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J. Math. Pures Appl. 82 (2003) 665–683
JOURNAL DE MATHÉMATIQUES PURES ET APPLIQUÉES
www.elsevier.com/locate/matpur

Mean field dynamics of fermions and the time-dependent Hartree–Fock equation

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Received 10 July 2002

Abstract

The time-dependent Hartree–Fock equations are derived from the N-body linear Schrödinger equation with the mean-field scaling in the limit $N \to +\infty$ and for initial data that are close to Slater determinants. Only the case of bounded, symmetric binary interaction potentials is treated in this work. We prove that, as $N \to +\infty$, the first partial trace of the N-body density operator approaches the solution of the time-dependent Hartree–Fock equations (in operator form) in the sense of the trace norm.

Résumé

On montre dans ce travail que les équations d'évolution de Hartree–Fock décrivent la limite de l'équation de Schrödinger à N corps pour N tendant vers l'infini et une constante de couplage en $O(1/N)$ et pour des données initiales proches de déterminants de Slater. On ne considère ici que le cas de potentiels d'interaction binaires, symétriques et bornés. Lorsque $N \to +\infty$, on montre que la suite des traces partielles "à un corps" de l'opérateur densité à N corps converge, au sens des opérateurs à trace, vers la solution de l'équation de Hartree–Fock sous forme opératorielle.

MSC: 35Q40; 35Q55; 47N50; 82C10; 82C22

Keywords: Hartree–Fock equations; Quantum N-body problem; Mean-field limit

Mots-clés : Equations de Hartree–Fock ; Problème à N corps quantique ; Approximation de champ moyen

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0021-7824/$ – see front matter
doi:10.1016/S0021-7824(03)00023-0

1. Introduction

In this article we consider the Hamiltonian dynamics of systems of fermions and derive the time-dependent Hartree–Fock equation in the mean field limit. We follow the approach of Spohn, who derived a mean field dynamical equation (the time-dependent Hartree equation) for mean field systems of distinguishable particles, remarking at the time that "the convergence of the mean field limit with statistics included is an open problem" [15]—see [2] for a complete proof of Spohn's theorem.

In Spohn's theory the initial N-body density operator D_N is assumed to be a product state $D^{\otimes N}$, i.e., the particles are statistically independent and identically distributed. The mean field limit is investigated in the Schrödinger picture, where $D_N(t)$ obeys the von Neumann equation:

$$\mathrm{i}\hbar \frac{\mathrm{d}}{\mathrm{d}t} D_N(t) = \sum_{1\leqslant j\leqslant N} \big[L_j, D_N(t)\big] + \frac{1}{N-1} \sum_{1\leqslant i<j\leqslant N} \big[V_{ij}, D_N(t)\big] \tag{1}$$

with V_{ij} denoting the two-body potential V acting between the ith and jth particles (and $[\ ,\ ]$ denoting the commutator). The limit as $N \to \infty$ of the n-body density operator $D_{N:n}(t)$ is shown to converge to $D(t)^{\otimes n}$, where $D(t)$ obeys a time-dependent Hartree equation. (The subscript $_{:n}$ appearing in $D_{N:n}$ is our notation for the nth partial trace, defined in Eq. (4) below.) Spohn's ideas have been refined in [1] and generalized to open systems. There are other theories of quantum mean field dynamics, e.g., the algebraic theory of [7], but to our knowledge the problem of including quantum statistical effects remains unsolved.

The problem is that Fermi–Dirac or Bose–Einstein statistics constrain the possible initial condition of (1) to have the appropriate symmetry, which is typically inconsistent with the product form $D^{\otimes N}$. An N-body density operator with Fermi–Dirac symmetry can never have the form $D^{\otimes N}$ and a Bose–Einstein density operator can only have the form $D^{\otimes N}$ if D is a pure state (i.e., if the system of bosons is in a condensed state). The remedy to this problem, for fermions, is to replace the hypothesis that the initial state be a product state with a hypothesis that is consistent with Fermi–Dirac statistics, e.g., that the initial states are Slater determinants.

The role of the factorization hypothesis $D_N(0) = D^{\otimes N}$ is to permit the closure of the BBGKY hierarchy by setting the two-body state $D_{N:2}$ equal to $D \otimes D$. Closing the hierarchy this way results in the time-dependent Hartree equation. This kind of closure hypothesis is implicit in the *Stosszahlansatz* that leads to Boltzmann's kinetic equation for gases [4]. Kac noted that, for Boltzmann's equation, the factorization $f_{N:2} = f \otimes f$ is only realized in the limit $N \to \infty$, and he called this behavior the *Boltzmann property* [11,12]. Later authors [10,13,16] developed Kac's ideas; what is now called the *propagation of chaos* is an important tool in rigorous kinetic theory [9,14,17]. We have noted that Boltzmann's closure Ansatz is inconsistent with the Pauli Exclusion Principle, and needs to be replaced by another closure Ansatz when the particles are fermions. The novelty of our approach consists in replacing the condition of asymptotic independence of the particles by a condition that describes the correlations of Slater determinants. This condition, called *Slater closure* is defined in Definition 2.1 below.

Assuming that $\{D_N(0)\}$ is a sequence of initial states for (1) that has Slater closure, we can prove that $\{D_N(t)\}$ has Slater closure for all $t > 0$. This phenomenon could be called the *propagation of Slater closure* because it is like the "propagation of chaos" mentioned above. Since $\{D_N(t)\}$ has Slater closure, the two-body density operator $D_{N:2}(t)$ is approximately equal to $(D_{N:1}(t) \otimes D_{N:1}(t))\Sigma_2$ when N is large, where Σ_2 is the two-body operator defined by:

$$\Sigma_2(x \otimes y) = x \otimes y - y \otimes x.$$

Substituting $(D_{N:1}(t) \otimes D_{N:1}(t))\Sigma_2$ for $D_{N:2}(t)$ in the BBGKY hierarchy leads one to conjecture that, when N is large, the single-body density operator should nearly obey the time-dependent Hartree–Fock (TDHF) equation:

$$\mathrm{i}\hbar \frac{\mathrm{d}}{\mathrm{d}t} F(t) = [L, F(t)] + \big[V, \big(F(t) \otimes F(t)\big)\Sigma_2\big]_{:1}, \quad F(0) = D_{N:1}(0).$$

Theorem 3.1 confirms this conjecture.

Theorem 3.1 states that the distance in the trace norm between $D_{N:1}(t)$ and the corresponding solution $F(t)$ of the TDHF equation tends to 0 as N tends to infinity. The trace norms of $D_{N:1}(t)$ and $F(t)$ are separately equal to 1, so it is significant that their difference $D_{N:1}(t) - F(t)$ converges to 0 in the trace norm. A crucial detail of the proof is Lemma 5.1, which states that the *operator* norm of $D_{N:1}$ tends to 0 if $\{D_N\}$ has Slater closure. Much of the rest of the proof lies in bounding the *trace norm* of $D_{N:1}(t) - F(t)$ by an expression involving the *operator norm* of $D_{N:1}(0)$.

