{2} \right)^n, \]

which gives immediately equation (102).

On the other hand we have that

\[ \sum_{n=0}^{N-p} \frac{(N-p)!}{(N-p-n)!N^n} \frac{p+n}{N} \left( \frac{1}{2} \right)^n \leq \sum_{n=0}^{N-p} \frac{p+n}{N} \left( \frac{1}{2} \right)^n \]

\[ \leq \frac{2(p+1)}{N}, \]

where in the last step we used equation (42) with \( p \to p + 1 \). This, together with equation (102) gives Lemma C.1. \( \square \)
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