A MICROSCOPIC DERIVATION OF THE TIME-DEPENDENT HARTREE-FOCK EQUATION WITH COULOMB TWO-BODY INTERACTION

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August 10, 2011

We study the dynamics of a Fermi gas with a Coulomb interaction potential, and show that, in a mean-field regime, the dynamics is described by the Hartree-Fock equation. This extends previous work of Bardos et al. [3] to the case of unbounded interaction potentials. We also express the mean-field limit as a "superhamiltonian" system, and state our main result in terms of the Heisenberg-picture dynamics of observables. This is a Egorov-type theorem.

1. Introduction

The Hartree-Fock equation is a fundamental tool, used throughout physics and chemistry, for describing a system consisting of a large number of fermions. Despite its importance for both conceptual and numerical applications, many questions surrounding it remain unsolved. One area in which significant progress has been made is the microscopic justification of the static Hartree-Fock equation, which is known to yield the correct asymptotic ground state energy of large atoms and molecules; see [1, 8, 9, 11, 13, 14]. The time-dependent Hartree-Fock equation, which is supposed to describe the dynamics of a large Fermi system, has received less attention. To our knowledge, the only work in which this equation is derived from microscopic Hamiltonian dynamics is [3]. The Cauchy problem for the time-dependent Hartree-Fock equation has also been studied in the literature; see [2, 5] and especially [19], where the Cauchy problem is solved for singular interaction potentials.

A key assumption in [3] is that the interaction potential be bounded. A goal of this article is to extend the result of [3] to a class of singular interaction potentials, which includes the physically relevant Coulomb potential. We also describe how this mean-field result can be formulated as a Egorov-type theorem.

A system of N spinless[1] fermions is described by a wave function $\Psi_N(x_1, \dots, x_N) \in \bigwedge^N L^2(\mathbb{R}^3, \mathrm{d}x)$ which is totally antisymmetric in its arguments. The dynamics of Ψ_N is governed by the usual Schrödinger

[1] For simplicity of exposition we omit the spin, whose inclusion is merely a notational complication.

equation. In order to obtain a mean-field limit, the Schrödinger equation is rescaled with N. In this article we adopt the scaling of [3]. The Schrödinger equation reads

$$\mathrm{i}\partial_t \Psi_N(t) \;=\; H_N \Psi_N(t)\,, \tag{1.1}$$

where the N-particle Hamiltonian H_N is defined by

$$H_N \;:=\; \sum_{i=1}^N h_i + \frac{1}{N}\sum_{i<j} w(x_i - x_j)\,. \tag{1.2}$$

Here, h_i is a one-particle Hamiltonian acting on the coordinate x_i, typically of the form $h_i = -\Delta_i + v(x_i)$, where Δ is the three-dimensional Laplacian and v is some external potential; w is the interaction potential. Under the assumptions on v and w we make below, it is easy to see that H_N is a well-defined self-adjoint operator with domain $\bigwedge^N H^2(\mathbb{R}^3)$.

We briefly sketch our main result. Consider a sequence of N orthonormal orbitals $\varphi_1, \dots, \varphi_N$, where φ_i is a one-particle wave function. This defines an N-particle fermionic state through the Slater determinant

$$\Psi_N \;:=\; \varphi_1 \wedge \cdots \wedge \varphi_N\,.$$

Let $\Psi_N(t)$ be the solution of the Schrödinger equation (1.1) with initial state Ψ_N. In general, $\Psi_N(t)$ is no longer a Slater determinant for $t \neq 0$. However, one expects that this holds asymptotically for large N:

$$\Psi_N(t) \;\approx\; \varphi_1(t) \wedge \cdots \wedge \varphi_N(t)\,.$$

Here the orbitals $\varphi_1(t), \dots, \varphi_N(t)$ are supposed to solve the Hartree-Fock equation

$$\mathrm{i}\partial_t \varphi_i \;=\; h\varphi_i + \frac{1}{N}\sum_{j=1}^N (w * |\varphi_j|^2)\varphi_i - \frac{1}{N}\sum_{j=1}^N \left(w * (\varphi_i \bar{\varphi}_j)\right)\varphi_j\,. \tag{1.3}$$

Our main result (Theorems 6.1 and 6.2 below) is a precise formulation of this asymptotic behaviour.