The use of the trace norm to measure the distance between two density operators is quite natural. A density operator D corresponds to a quantum state through the assignment $B \mapsto \mathrm{Tr}(DB)$ of expectation values to bounded observables B. Thus, two density operators D and D' are within ε of one another in the trace norm if and only if they correspond to quantum states that give expectations differing by no more than ε for all observables B with $\|B\| \leqslant 1$.

In this article, we assume that the two-body potential V is a bounded operator. We find the error in approximating $D_{N:1}$ by the solution of the TDHF equation to be (at worst) proportional to $\|V\|$. Because of this, our estimates are not of much use for real N-particle systems (where there is no mean field scaling), for then the error becomes proportional to $N\|V\|$ and this is not likely to be small. It would be better, from a physical point of view, to prove that the accuracy of the TDHF approximation is proportional to the *average* interaction energy $\mathrm{Tr}(D_N V)$ rather than the *maximum* interaction energy $\|V\|$.

Recent work on the time-dependent Schrödinger–Poisson equation [3,8] suggests that it may be possible to prove a theorem similar to our Theorem 3.1 when V is the Coulomb potential. This work shall be published in a separate paper.

This rest of this article is organized as follows: The next section discusses fermionic density operators and defines Slater closure. The N-particle Hamiltonian and the associated time-dependent Hartree–Fock equation are described in Section 3. This section concludes with the statement of our main result, Theorem 3.1, whose proof spans Sections 4–6. Sections 7 is an appendix relating the von Neumann form of the TDHF equation, used throughout this paper, to the formulation of the TDHF equation as a coupled system of wave equations, which may be more familiar to some readers.

2. Fermionic density operators and Slater closure

Let $\mathcal{H}$ be a Hilbert space, supposed to be the space of wavefunctions for a certain type of quantum system (a "component" or "particle"). Then the Hilbert space of wavefunctions for a system consisting of N distinguishable components or particles of that type is $\mathcal{H}_N = \mathcal{H}^{\otimes N}$. If the components are not distinguishable, but obey Fermi–Dirac statistics, then the appropriate Hilbert space of wavefunctions is the antisymmetric subspace $\mathcal{A}_N \subset \mathcal{H}_N$. To define this subspace, it is convenient first to define unitary *transposition* and *permutation* operators on $\mathcal{H}_N$. The transposition operator $U_{(ij)}$ is defined by extending the following isometry defined on *simple tensors*:

$$U_{(ij)}(x_1 \otimes x_2 \otimes \cdots x_i \cdots x_j \cdots \otimes x_N) = x_1 \otimes x_2 \otimes \cdots x_j \cdots x_i \cdots \otimes x_N$$

to all of $\mathcal{H}_N$. For any π in the group Π_N of permutations of $\{1, 2, \ldots, N\}$, one may define the permutation operator U_π as $U_{(i_k j_k)} \cdots U_{(i_2 j_2)} U_{(i_1 j_1)}$, where $(i_k j_k) \cdots (i_2 j_2)(i_1 j_1)$ is any product of transpositions that equals π.

The antisymmetric subspace may now be defined as:

$$\mathcal{A}_N = \bigl\{\psi \in \mathcal{H}_N \colon U_\pi \psi = \operatorname{sgn}(\pi)\psi \ \forall \pi \in \Pi_N\bigr\}.$$

One may verify that

$$P_{\mathcal{A}_N} = \frac{1}{N!} \sum_{\pi \in \Pi_N} \operatorname{sgn}(\pi) U_\pi$$

is the orthogonal projector whose range is $\mathcal{A}_N$.

The *pure states* of an N-fermion system correspond to the orthogonal projectors P_ψ onto one-dimensional subspaces of $\mathcal{A}_N$. That is, a pure state is given by:

$$P_\psi(\phi) = \langle \phi, \psi \rangle \psi$$

for some $\psi \in \mathcal{A}_N$ of unit length. The *statistical states* of the N-fermion system are the positive trace class operators or *density operators* D on $\mathcal{A}_N$ of trace 1. These can be identified with density operators D on all of $\mathcal{H}_N$ whose eigenvectors lie in $\mathcal{A}_N$, i.e., such that

$$D = \sum_{i=1}^{\infty} \lambda_i P_{\psi_i}$$

for some orthonormal system $\{\psi_i\}$ in $\mathcal{A}_N$ and a family of positive numbers λ_i that sum to 1. It follows that these *fermionic densities* are those density operators that satisfy:

$$DU_\pi = U_\pi D = \operatorname{sgn}(\pi) D \quad \forall \pi \in \Pi_N. \tag{2}$$

If a density operator D on $\mathcal{H}_N$ commutes with every permutation operator U_π then it is *symmetric*. In particular, fermionic densities are symmetric by (2).

If $\{e_j\}_{j\in J}$ is an orthonormal basis of $\mathcal{H}$ then

$$\{e_{j_1} \otimes e_{j_2} \otimes \cdots \otimes e_{j_N}\colon\ j_1, j_2, \ldots, j_N \in J\}$$

is an orthonormal basis of $\mathcal{H}_N$. Since $\mathcal{A}_N$ is the range of $P_{\mathcal{A}_N}$ and since

$$P_{\mathcal{A}_N}(e_{j_1} \otimes e_{j_2} \otimes \cdots \otimes e_{j_N}) = 0$$

unless all of the indices j_i are distinct, the set

$$\bigl\{P_{\mathcal{A}_N}(e_{j_1} \otimes e_{j_2} \otimes \cdots \otimes e_{j_N})\colon\ j_1, j_2, \ldots, j_n \text{ all distinct}\bigr\}$$

is a spanning set for $\mathcal{A}_N$. In fact it is an orthogonal basis for $\mathcal{A}_N$, each vector having norm $1/\sqrt{N!}$. Vectors of the form $\sqrt{N!}P_{\mathcal{A}_N}(e_{j_1} \otimes e_{j_2} \otimes \cdots \otimes e_{j_N})$ are known as *Slater determinants*.

The trace class operators on a Hilbert space $\mathcal{H}$ form a Banach space $\mathcal{T}(\mathcal{H})$ with the norm $\|T\|_{\mathrm{tr}} = \operatorname{Tr}(|T|)$. The important inequality

$$\|TB\|_{\mathrm{tr}} \leqslant \|T\|_{\mathrm{tr}}\|B\| \tag{3}$$

holds whenever B is a bounded operator of norm $\|B\|$ and $T \in \mathcal{T}(\mathcal{H})$. It is this basic inequality that will produce our key estimates.