Aside from the mathematical question of generalizing the result of [3] to singular potentials, this result is of some physical relevance when studying the dynamics of electrons of a large atom in the Born-Oppenheimer approximation. Consider an atom of atomic number N (commonly also denoted by Z). The nucleus has charge Ne, where e is the positive unit charge, and is surrounded by N electrons of charge $-e$. We assume that the nucleus is immobile; this is heuristically justified by the fact that the nucleus is much heavier than the electrons. The Hamiltonian of the electrons reads, in appropriately chosen units,

$$\sum_{i=1}^N \left(-\Delta_i - \frac{e^2 N}{|x_i|}\right) + \sum_{1 \leqslant i < j \leqslant N} \frac{e^2}{|x_i - x_j|}\,. \tag{1.4}$$

After conjugation with the unitary dilation defined by $x_i \mapsto N^{-1} x_i$ for all i, the Hamiltonian (1.4) becomes

$$N^2 \left[\sum_{i=1}^N \left(-\Delta_i - \frac{e^2}{|x_i|}\right) + \frac{1}{N}\sum_{1 \leqslant i < j \leqslant N} \frac{e^2}{|x_i - x_j|}\right],$$

which is of the form $N^2 H_N$. We conclude that our results describe the dynamics of atomic electrons at length scales of order N^{-1} and time scales of order N^{-2}. The approximation is therefore quite crude. For

instance in the Thomas-Fermi atom, most electrons are to be found at length scales of order $N^{-1/3}$, while the innermost electrons (K-shell, etc.) reside at length scales of order N^{-1}.

One problem in the above physical model, as well as in the works [1,8,9,11,13,14], is that, as N becomes large, relativistic effects should be taken into account. Indeed, a simple argument shows that the speeds of the innermost electrons are of order N. Another problem in applying the time-dependent Hartree-Fock theory to the dynamics of excited states is that the interaction with the radiation field is neglected. This interaction is responsible for the relaxation of excited states to the ground state of the atom.

A somewhat different physical scenario is an interacting Fermi gas confined to a box of fixed size. As discussed in [6, 15], the natural scaling in this situation may be viewed as a combination of mean-field and semiclassical scalings. This problem was first studied in [15, 18]. The authors show that the limiting dynamics is governed by the Vlasov equation. These results were sharpened in [6], where the authors compare the Hamiltonian dynamics with the dynamics of the Hartree equation, and derive estimates on the rate of convergence.

A further, physically very different, scenario studied in the literature is an interacting Fermi gas in the weak coupling regime. Here the limiting dynamics is given by a nonlinear Boltzmann equation. See for instance [7], in which a nonrigorous derivation is given for a model of interacting fermions on a lattice.

Finally, we outline the key ideas of our proof. It relies on the diagrammatic Schwinger-Dyson expansion and Kato smoothing estimates developed in [10]. The main steps are:

(a) Use the Schwinger-Dyson expansion to express the Hamiltonian time evolution of a p-particle observable.

(b) Show that, in the limit $N \to \infty$, only the tree terms of the Schwinger-Dyson expansion survive.

(c) Show that the time evolution of a p-particle observable under the Hartree-Fock equation converges to the tree terms of the Schwinger-Dyson series as $N \to \infty$.

Steps (a) and (b) have been addressed in [10]. Thus, the argument in this paper consists in doing step (c).

This article is organized as follows. In Section 2 we introduce the Hartree-Fock equation, discuss its Hamiltonian structure and prove a Schwinger-Dyson series for its time evolution. In Section 3 we rewrite the Hartree-Fock equation using density matrices. In Sections 4 and 5 we introduce second quantized notation and Slater determinants. After these preparations, we state our main result in Section 6. The proof is given in Section 7. Finally, Section 8 is devoted to a Egorov-type formulation of our main result, whereby the microscopic dynamics is recognized as a quantization of a classical "superhamiltonian" theory.

Conventions. In the following, the expression "$A(t)$ holds for small times" is understood to mean that there is a constant T such that $A(t)$ is true for all $|t| < T$. The precise value of T can always be inferred from the context. To simplify notation, we assume in the following that $t \geqslant 0$.

The norm of a Hilbert space $\mathcal{H}$ is denoted by $\|\cdot\|$. We denote by

$$\mathcal{H}_{\pm}^{(n)} := P_{\pm}\mathcal{H}^{\otimes n}$$

the symmetric/antisymmetric subspaces of the tensor product space $\mathcal{H}^{\otimes n}$. Here, $P_{\pm}$ is the orthogonal projector onto the symmetric/antisymmetric subspace. The Banach space of bounded operators on $\mathcal{H}$ with operator norm is denoted by $(\mathcal{L}(\mathcal{H}), \|\cdot\|)$, and the Banach space of trace-class operators on $\mathcal{H}$ with trace norm is denoted by $(\mathcal{L}^1(\mathcal{H}), \|\cdot\|_1)$.

We use the notation $a^{(p)}_{i_1\dots i_p} \in \mathcal{L}(\mathcal{H}^{\otimes n})$ to denote a p-particle operator $a^{(p)} \in \mathcal{L}(\mathcal{H}^{\otimes p})$ acting on the coordinates $x_{i_1}, \dots, x_{i_p}$ of n-particle space. Similarly, $\mathrm{Tr}_{i_1\dots i_p}$ denotes a partial trace over the p-particle space corresponding to the coordinates $x_{i_1}, \dots, x_{i_p}$.

A time subscript of the form $(\cdot)_t$ is always understood to mean time evolution up to time t of $(\cdot)$ with respect to the appropriate free dynamics. We shall explain this in greater detail whenever this notation is used.

The symbol C is reserved for a constant whose dependence on some parameters may be indicated. The value of C need not be the same from one equation to the next.

Acknowledgements. We would like to thank two referees for pointing out inaccuracies in an earlier version of this manuscript.

2. The Hartree-Fock equation

For simplicity of notation, we only consider spinless fermions in the following; the one-particle Hilbert space is $\mathcal{H} := L^2(\mathbb{R}^3, \mathrm{d}x) \equiv L^2(\mathbb{R}^3)$. Merely cosmetic modifications extend our results to the case of spin-s fermions for which the one-particle Hilbert space is $L^2(\mathbb{R}^3) \otimes \mathbb{C}^{2s+1}$. To fix ideas, we consider the free Hamiltonian $h := -\Delta$ and a Coulomb two-body interaction potential $w(x) := \kappa|x|^{-1}$. By a simple extension of the results of [10], Section 8, our results remain valid for a free Hamiltonian of the form $h = -\Delta + v$ and a two-body interaction potential w, where w is even and $v, w \in L^\infty(\mathbb{R}^3) + L^3_w(\mathbb{R}^3)$ are both real. Here, L^p_w denotes the weak L^p-space (see e.g. [16]). In particular, we may treat Hamiltonians of the form

$$\sum_{i=1}^{N} \left(-\Delta_i - \frac{e^2}{|x_i|} \right) + \frac{1}{N} \sum_{1 \leqslant i < j \leqslant N} \frac{e^2}{|x_i - x_j|} \,,$$

describing the dynamics of electrons in a large atom, as discussed in Section 1.

2.1. Some notation. It is convenient to state the time-dependent Hartree-Fock equation in terms of an infinite sequence of orbitals $\Phi = (\varphi_i)_{i \in \mathbb{N}}$ which is an element of the Hilbert space

$$\tilde{\mathcal{H}} \;:=\; l^2(\mathbb{N}; L^2(\mathbb{R}^3)) \;=\; l^2(\mathbb{N}) \otimes L^2(\mathbb{R}^3) \,.$$

To simplify notation, we set $\alpha = (x, i)$ and write $\Phi(\alpha) = \varphi_i(x)$. Furthermore, we abbreviate

$$\int \mathrm{d}\alpha \;:=\; \sum_{i \in \mathbb{N}} \int \mathrm{d}x \,, \qquad \delta(\alpha - \alpha') \;:=\; \delta_{ii'} \delta(x - x') \,.$$

The scalar product on $\tilde{\mathcal{H}}$ is then given by

$$\langle \Phi \,, \Phi' \rangle \;=\; \int \mathrm{d}\alpha \; \overline{\Phi(\alpha)} \Phi'(\alpha) \,.$$

Let $a^{(p)} \in \mathcal{L}(\mathcal{H}^{\otimes p})$ and define $\tilde{a}^{(p)} \in \mathcal{L}(\tilde{\mathcal{H}}^{\otimes p})$ through

$$\tilde{a}^{(p)} \;:=\; \mathbb{1}_{(l^2(\mathbb{N}))^{\otimes p}} \otimes a^{(p)} \,.$$