For $n \leqslant N$, the nth *partial trace* is a contraction from $\mathcal{T}(\mathcal{H}^{\otimes N})$ onto $\mathcal{T}(\mathcal{H}^{\otimes n})$. The nth partial trace of T will be denoted $T_{:n}$, and may be defined as follows: Let $\mathcal{O}$ be any orthonormal basis of $\mathcal{H}$. If $T \in \mathcal{T}(\mathcal{H}^{\otimes N})$ and $n < N$ then

$$\bigl\langle T_{:n}(w), x\bigr\rangle = \sum_{z_1,\ldots,z_{N-n}\in\mathcal{O}} \bigl\langle T(w \otimes z_1 \otimes \cdots \otimes z_{N-n}), x \otimes z_1 \otimes \cdots \otimes z_{N-n}\bigr\rangle \tag{4}$$

for any $w, x \in \mathcal{H}^{\otimes n}$. If a trace class operator $T \in \mathcal{T}(\mathcal{H}^{\otimes N})$ satisfies (2) then so does $T_{:n}$, i.e., the partial trace defines a positive contraction from $\mathcal{T}(\mathcal{H}^{\otimes N})$ to $\mathcal{T}(\mathcal{H}^{\otimes n})$ that carries fermionic densities to fermionic densities.

In the following definition, and throughout this article, we use the superscript ${}^{\otimes n}$ to denote the nth tensor power of an operator, and we use the notation Σ_n for $n!P_{\mathcal{A}_n}$, i.e.,

$$\Sigma_n = \sum_{\pi\in\Pi_n} \operatorname{sgn}(\pi) U_\pi.$$

The nth *tensor power* of an operator A on $\mathcal{H}$ is the operator $A^{\otimes n}$ on $\mathcal{H}_n$ defined on simple tensors by:

$$A^{\otimes n}(x_1 \otimes x_2 \otimes \cdots \otimes x_n) = Ax_1 \otimes Ax_2 \otimes \cdots \otimes Ax_n.$$

Definition 2.1. For each N, let D_N be a symmetric density operator on $\mathcal{H}_N$. The sequence $\{D_N\}$ *has Slater closure* if, for each fixed n,

$$\lim_{N\to\infty} \left\| D_{N:n} - D_{N:1}^{\otimes n}\Sigma_n \right\|_{\mathrm{tr}} = 0.$$

This terminology is motivated by the observation that, if Ψ_N is a Slater determinant in $\mathcal{A}_N$ and P_{Ψ_N} denotes the orthogonal projector onto the span of Ψ_N, then

$$\left(P_{\Psi_N}\right)_{:n} = \frac{N^n(N-n)!}{N!}(P_{\Psi_N})_{:1}^{\otimes n} \sum_{\pi\in\Pi_n} \operatorname{sgn}(\pi)U_\pi, \tag{5}$$

for this implies the following:

Proposition 2.2. *For each N let Ψ_N be a Slater determinant in $\mathcal{A}_N$, and let P_{Ψ_N} denote the orthoprojector onto the span of Ψ_N. Then $\{P_{\Psi_N}\}$ has Slater closure.*

3. The time-dependent Hartree–Fock equation

We are going to prove that, in the mean field limit, the time-dependent Hartree–Fock equation describes the time-evolution of the single-particle state in systems of fermions. We state our theorem in this section and go on to prove it in the three subsequent sections.

First we describe the N-particle Hamiltonian. Let $\mathrm{i}L^{(N)}$ be a self-adjoint operator on $\mathcal{H}$, where $L^{(N)}$ may depend on N in an arbitrary manner. The free motion of the jth particle is governed by:

$$L_j^{(N)} = I^{\otimes j-1} \otimes L^{(N)} \otimes I^{\otimes N-j},$$

where I denotes the identity operator on $\mathcal{H}$. The interaction between the particles has the form $1/(N-1)$ times the sum over pairs of distinct particles of a two-body potential V. Let V be a bounded Hermitian operator on $\mathcal{H}\otimes\mathcal{H}$ that commutes with the transposition operator $U_{(12)}$. Define the operator V_{12} on $\mathcal{H}_N$ by:

$$V_{12}(x_1 \otimes x_2 \otimes \cdots \otimes x_N) = V(x_1 \otimes x_2) \otimes x_3 \otimes \cdots \otimes x_N$$

and for each $1 \leqslant i < j \leqslant N$ define $V_{ij} = U_\pi^* V_{12} U_\pi$ where π is any permutation with $\pi(i) = 1$ and $\pi(j) = 2$. Let

$$H_N = \sum_{1\leqslant j\leqslant N} L_j^{(N)} + \frac{1}{N-1} \sum_{1\leqslant i<j\leqslant N} V_{ij} \tag{6}$$

be the *N-particle Hamiltonian* operator on $\mathcal{H}_N$. The von Neumann equation for the N-particle density operator $D_N(t)$ is

$$\mathrm{i}\hbar \frac{\mathrm{d}}{\mathrm{d}t} D_N(t) = \sum_{1 \leqslant j \leqslant N} \left[L_j^{(N)}, D_N(t)\right] + \frac{1}{N-1} \sum_{1 \leqslant i < j \leqslant N} \left[V_{ij}, D_N(t)\right] \tag{7}$$

and has the solution

$$\mathrm{e}^{-\mathrm{i}H_N t/\hbar} D_N(0) \mathrm{e}^{\mathrm{i}H_N t/\hbar}. \tag{8}$$

Next we define the time-dependent Hartree–Fock equation. Let $L^{(N)}$ and V be as above, and let $U_{(12)}$ denote the transposition operator on $\mathcal{H} \otimes \mathcal{H}$. The time-dependent Hartree–Fock (TDHF) equation for a density operator $F(t)$ on $\mathcal{H}$ is

$$\begin{aligned} &\mathrm{i}\hbar \frac{\mathrm{d}}{\mathrm{d}t} F(t) = \left[L^{(N)}, F(t)\right] + \left[V, F_2^-(t)\right]_{:1}, \\ &F_2^-(t) = \big(F(t) \otimes F(t)\big)(I - U_{(12)}) = F(t)^{\otimes 2} \Sigma_2 \end{aligned} \tag{9}$$

(the subscript $_{:1}$ on the last commutator denotes partial contraction). Following [5], we define a *strong solution* of equation of (9) to be a continuously differentiable function $F(t)$ from $[0, \infty)$ to the real Banach space of Hermitian trace class operators such that the domain of $L^{(N)}$ is invariant under $F(t)$ for all $t \geqslant 0$ and

$$\mathrm{i}\hbar \frac{\mathrm{d}F(t)}{\mathrm{d}t} x = L^{(N)} F(t) x - F(t) L^{(N)} x + \left[V, F_2^-(t)\right]_{:1} x$$

for all x in the domain of $L^{(N)}$. The results proved in [5] show that (9) has a global strong solution[1] if the domain of $L^{(N)}$ contains the range of the initial condition $F(0)$. Furthermore,

$$F(t) = U^* F(0) U \tag{10}$$

for some unitary operator depending on t and $F(0)$. In particular, the operator norm of $F(t)$ is constant.

The relationship between the N-particle system and the TDHF equation is the subject of our main theorem. Recall the Definition 2.1 of Slater closure.

Theorem 3.1. *For each N, let $D_N(t)$ be a solution to* (7) *whose initial value $D_N(0)$ is a symmetric density. Let $F^{(N)}(t)$ be the solution of the TDHF equation* (9) *whose initial value is $F^{(N)}(0) = D_{N:1}(0)$.*

[1] The solution obtained in Theorem 4.2 of [5] is indeed defined for all positive times because the nonlinearity of TDHF satisfies condition (4.1) of [5]—see Proposition 3.5 there.

If $\{D_N(0)\}$ *has Slater closure then* $\{D_N(t)\}$ *has Slater closure and*

$$\lim_{N\to\infty} \left\| D_{N:1}(t) - F^{(N)}(t) \right\|_{\mathrm{tr}} = 0$$

for all $t > 0$.

4. Two hierarchies and their difference

Consider the N-particle von Neumann equation (7). From now on we will suppose that the initial N-particle density operator $D_N(0)$ is symmetric, i.e., that

$$U_\pi^* D_N(0) U_\pi = D_N(0)$$

for all $\pi \in \Pi_N$. (Recall that, in particular, fermionic densities are symmetric.) The symmetry of the Hamiltonian (6) ensures that $D_N(t)$ remains symmetric for all t. From (7) and the symmetry of $D_N(t)$, it follows that the partial trace $D_{N:n}(t)$ satisfies:

$$\begin{aligned} \mathrm{i}\hbar \frac{\mathrm{d}}{\mathrm{d}t} D_{N:n}(t) = {} & \sum_{1\leqslant j\leqslant n} \left[L_j^{(N)}, D_{N:n}(t)\right] + \frac{1}{N-1} \sum_{1\leqslant i<j\leqslant n} \left[V_{ij}, D_{N:n}(t)\right] \\ & + \frac{N-n}{N-1} \sum_{1\leqslant i\leqslant n} \left[V_{i,n+1}, D_{N:n+1}(t)\right]_{:n}. \end{aligned} \tag{11}$$

The system of Eqs. (11) for $D_{N:1}, D_{N:2}, \ldots, D_{N:N-1}$ together with Eq. (7) for D_N is called the *N-particle hierarchy*. For our estimates later on, it is convenient to rewrite Eqs. (11) of the hierarchy as

$$\mathrm{i}\hbar \frac{\mathrm{d}}{\mathrm{d}t} D_{N:n}(t) = \mathcal{L}_n^{(N)}\big(D_{N:n}(t)\big) + \sum_{1\leqslant i\leqslant n} \left[V_{i,n+1}, D_{N:n+1}(t)\right]_{:n} + \mathcal{E}_n\big(N, D_N(t)\big) \tag{12}$$

with

$$\begin{aligned} \mathcal{L}_n^{(N)}(\cdot) &= \sum_{1\leqslant j\leqslant n} \left[L_j^{(N)}, \cdot\right], \\ \mathcal{E}_n\big(t, N, D_N(0)\big) &= \frac{1}{N-1} \sum_{1\leqslant i<j\leqslant n} \left[V_{ij}, D_{N:n}(t)\right] \\ &\quad - \frac{n-1}{N-1} \sum_{1\leqslant i\leqslant n} \left[V_{i,n+1}, D_{N:n+1}(t)\right]_{:n}. \end{aligned} \tag{13}$$

Next we describe another hierarchy, built from "the bottom up" out of solutions to the TDHF equation, in contrast to the hierarchy we have just considered, which is built from "the top down" starting with solutions to (7). If F is a trace class operator, define $F_1^- = F$ and

$$F_n^- = F^{\otimes n}\Sigma_n$$

for $n > 1$. When F depends on t we write $F_n^-(t)$ instead of $F(t)_n^-$. The notation $F_2^-(t)$ has already been used in the TDHF equation (9).

Proposition 4.1. *If $F(t)$ is a strong solution of the TDHF equation* (9)*, then*

$$\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}F_n^-(t) = \sum_{j=1}^{n}\bigl[L_j^{(N)}, F_n^-(t)\bigr] + \sum_{j=1}^{n}\bigl[V_{j,n+1}, F_{n+1}^-(t)\bigr]_{:n} + \mathcal{R}_n\bigl(F(t)\bigr),$$

where $\mathcal{R}_n$ is defined on trace class operators by $\mathcal{R}_1(X) = \mathbf{0}$ (the zero operator) and

$$\mathcal{R}_n(X) = \sum_{j=1}^{n}\Biggl[V_{j,n+1}, X^{\otimes n+1}\sum_{k\neq j}U_{(k,n+1)}\Biggr]_{:n}\Sigma_n \tag{14}$$

for $n > 1$.

Proof. For any trace class operator X,

$$\begin{aligned}\sum_{j=1}^{n}[V_{j,n+1}, X_{n+1}^-]_{:n} &= \sum_{j=1}^{n}\Biggl[V_{j,n+1}, X^{\otimes n+1}\Biggl(I - \sum_{k=1}^{n}U_{(k,n+1)}\Biggr)\Sigma_n\otimes I_{\mathcal{B}(\mathcal{H})}\Biggr]_{:n}\\ &= \sum_{j=1}^{n}\Biggl[V_{j,n+1}, X^{\otimes n+1}\Biggl(I - \sum_{k=1}^{n}U_{(k,n+1)}\Biggr)\Biggr]_{:n}\Sigma_n.\end{aligned} \tag{15}$$

The first equality in (15) holds because

$$\Sigma_{n+1} = \Biggl(I - \sum_{k=1}^{n}U_{(k,n+1)}\Biggr)\Sigma_n\otimes I_{\mathcal{B}(\mathcal{H})},$$

and the second equality in (15) holds because $\Sigma_n\otimes I_{\mathcal{B}(\mathcal{H})}$ commutes with $\sum_{j=1}^{n}V_{j,n+1}$. From the TDHF equation (9) we calculate,

$$\begin{aligned}\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}F_n^-(t) &= \mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}F(t)^{\otimes n}\Sigma_n = \mathrm{i}\hbar\Biggl\{\sum_{j=1}^{n}F(t)^{\otimes j-1}\otimes\frac{\mathrm{d}}{\mathrm{d}t}F(t)\otimes F(t)^{\otimes n-j}\Biggr\}\Sigma_n\\ &= \sum_{j=1}^{n}\bigl\{\bigl[L_j^{(N)}, F(t)^{\otimes n}\bigr] + \bigl[V_{j,n+1}, F(t)^{\otimes n+1}\bigl(I - U_{(j,n+1)}\bigr)\bigr]_{:n}\bigr\}\Sigma_n\end{aligned}$$

$$= \sum_{j=1}^{n} \left[L_j^{(N)}, F_n^-(t)\right] + \mathcal{R}_n(F(t))$$
$$+ \sum_{j=1}^{n} \left[V_{j,n+1}, F(t)^{\otimes n+1} \left(I - \sum_{k=1}^{n} U_{(k,n+1)} \right) \right]_{:n} \Sigma_n. \tag{16}$$