We have the identity

$$\|\tilde{a}^{(p)}\| \;=\; \|a^{(p)}\| \,. \tag{2.1}$$

Furthermore, one easily finds that

$$\left\langle \Phi^{\otimes p} \,, \tilde{a}^{(p)} \Phi^{\otimes p} \right\rangle \;=\; \sum_{i_1, \ldots, i_p \in \mathbb{N}} \left\langle \varphi_{i_1} \otimes \cdots \otimes \varphi_{i_p} \,, a^{(p)} \, \varphi_{i_1} \otimes \cdots \otimes \varphi_{i_p} \right\rangle . \tag{2.2}$$

2.2. Hamiltonian formulation of the Hartree-Fock equation. The time-dependent Hartree-Fock equation for the sequence Φ reads

$$\mathrm{i}\partial_t\varphi_i \;=\; h\varphi_i + \sum_{j\in\mathbb{N}}(w * |\varphi_j|^2)\varphi_i - \sum_{j\in\mathbb{N}}\left(w * (\varphi_i\bar{\varphi}_j)\right)\varphi_j\,. \tag{2.3}$$

We begin by noting that (2.3) is the Hamiltonian equation of motion of a classical Hamiltonian system with phase space $\Gamma := l^2(\mathbb{N}) \otimes H^1(\mathbb{R}^3)$.

Define the map $\mathbb{A}$, from closed operators $A^{(p)}$ on $\tilde{\mathcal{H}}_+^{(p)}$ to "polynomial" functions on phase space, through

$$\begin{aligned}\mathbb{A}(A^{(p)})(\Phi) \;&:=\; \left\langle \Phi^{\otimes p}, A^{(p)}\Phi^{\otimes p}\right\rangle \\ &=\; \int \mathrm{d}\alpha_1\cdots\mathrm{d}\alpha_p\,\mathrm{d}\beta_1\cdots\mathrm{d}\beta_p\,\overline{\Phi(\alpha_p)}\cdots\overline{\Phi(\alpha_1)}A^{(p)}(\alpha_1,\ldots,\alpha_p;\beta_1,\ldots,\beta_p)\,\Phi(\beta_1)\cdots\Phi(\beta_p)\,,\end{aligned}$$

where $A^{(p)}(\alpha_1,\ldots,\alpha_p;\beta_1,\ldots,\beta_p)$ is the distribution kernel of $A^{(p)}$ (see [10] for details). We denote by $\mathfrak{A}$ the linear hull of functions of the form $\mathbb{A}(A^{(p)})$, with $A^{(p)} \in \mathcal{L}(\tilde{\mathcal{H}}_+^{(p)})$.

The Hamilton function is given by

$$H \;:=\; \mathbb{A}(\tilde{h}) + \frac{1}{2}\mathbb{A}(\tilde{\mathcal{W}})\,, \tag{2.4}$$

where

$$\mathcal{W} \;:=\; W(\mathbb{1} - E)\,;$$

here $(E\Psi)(x_1,x_2) := \Psi(x_2,x_1)$ is the exchange operator and W is the two-particle operator defined by multiplication by $w(x_1-x_2)$. Written out in terms of components, (2.4) reads

$$H(\Phi) \;=\; \sum_{i\in\mathbb{N}}\langle\varphi_i\,, h\varphi_i\rangle + \frac{1}{2}\sum_{i,j\in\mathbb{N}}\left(\langle\varphi_i\otimes\varphi_j\,, W\,\varphi_i\otimes\varphi_j\rangle - \langle\varphi_i\otimes\varphi_j\,, W\,\varphi_j\otimes\varphi_i\rangle\right).$$

Using Sobolev-type inequalities, one readily sees that H is well-defined on Γ.

A short calculation shows that the Hartree-Fock equation is equivalent to

$$\mathrm{i}\partial_t\Phi \;=\; \partial_{\bar{\Phi}}H(\Phi)\,.$$

The symplectic form on Γ is given by

$$\omega \;=\; \mathrm{i}\int \mathrm{d}\alpha\;\mathrm{d}\overline{\Phi}(\alpha)\wedge\mathrm{d}\Phi(\alpha)\,,$$

which induces the Poisson bracket

$$\{\Phi(\alpha),\overline{\Phi}(\beta)\} \;=\; \mathrm{i}\delta(\alpha-\beta)\,,\qquad \{\Phi(\alpha),\Phi(\beta)\} \;=\; \{\overline{\Phi}(\alpha),\overline{\Phi}(\beta)\} \;=\; 0\,. \tag{2.5}$$

Thus, for two observables $A, B \in \mathfrak{A}$,

$$\{A,B\}(\Phi) \;=\; \mathrm{i}\int \mathrm{d}\alpha\;\left(\frac{\delta A}{\delta\Phi(\alpha)}(\Phi)\frac{\delta B}{\delta\overline{\Phi}(\alpha)}(\Phi) - \frac{\delta B}{\delta\Phi(\alpha)}(\Phi)\frac{\delta A}{\delta\overline{\Phi}(\alpha)}(\Phi)\right).$$

The Hamiltonian equation of motion on Γ is the Hartree-Fock equation (2.3).

The conservation laws of the Hartree-Fock flow can be understood in terms of symmetries of the Hamiltonian (2.4). One immediately sees that (2.4) is invariant under the rotation $\Phi \mapsto (U \otimes \mathbb{1}_{L^2(\mathbb{R}^3)})\Phi$, where $U \in \mathcal{L}(l^2(\mathbb{N}))$ is unitary. A one-parameter group of such unitary transformations is generated by linear combinations of the functions $\mathrm{Re}\langle\varphi_i\,,\varphi_j\rangle$ and $\mathrm{Im}\langle\varphi_i\,,\varphi_j\rangle$, which Poisson-commute with the Hamiltonian (2.4). By Noether's principle, it follows that $\langle\varphi_i\,,\varphi_j\rangle$ is (at least formally) conserved. The energy H is of course formally conserved as well.

In order to solve the Hartree-Fock equation (2.3) with initial state Φ, we rewrite it as an integral equation

$$\varphi_i(t) \;=\; \mathrm{e}^{-\mathrm{i}th}\varphi_i - \mathrm{i}\int_0^t \mathrm{d}s\; \mathrm{e}^{-\mathrm{i}(t-s)h} \sum_{j\in\mathbb{N}} \big((w * |\varphi_j(s)|^2)\varphi_i(s) - (w * (\varphi_i(s)\bar{\varphi}_j(s)))\,\varphi_j(s)\big)\,. \tag{2.6}$$

The Cauchy-problem for (2.6) was solved in [19]. We quote the relevant results:

LEMMA 2.1. *Let $\Phi \in \tilde{\mathcal{H}}$. Then (2.6) has a unique global solution $\Phi(\cdot) \in C(\mathbb{R};\tilde{\mathcal{H}})$. Furthermore, the quantities $\langle\varphi_i\,,\varphi_j\rangle$ are conserved. In particular, $\|\Phi(t)\| = \|\Phi\|$.*

2.3. A Schwinger-Dyson expansion for the Hartree-Fock equation. Our main tool is the Schwinger-Dyson expansion for the flow of the Hartree-Fock equation. We use the notation $(\cdot)_t$ to denote free time evolution generated by the free Hamiltonian $\mathbb{A}(\tilde{h})$. Explicitly,

$$A_t(\varphi_1,\varphi_2,\dots) \;=\; A\big(\mathrm{e}^{-\mathrm{i}th}\varphi_1, \mathrm{e}^{-\mathrm{i}th}\varphi_2,\dots\big)\,.$$

LEMMA 2.2. *Let $A \in \mathfrak{A}$, $\nu > 0$, and $\Phi(t)$ be the solution of (2.6) with initial data $\Phi \in \tilde{\mathcal{H}}$. Then, for small times t, we have that*

$$\begin{aligned} A(\Phi(t)) \;&=\; A_t(\Phi) + \int_0^t \mathrm{d}s\; \frac{1}{2}\big\{\mathbb{A}(\tilde{\mathcal{W}}), A_{t-s}\big\}(\Phi(s)) \\ &=\; \sum_{k=0}^{\infty} \frac{1}{2^k} \int_{\Delta^k(t)} \mathrm{d}\underline{t}\, \Big\{\mathbb{A}(\tilde{\mathcal{W}}_{t_k}), \dots \big\{\mathbb{A}(\tilde{\mathcal{W}}_{t_1}), A_t\big\}\Big\}(\Phi)\,, \end{aligned}$$

uniformly for $\Phi \in B_\nu := \{\Phi \in \tilde{\mathcal{H}} \,:\, \|\Phi\|^2 \leqslant \nu\}$.