By the identity (15), the last sum in (16) equals $\sum_{j=1}^{n} \left[V_{j,n+1},\ F_{n+1}^-(t)\right]_{:n}$, proving the proposition. $\square$

Now let $D_N(t)$ be a solution of the N-particle von Neumann equation (7) and let $F(t)$ be a solution of the TDHF equation (9). For $1 \leqslant n \leqslant N$ define the nth *difference*:

$$E_{N,n}(t) = D_{N:n}(t) - F_n^-(t). \tag{17}$$

From the N-particle hierarchy equations (12) and (13) and Proposition 4.1, it follows that

$$\mathrm{i}\hbar \frac{\mathrm{d}}{\mathrm{d}t} E_{N,n}(t) = \mathcal{L}_n^{(N)}\big(E_{N,n}(t)\big) + \sum_{j=1}^{n} \left[V_{j,n+1}, E_{N,n+1}(t)\right]_{:n}$$
$$+ \mathcal{E}_n\big(N, D_N(t)\big) - \mathcal{R}_n\big(F(t)\big) \tag{18}$$

for $n = 1, 2, \ldots, N-1$. The characters $\mathcal{E}$ and $\mathcal{R}$ were chosen to evoke the words “error” and “remainder”. Indeed, in the next section we find bounds on these error terms under conditions on $D_N(0)$ and $F(0)$. The rest of this section is devoted to show how such bounds lead to an upper bound on the differences $E_{N,n}(t)$.

To this end, let us define:

$$\mathrm{Err}(t, N, n) = \mathcal{E}_n\big(N, D_N(t)\big) - \mathcal{R}_n\big(F(t)\big). \tag{19}$$

Let $U_{n,t}^{(N)}$ denote the unitary operator $\exp(\frac{\mathrm{i}t}{\hbar} \sum_{j=1}^{n} L_j^{(N)})$ on $\mathcal{H}_n$ and define isometries $\mathcal{U}_{n,t}^{(N)}$ on the trace class operators by:

$$\mathcal{U}_{n,t}^{(N)}(\cdot) = \mathrm{e}^{\frac{\mathrm{i}t}{\hbar}\mathcal{L}_n^{(N)}}(\cdot) = U_{n,t}^{(N)}(\cdot)U_{n,-t}^{(N)}.$$

Then $Z_{N,n}(t) = \mathcal{U}_{n,t}^{(N)}(E_{N,n}(t))$ has the same trace norm as $E_{N,n}(t)$ and satisfies:

$$\frac{\mathrm{d}}{\mathrm{d}t} Z_{N,n}(t) = -\frac{\mathrm{i}}{\hbar} \sum_{j=1}^{n} \left[V_{j,n+1}, Z_{N,n+1}(t)\right]_{:n} - \frac{\mathrm{i}}{\hbar} \mathcal{U}_{n,t}^{(N)} \,\mathrm{Err}(t, N, n) \tag{20}$$

for $n = 1, 2, \ldots, N-1$. From (20) it follows that

$$\left\|E_{N,n}(t)\right\|_{\mathrm{tr}} = \left\|Z_{N,n}(t)\right\|_{\mathrm{tr}} \leqslant \left\|Z_{N,n}(0)\right\|_{\mathrm{tr}} + \frac{2\|V\|n}{\hbar}\int_0^t \left\|Z_{N,n+1}(s)\right\|_{\mathrm{tr}}\,\mathrm{d}s + \frac{1}{\hbar}\int_0^t \left\|\mathcal{U}_{n,t}^{(N)}\big(\mathrm{Err}(s,N,n)\big)\right\|_{\mathrm{tr}}\,\mathrm{d}s$$

for $n = 1, 2, \ldots, N-1$. Recalling that $\|Z_{N,n+1}(s)\|_{\mathrm{tr}} = \|E_{N,n+1}(s)\|_{\mathrm{tr}}$ and that $\|\mathcal{U}_{n,t}^{(N)}(\mathrm{Err}(s,N,n))\|_{\mathrm{tr}} = \|\mathrm{Err}(s,N,n)\|_{\mathrm{tr}}$, the preceding inequality becomes:

$$\left\|E_{N,n}(t)\right\|_{\mathrm{tr}} \leqslant \varepsilon(N,n,t) + \frac{2\|V\|n}{\hbar}\int_0^t \left\|E_{N,n+1}(s)\right\|_{\mathrm{tr}}\,\mathrm{d}s, \tag{21}$$

if we define

$$\varepsilon(N,n,t) = \left\|E_{N,n}(0)\right\|_{\mathrm{tr}} + \frac{1}{\hbar}\int_0^t \left\|\mathrm{Err}(s,N,n)\right\|_{\mathrm{tr}}\,\mathrm{d}s. \tag{22}$$

Beginning from (21) and iterating the inequality m times (for some $m \leqslant N-n-1$) we obtain our desired bound on the trace norm of $E_{N,n}(t)$:

$$\left\|E_{N,n}(t)\right\|_{\mathrm{tr}} \leqslant \sum_{k=0}^{m}\binom{n+k-1}{n-1}\left(\frac{2\|V\|t}{\hbar}\right)^k \varepsilon(N,n+k,t) + \binom{n+m-1}{n-1}\left(\frac{2\|V\|t}{\hbar}\right)^m \sup_{s\in[0,t]}\left\{\left\|E_{N,n+m+1}(s)\right\|_{\mathrm{tr}}\right\}. \tag{23}$$

5. Error estimates

In this section we collect the error estimates that will be used to prove Theorem 3.1.

If $D_N(0)$ is a density operator then the solution $D_N(t)$ of the N-particle von Neumann equation (7) is a density operator for all $t > 0$, and it is clear from (13) that

$$\left\|\mathcal{E}_n\big(N, D_N(t)\big)\right\|_{\mathrm{tr}} \leqslant \frac{4n(n-1)}{N-1}\|V\| \tag{24}$$

for all t.