PROOF. The proof of Lemma 7.1 in [10] applies with virtually no modifications. One uses (2.1), the identity

$$\mathbb{A}(\tilde{\mathcal{W}})_t \;=\; \mathbb{A}(\tilde{\mathcal{W}}_t) \;=\; \mathbb{A}\big((W_t(\mathbb{1}-E))\tilde{}\,\big)\,,$$

and $\|E\| = 1$. □

3. The density matrix Hartree-Fock equation

From now on, we only work with orthogonal sequence of orbitals belonging to the set

$$\mathcal{K} \;:=\; \{\Phi \in \tilde{\mathcal{H}} \,:\, \langle\varphi_i\,,\varphi_j\rangle = 0 \text{ for } i \neq j\}\,.$$

By Lemma 2.1, $\Phi \in \mathcal{K}$ implies that $\Phi(t) \in \mathcal{K}$ for all t. To each sequence of orbitals Φ we assign a one-particle density matrix

$$\gamma_\Phi \;:=\; \sum_{i\in\mathbb{N}} |\varphi_i\rangle\langle\varphi_i|\,. \tag{3.1}$$

It is easy to see that this defines a mapping from $\mathcal{K}$ onto the set of density matrices

$$\mathcal{D} \;:=\; \big\{\gamma \in \mathcal{L}^1(\mathcal{H}) \,:\, \gamma \geqslant 0\big\}\;.$$

Furthermore,

$$\|\gamma_\Phi\|_1 \;=\; \|\Phi\|^2\,.$$

Conversely, one may recover Φ from γ_Φ, up to ordering of the orbitals, by spectral decomposition. Also, (2.2) implies that

$$\mathbb{A}(\tilde{a}^{(p)})(\Phi) \;=\; \mathrm{Tr}(a^{(p)}\gamma_\Phi^{\otimes p})\,. \tag{3.2}$$

Next, we note that the Hartree-Fock equation may be formulated in terms of density matrices. Let $\Phi(t)$ be a solution of the Hartree-Fock equation (2.3), and abbreviate

$$\gamma(t) \;=\; \gamma_{\Phi(t)}\,.$$

Then a short calculation shows that

$$\mathrm{i}\partial_t\gamma \;=\; [h,\gamma] + \mathrm{Tr}_2\,[\mathcal{W},\gamma\otimes\gamma]\;, \tag{3.3}$$

which is the Hartree-Fock equation for density matrices. As an integral equation in the interaction picture, this reads

$$\gamma(t) \;=\; \mathrm{e}^{-\mathrm{i}th}\,\gamma\,\mathrm{e}^{\mathrm{i}th} - \mathrm{i}\int_0^t \mathrm{d}s\;\mathrm{e}^{-\mathrm{i}(t-s)h}\;\mathrm{Tr}_2\,[\mathcal{W},\gamma(s)\otimes\gamma(s)]\;\mathrm{e}^{\mathrm{i}(t-s)h}\,. \tag{3.4}$$

Sometimes it is convenient to rewrite this using the shorthand

$$\tilde{\gamma}(t) \;:=\; \mathrm{e}^{\mathrm{i}th}\,\gamma(t)\,\mathrm{e}^{-\mathrm{i}th}\,. \tag{3.5}$$

Then (3.4) is equivalent to

$$\tilde{\gamma}(t) \;=\; \gamma - \mathrm{i}\int_0^t \mathrm{d}s\;\mathrm{Tr}_2\,[\mathcal{W}_s,\tilde{\gamma}(s)\otimes\tilde{\gamma}(s)]\;. \tag{3.6}$$

The next lemma ensures that if $\Phi(t)$ is a general solution of the integral Hartree-Fock equation (2.6) then $\gamma_{\Phi(t)}$ solves the integral density matrix equation (3.4).