Lemma 5.1. *If $\{D_N\}$ has Slater closure, then*

$$\lim_{N\to\infty}\|D_{N:1}\| = 0.$$

Proof. The trace norm of $D_{N:1}^2$ equals the sum of the squares of the eigenvalues of $D_{N:1}$. Since the operator norm of $D_{N:1}$ equals its largest eigenvalue, it follows that $\|D_{N:1}\| \leqslant \|D_{N:1}^2\|_{\mathrm{tr}}^{1/2}$. But $D_{N:1}^2 = \{D_{N:1}^{\otimes 2} U_{(12)}\}_{:1}$, whence

$$\left\|D_{N:1}^2\right\|_{\mathrm{tr}} = \left\|\left\{D_{N:2} - D_{N:1}^{\otimes 2}(I - U_{(12)})\right\}_{:1}\right\|_{\mathrm{tr}} \leqslant \left\|D_{N:2} - D_{N:1}^{\otimes 2}\Sigma_2\right\|_{\mathrm{tr}}.$$

The Slater closure of $\{D_N\}$ implies that the right-hand side of the preceding inequality tends to 0 as $N \to \infty$. □

Lemma 5.2. *If F is a density operator, then $\|F_n^-\|_{\mathrm{tr}} \leqslant 1$ for all n.*

Proof. Since $\Sigma_n = (\Sigma_n)^* = \frac{1}{n!}(\Sigma_n)^2$ commutes with $F^{\otimes n}$, it follows that

$$F_n^- = F^{\otimes n}\Sigma_n = \frac{1}{n!}\Sigma_n\left(F^{\otimes n}\right)\Sigma_n$$

is a nonnegative operator. Thus, the trace norm of F_n^- equals its trace. This trace is:

$$\sum_{j_1,\ldots,j_n \in J} \left\langle e_{j_1} \otimes \cdots \otimes e_{j_n}, F^{\otimes n}\Sigma_n(e_{j_1} \otimes \cdots \otimes e_{j_n})\right\rangle,$$

where $\{e_j\}_{j\in J}$ is an orthonormal basis for $\mathcal{H}$ consisting of eigenvectors of F. This sum may be taken over distinct indices $j_1, \ldots, j_n \in J$, since Σ_n annihilates all tensor products $e_{j_1} \otimes \cdots \otimes e_{j_n}$ with repeating factors, so that

$$\begin{aligned}
\mathrm{Tr}(F_n^-) &= \sum_{\substack{\text{distinct} \\ j_1,\ldots,j_n \in J}} \left\langle e_{j_1} \otimes \cdots \otimes e_{j_n}, F^{\otimes n}\Sigma_n(e_{j_1} \otimes \cdots \otimes e_{j_n})\right\rangle \\
&= \sum_{\substack{\text{distinct} \\ j_1,\ldots,j_n \in J}} \left\langle e_{j_1} \otimes \cdots \otimes e_{j_n}, F^{\otimes n}(e_{j_1} \otimes \cdots \otimes e_{j_n})\right\rangle \\
&\leqslant \mathrm{Tr}\left(F^{\otimes n}\right) = 1
\end{aligned}$$

as asserted. □

The next lemma provides a bound on the trace norm of the remainder term $\mathcal{R}_n(F)$ when F is a density operator. The bound is proportional to the *operator* norm of F.

Lemma 5.3. *Let $\mathcal{R}_n$ be as in* (14) *and let F be a density operator. Then*

$$\left\|\mathcal{R}_n(F)\right\|_{\mathrm{tr}} \leqslant 2n(n-1)\|V\|\|F\|. \tag{25}$$

Proof. From (14) we see that $\mathcal{R}_n(F)$ equals:

$$\left\{\sum_{\substack{j,k=1\\ j\neq k}}^{n}\bigl(V_{j,n+1}F^{\otimes n+1}U_{(k,n+1)}-F^{\otimes n+1}U_{(k,n+1)}V_{j,n+1}\bigr)(\Sigma_n\otimes I_{\mathcal{B}(\mathcal{H})})\right\}_{:n}.$$

Since $U_{(k,n+1)}$ commutes with $F^{\otimes n+1}$ and since $\Sigma_n\otimes I_{\mathcal{B}(\mathcal{H})}$ commutes with $\sum_{j,k:\,j\neq k}U_{(k,n+1)}V_{j,n+1}$, it follows that $\mathcal{R}_n(F)$ equals

$$\left\{\sum_{\substack{j,k=1\\ j\neq k}}^{n}V_{j,n+1}U_{(k,n+1)}(F_n^-\otimes F)\right\}_{:n}-\left\{(F_n^-\otimes F)\sum_{\substack{j,k=1\\ j\neq k}}^{n}U_{(k,n+1)}V_{j,n+1}\right\}_{:n}.$$

Since the trace norm of a trace class operator equal the trace norm of its adjoint, it follows that

$$\begin{aligned}\bigl\|\mathcal{R}_n(F)\bigr\|_{\mathrm{tr}}&\leqslant 2\left\|\sum_{\substack{j,k=1\\ j\neq k}}^{n}\bigl\{V_{j,n+1}U_{(k,n+1)}(F_n^-\otimes F)\bigr\}_{:n}\right\|_{\mathrm{tr}}\\ &\leqslant 2n(n-1)\bigl\|\bigl\{V_{n-1,n+1}U_{(n,n+1)}(F_n^-\otimes F)\bigr\}_{:n}\bigr\|_{\mathrm{tr}}.\end{aligned}\tag{26}$$

But one may verify directly that

$$\bigl\{V_{n-1,n+1}U_{(n,n+1)}(F_n^-\otimes F)\bigr\}_{:n}=\bigl(I^{\otimes n-1}\otimes F\bigr)V_{n-1,n}F_n^-,\tag{27}$$

so that, by (3) and Lemma 5.2,

$$\bigl\|\bigl\{V_{n-1,n+1}U_{(n,n+1)}(F_n^-\otimes F)\bigr\}_{:n}\bigr\|_{\mathrm{tr}}\leqslant\|F\|\|V\|\|F_n^-\|_{\mathrm{tr}}\leqslant\|F\|\|V\|.$$

Substituting this in (26) yields (25).

To verify (27), we can assume $n=3$; choose an orthonormal basis $\{e_j\}_{j\in J}$ for $\mathcal{H}$ and check that the operators on both sides of (27) have the same matrix elements relative to the basis $\{e_i\otimes e_j\otimes e_k\colon i,j,k\in J\}$. □

Let $F(t)$ be a solution of the TDHF equation (9). Since the (operator) norm of $F(t)$ is constant, it follows from Lemma 25 that

$$\bigl\|\mathcal{R}_n\bigl(F(t)\bigr)\bigr\|_{\mathrm{tr}}\leqslant 2n(n-1)\|V\|\bigl\|F(0)\bigr\|$$

for all $t\geqslant 0$. Thus, $\mathrm{Err}(t,N,n)$ of Eq. (19) satisfies:

$$\bigl\|\mathrm{Err}(t,N,n)\bigr\|_{\mathrm{tr}}\leqslant 2n(n-1)\|V\|\left(\frac{2}{N-1}+\bigl\|F(0)\bigr\|\right)$$

and $\varepsilon(N,n,t)$ of Eq. (22) satisfies:

$$\varepsilon(N,n,t) = 2n(n-1)\|V\|\frac{t}{\hbar}\left(\frac{2}{N-1} + \big\|F(0)\big\|\right) + \big\|E_{N,n}(0)\big\|_{\mathrm{tr}}. \tag{28}$$

6. Proof of the theorem

Equipped with the estimates of the preceding sections, we proceed to the proof of Theorem 3.1.