LEMMA 3.1. *Let $\Phi(t)$ be the solution of* (2.6)*. Then $\gamma_{\Phi(t)}$ solves* (3.4)*.*

PROOF. Let $a^{(1)} \equiv a \in \mathcal{L}(\mathcal{H})$. From Lemma 2.2 we get

$$\mathbb{A}(\tilde{a})(\Phi(t)) \;=\; \mathbb{A}(\tilde{a}_t)(\Phi) + \int_0^t \mathrm{d}s\;\big\{\mathbb{A}(\tilde{\mathcal{W}}),\mathbb{A}(\tilde{a}_{t-s})\big\}(\Phi(s))\,. \tag{3.7}$$

Now (2.5) and (3.2) imply

$$\begin{aligned}\big\{\mathbb{A}(\tilde{\mathcal{W}}),\mathbb{A}(\tilde{a})\big\}(\Phi) \;&=\; \mathrm{i}\mathbb{A}\big(\big[\tilde{\mathcal{W}},\tilde{a}\otimes\mathbb{1}\big]\big)(\Phi)\\ &=\; \mathrm{i}\,\mathrm{Tr}\big(\big[\mathcal{W},a\otimes\mathbb{1}\big]\gamma_\Phi\otimes\gamma_\Phi\big)\\ &=\; -\mathrm{i}\,\mathrm{Tr}\big((a\otimes\mathbb{1})\big[\mathcal{W},\gamma_\Phi\otimes\gamma_\Phi\big]\big)\,.\end{aligned}$$

Thus (3.7) reads

$$\begin{aligned}\mathrm{Tr}(a\,\gamma_{\Phi(t)}) \;&=\; \mathrm{Tr}(a_t\,\gamma_\Phi) - \mathrm{i}\int_0^t \mathrm{d}s\;\mathrm{Tr}\big((a_{t-s}\otimes\mathbb{1})\big[\mathcal{W},\gamma_{\Phi(s)}\otimes\gamma_{\Phi(s)}\big]\big)\\ &=\; \mathrm{Tr}\big(a\,\mathrm{e}^{\mathrm{i}th}\gamma_\Phi\mathrm{e}^{-\mathrm{i}th}\big) - \mathrm{i}\int_0^t \mathrm{d}s\;\mathrm{Tr}\Big(a\,\mathrm{e}^{-\mathrm{i}(t-s)h}\;\mathrm{Tr}_2\,\big[\mathcal{W},\gamma_{\Phi(s)}\otimes\gamma_{\Phi(s)}\big]\;\mathrm{e}^{\mathrm{i}(t-s)h}\Big)\,.\end{aligned}$$

Since $a \in \mathcal{L}(\mathcal{H})$ was arbitrary, this is equivalent to (3.4). □

4. Second quantization

For the following it is convenient to use second quantized notation; see e.g. [4] and [10] for a full account. We introduce the fermionic Fock space

$$\mathcal{F} \,:=\, \bigoplus_{N\geqslant 0} \mathcal{H}_-^{(N)}\,,$$

where we adopt the usual convention that $\mathcal{H}_-^{(0)} = \mathbb{C}$. A vector $\Psi \in \mathcal{F}$ is a sequence $\Psi = (\Psi_0, \Psi_1, \Psi_2, \dots)$ with $\Psi_N \in \mathcal{H}_-^{(N)}$ for all N. By a slight abuse of notation, we often identify an N-particle vector $\Psi_N \in \mathcal{H}_-^{(N)}$ with the vector in Fock space whose N-particle component equals Ψ_N and whose other components vanish.

On $\mathcal{F}$ act the usual fermionic creation and annihilation operators, a^* and a, which map the one-particle space into densely defined closable operators on $\mathcal{F}$. For $\varphi \in \mathcal{H}$ and $\Psi \in \mathcal{F}$, they are defined by

$$\begin{aligned}
\big(a^*(\varphi)\Phi\big)_N(x_1,\dots,x_N) \,&:=\, \frac{1}{\sqrt{N}} \sum_{i=1}^{N} (-1)^{i+1} \varphi(x_i) \Psi_{N-1}(x_1,\dots,x_{i-i},x_{i+1},\dots,x_N)\,,\\
\big(a(\varphi)\Phi\big)_N(x_1,\dots,x_N) \,&:=\, \sqrt{N+1} \int \mathrm{d}y\, \overline{\varphi(y)} \Psi_{N+1}(y,x_1,\dots,x_N)\,.
\end{aligned}$$

It is not hard to see that $a^*(\varphi)$ and $a(\varphi)$ are each other's adjoints. Moreover, they satisfy the canonical anticommutation relations

$$\big[a(\varphi)\,, a^*(\varphi')\big]_+ \;=\; \langle \varphi, \varphi' \rangle\,, \qquad \big[a^\sharp(\varphi)\,, a^\sharp(\varphi')\big]_+ \;=\; 0\,,$$

where $[A\,,B]_+ := AB + BA$ is the anticommutator and $a^\sharp$ stands for either a^* or a.