Proof. So, let us assume that $D_N(0)$ is a symmetric density for each N and that the sequence $\{D_N(0)\}$ has Slater closure. Let $D_N(t)$ be the solution of (7) with initial value $D_N(0)$, and let $F^{(N)}(t)$ be the solution of the TDHF equation (9) whose initial value is $F^{(N)}(0) = D_{N:1}(0)$. Let $\{F^{(N)}\}_n^-(t)$ denote $\{F^{(N)}(t)\}^{\otimes n}\Sigma_n$ and let $E_{N,n}(t)$ denote the difference between $D_{N:n}(t)$ and $\{F^{(N)}\}_n^-(t)$.

We have the upper bound (23) for the trace norm of $E_{N,n}(t)$, into which we now substitute the estimates (28). In the same stroke, we will replace the binomial coefficients $\binom{n+k-1}{n-1}$ with the larger quantities $(n+k)^n/n!$ and we will use the fact that $\sup_{s\in[0,t]}\{\|E_{N,n+m+1}(s)\|_{\mathrm{tr}}\} \leqslant 2$ by Lemma 5.2. Also, let us set $T = 2\|V\|t/\hbar$. We obtain:

$$\begin{aligned}\big\|E_{N,n}(t)\big\|_{\mathrm{tr}} \leqslant{} & \frac{1}{n!}\sum_{k=0}^{m}(n+k)^n\big\|E_{N,n+k}(0)\big\|_{\mathrm{tr}}T^k \\ & + \frac{1}{n!}\sum_{k=0}^{m}(n+k)^{n+2}\left(\frac{2}{N-1} + \big\|F^{(N)}(0)\big\|\right)T^{k+1} \\ & + \frac{2}{n!}(n+m)^n T^m \end{aligned} \tag{29}$$

for $m \leqslant N-n-1$. Fix T to be less than 1, i.e., fix $t < \hbar/(2\|V\|)$. For fixed n, consider the limit of the right-hand side of (29) as N and m tend to infinity. The individual terms (fixed k) tend to 0, for $\|F^{(N)}(0)\|$ tends to 0 by Lemma 5.1 and $\|E_{N,n+k}(0)\|_{\mathrm{tr}}$ tends to 0 thanks to the hypothesis that $\{D_N(0)\}$ has Slater closure (recall that $F^{(N)}(0) = D_{N:1}(0)$). On the other hand, the series on the right-hand side of (29) are dominated, uniformly with respect to m, by a series that converges absolutely for $T < 1$. It follows that

$$\lim_{N\to\infty}\big\|E_{N,n}(t)\big\|_{\mathrm{tr}} = 0 \tag{30}$$

if $t < \hbar/(2\|V\|)$. When $n = 1$, this shows that $\lim_{N\to\infty}\|D_{N:1}(t) - F^{(N)}(t)\|_{\mathrm{tr}} = 0$ and consequently

$$\lim_{N\to\infty}\big\|D_{N:1}^{\otimes n}(t)\Sigma_n - \big\{F^{(N)}\big\}_n^-(t)\big\|_{\mathrm{tr}} = 0$$

for $n > 1$ and $t < \hbar/(2\|V\|)$. From (30) again it follows that, for any n and any $t < \hbar/(2\|V\|)$,

$$\lim_{N\to\infty} \left\| D_{N:n}(t) - D_{N:1}^{\otimes n}(t)\Sigma_n \right\|_{\mathrm{tr}} = 0,$$

i.e., $\{D_N(t)\}$ has Slater closure. This proves the theorem up to $t = \hbar/(2\|V\|)$.

Let $\tau = \hbar/(3\|V\|)$; the previous argument shows that the theorem holds for $t \in [0, \tau]$. At time τ, it is in general no longer the case that $D_{N:1}(\tau) = F^{(N)}(\tau)$. However, $\|E_{N,n+k}(\tau)\|_{\mathrm{tr}} \to 0$ and $\|F^{(N)}(\tau)\| \to 0$ as N tends to infinity—to see this, use (10) and the fact that $\|F^{(N)}(0)\| \to 0$ recalled above. An argument nearly identical to the one above shows that the theorem holds for $t \in [\tau, 2\tau]$. This argument may be repeated to establish the conclusion of the theorem on each interval of the form $[k\tau, (k+1)\tau]$ for each nonnegative integer k, and hence for all $t > 0$. $\square$

Acknowledgements

This research was supported by the French–Austrian “Amadeus” program (ÖAD V6) and by the Austrian START project “Nonlinear Schrödinger and quantum Boltzmann equations” of N.J.M. Also, F.G. was supported by the Institut Universitaire de France. The first three authors thank the ESI in Vienna for its hospitality. We also express our gratitude to Xavier Blanc, Eric Cancès and Claude Le Bris for numerous and helpful discussions on this paper.

Appendix A. TDHF equations for wavefunctions

The main body of this text describes time-dependent Hartree–Fock equations in the language of density matrices and operator calculus. In another formulation—which may be more familiar to some readers—the TDHF equations are written as a system of coupled Schrödinger equations for N time-dependent orbitals. This appendix explains how to recast the wavefunction formulation of the TDHF equations into the language of density operators used in this paper.

The starting point in this discussion is the linear N-body Schrödinger:

$$\mathrm{i}\hbar\frac{\partial}{\partial t}\Psi_N = -\frac{\hbar^2}{2}\sum_{k=1}^{N}\Delta_{x_k}\Psi_N + \frac{1}{N-1}\sum_{1\leqslant k<l\leqslant N} V(x_k - x_l)\Psi_N, \tag{31}$$

where $\Psi_N \equiv \Psi_N(t, x_1, \ldots, x_N)$ is the N-particle wavefunction. (Note that the interaction term has been multiplied by $1/(N-1)$.) This scaling has been introduced so that $N \to \infty$ may yield a *mean-field* equation for the single-particle density, namely, the TDHF equation.) The dynamics defined by (31) is unitary on $L^2((\mathbb{R}^3)^N)$. Therefore,

$$\int \left|\Psi_N(t, x_1, \ldots, x_N)\right|^2 \mathrm{d}x_1 \cdots \mathrm{d}x_N = 1$$

for all $t \geqslant 0$ if the same equality holds at $t = 0$ (as is the case if $|\Psi_N|^2$ is meant to be interpreted as the probability density of the system of N particles in its configuration space). In the language of (1), $L_k = -\hbar^2 \Delta_{x_k}/2$ while V_{kl} denotes the multiplication by $V(x_k - x_l)$. The TDHF equations corresponding to (31) may be written as a system of N coupled Schrödinger equations for orthonormal orbitals $\psi_1(t,x), \psi_2(t,x), \ldots, \psi_N(t,x)$:

$$\begin{aligned} \mathrm{i}\hbar \frac{\partial}{\partial t}\psi_k(t,x) &= -\frac{\hbar^2}{2}\Delta_x \psi_k(t,x) + \psi_k(t,x)\frac{1}{N}\sum_{l=1}^{N}\int V(x-z)\big|\psi_l(t,z)\big|^2\,\mathrm{d}z \\ &\quad - \frac{1}{N}\sum_{l=1}^{N}\psi_l(t,x)\int V(x-z)\psi_k(t,z)\overline{\psi_l(t,z)}\,\mathrm{d}z. \end{aligned} \tag{32}$$

The N orbitals remain orthonormal at all times; if $\psi_1(t,x), \psi_2(t,x), \ldots, \psi_N(t,x)$ is a solution of (32) and

$$\int \psi_k(0,x)\overline{\psi_l(0,x)}\,\mathrm{d}x = \delta_{kl},$$

then

$$\int \psi_k(t,x)\overline{\psi_l(t,x)}\,\mathrm{d}x = \delta_{kl} \quad \text{for all } t \geqslant 0.$$

One way to obtain the TDHF equations (32) from the linear N-particle Schrödinger equation (31) is to solve a variational problem which would lead to (31) if unconstrained, but with the constraint that the N-particle wave function remains a Slater determinant at all times [6]. This constraint is imposed for the sake of obtaining an computationally amenable approximation to (31), and it is not justified on physical grounds. In effect, this paper proves that the constraint maintaining Slater determinants at all times is rigorously justified *in the mean-field limit*.

To see how the orbital form (32) of the TDHF equations relates to the TDHF equation (9) discussed in this paper, we shall first rewrite (9) as an equation for the integral kernel of a time-dependent density operator. To do this, we need to know how to translate the partial trace into the language of integral operators, for Eq. (9) involves a partial trace. Let T be a trace class operator on $L^2(\mathbb{R}^m \times \mathbb{R}^n)$ having an integral kernel $\rho(x,\xi,y,\eta)$ with $x, y \in \mathbb{R}^m$ and $\xi, \eta \in \mathbb{R}^n$. The partial trace:

$$T_{:m} \text{ is the operator with integral kernel } \int \rho(x,z,y,z)\,\mathrm{d}z.$$

We may now convert the TDHF equation (9) into an integro-differential equation for a time-dependent integral kernel: let $\rho \equiv \rho(t,x,y)$ be the integral kernel of the operator $F(t)$ that appears in (9). Then $F_2^-(t)$ has integral kernel:

$$\rho(t,x_1,y_1)\rho(t,x_2,y_2) - \rho(t,x_1,y_2)\rho(t,x_2,y_1),$$

while $[V, F_2^-(t)]_{:1}$ has integral kernel:

$$\int \bigl(V(x_1-z)-V(y_1-z)\bigr)\bigl(\rho(t,x_1,y_1)\rho(t,z,z)-\rho(t,x_1,z)\rho(t,z,y_1)\bigr)\,\mathrm{d}z,$$

and the TDHF equation (9) in the language of integral kernels is:

$$\begin{aligned}\mathrm{i}\hbar\frac{\partial}{\partial t}\rho(t,x,y) = {} & -\frac{\hbar^2}{2}(\Delta_x-\Delta_y)\rho(t,x,y)\\ & + \int \bigl(V(x-z)-V(y-z)\bigr)\\ & \times \bigl(\rho(t,x,y)\rho(t,z,z)-\rho(t,x,z)\rho(t,z,y)\bigr)\,\mathrm{d}z. \end{aligned} \tag{33}$$

It may be verified that a solution $\psi_1(t,x), \psi_2(t,x), \ldots, \psi_N(t,x)$ to the orbital form of the TDHF equations (32) yields a solution $\rho(t,x,y)$ to the integro-differential equation (33) via

$$\rho(t,x,y) = \frac{1}{N}\sum_{k=1}^{N}\psi_k(t,x)\overline{\psi_k(t,y)}.$$

The rest of this Appendix is meant to serve as a key for reading this paper with the Schrödinger wave equation (31) in mind.

To the wavefunction $\Psi_N(t,\cdot)$ solution of the N-particle Schrödinger equation (31) one associates the operator $D_N(t)$ with integral kernel:

$$\rho_N(t,x_1,\ldots,x_N,y_1,\ldots,y_N) = \Psi_N(t,x_1,\ldots,x_N)\overline{\Psi_N(t,y_1,\ldots,y_N)}. \tag{34}$$

The natural Hilbert space $\mathcal{H}$ in this context is $\mathcal{H} = L^2(\mathbb{R}^3)$, and $\mathcal{H}^{\otimes N}$ is isomorphic to $L^2((\mathbb{R}^3)^N)$ through the identification:

$$\psi_1\otimes\cdots\otimes\psi_N \quad\leftrightarrow\quad \prod_{k=1}^{N}\psi_k(x_k).$$

The corresponding representation of the permutation group Π_N is given by the formula:

$$(U_\pi\Psi)(x_1,\ldots,x_N) = \Psi(x_{\pi^{-1}(1)},\ldots,x_{\pi^{-1}(N)})$$

for $\pi\in\Pi_N$ and $\Psi_N\in L^2((\mathbb{R}^3)^N)$. Hence the projection $P_{\mathcal{A}_N}$ is given by the formula:

$$(P_{\mathcal{A}_N}\Psi_N)(x_1,\ldots,x_N) = \frac{1}{N!}\sum_{\pi\in\Pi_N}\operatorname{sgn}(\pi)\Psi_N(x_{\pi(1)},\ldots,x_{\pi(N)}).$$

A wavefunction Ψ is antisymmetric if it is in the image of $P_{\mathcal{A}_N}$, or equivalently, if

$$\Psi(x_{\pi(1)}, \dots, x_{\pi(N)}) = \operatorname{sgn}(\pi)\Psi(x_1, \dots, x_N)$$

for all $\pi \in \Pi_N$. If Ψ_N is antisymmetric then the rank 1 orthogonal projector P_{Ψ_N} with integral kernel as in (34) is fermionic in the sense of (2). Property (2) extends to all convex combinations of such projectors P_{Ψ_N}, the fermionic density operators discussed in this article. Property (2) implies that fermionic density operators commute with all of the operators U_π, so that the integral kernel of a fermionic density operator is symmetric in the sense that

$$\rho_N(x_1, \dots, x_N, y_1, \dots, y_N) = \rho_N(x_{\pi(1)}, \dots, x_{\pi(N)}, y_{\pi(1)}, \dots, y_{\pi(N)})$$

for all $\pi \in \Pi_N$.

In the case where $\Psi_N = \psi_1 \otimes \cdots \otimes \psi_N$ with $\psi_1, \dots, \psi_N$ orthonormal, one finds that the Slater determinant $\sqrt{N!}P_{\mathcal{A}_N}(\Psi_N)$ truly is a determinant:

$$\sqrt{N!}(P_{\mathcal{A}_N}\Psi_N)(x_1, \dots, x_N) = \frac{1}{\sqrt{N!}} \begin{vmatrix} \psi_1(x_1) & \psi_1(x_2) & \cdots & \psi_1(x_N) \\ \psi_2(x_1) & \psi_2(x_2) & \cdots & \psi_2(x_N) \\ \vdots & \vdots & \ddots & \vdots \\ \psi_N(x_1) & \psi_N(x_2) & \cdots & \psi_N(x_N) \end{vmatrix}.$$

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