Define the operator-valued distributions $a^*(x) := a^*(\delta_x)$ and $a(x) := a(\delta_x)$, where δ_x is Dirac's delta function centred at x. In other words,

$$a^*(\varphi) \;=\; \int \mathrm{d}x\; \varphi(x)\, a^*(x)\,, \qquad a(\varphi) \;=\; \int \mathrm{d}x\; \overline{\varphi(x)}\, a(x)\,.$$

To streamline notation, it is convenient to introduce the rescaled creation and annihilation operators, defined by

$$a_\nu^\sharp(x) \;:=\; \frac{1}{\sqrt{\nu}}\, a^\sharp(x)\,.$$

Here $\nu > 0$ is a parameter that will ultimately be taken to equal N, the number of particles.

Let $a^{(p)} \in \mathcal{L}(\mathcal{H}^{(p)})$ and define its second quantization $\widehat{\mathbb{A}}_\nu(a^{(p)})$, a closed operator on $\mathcal{F}$, through

$$\widehat{\mathbb{A}}_\nu(a^{(p)}) \;:=\; \int \mathrm{d}x_1 \cdots \mathrm{d}x_p\, \mathrm{d}y_1 \cdots \mathrm{d}y_p\, a_\nu^*(x_p) \cdots a_\nu^*(x_1)\, a^{(p)}(x_1,\dots,x_p;y_1,\dots,y_p)\, a_\nu(y_1) \cdots a_\nu(y_p)\,,$$

where $a^{(p)}(x_1,\dots,x_p;y_1,\dots,y_p)$ denotes the distribution kernel of $a^{(p)}$. Explicitly, $\widehat{\mathbb{A}}_\nu(a^{(p)})$ is given by (see [10])

$$\widehat{\mathbb{A}}_\nu(a^{(p)})\Big|_{\mathcal{H}_-^{(N)}} \;=\; \begin{cases} \frac{p!}{\nu^p} \binom{N}{p} P_-(a^{(p)} \otimes \mathbb{1}^{(N-p)}) P_- & \text{if } N \geqslant p \\ 0 & \text{if } N < p\,, \end{cases} \tag{4.1}$$

which may be viewed as an alternative definition of $\widehat{\mathbb{A}}_\nu(a^{(p)})$. In particular, when restricted to $\mathcal{H}_-^{(N)}$, the operator $\widehat{\mathbb{A}}_N(a^{(p)})$ is of order one as $N \to \infty$.

5. Slater determinants

Next, we introduce quasi-free states (see [4] for more details). Their importance for our purposes stems from the fact that the Hartree-Fock equation naturally describes the time evolution of quasi-free states. Let $\gamma \in \mathcal{D}$ be a one-particle density matrix. The *quasi-free state* ω_γ associated with γ satisfies by definition

$$\gamma^{(p)}(x_1, \dots, x_p; y_1, \dots, y_p) \;=\; \det\left(\gamma(x_i; y_j)\right)_{i,j} \,,$$

where

$$\gamma^{(p)}(x_1, \dots, x_p; y_1, \dots, y_p) \;:=\; \omega_\gamma\big(a^*(y_p) \cdots a^*(y_1) a(x_1) \cdots a(x_p)\big)$$

is the reduced p-particle density matrix of ω_γ. In other words, $\gamma^{(p)}$ is the operator kernel of

$$\gamma^{(p)} \;=\; \gamma^{\otimes p}\, \Sigma_-^{(p)} \,, \tag{5.1}$$

where

$$\Sigma_-^{(p)} \;:=\; p! P_-^{(p)} \,.$$

For the following calculations it is convenient to introduce the symbol $\varepsilon_{i_1 \dots i_p}^{j_1 \dots j_p}$, which is equal to $\operatorname{sgn}\sigma$ if $i_1, \dots, i_p$ are disjoint and there is a permutation $\sigma \in S_p$ such that $(i_1, \dots, i_p) = (j_{\sigma(1)}, \dots, j_{\sigma(p)})$, and equal to 0 otherwise. Also, for the remainder of this section, summation over any index appearing twice in an equation is implied.

Lemma 5.1. *Let $\gamma \in \mathcal{D}$ with $\operatorname{Tr}\gamma = 1$. Then $\operatorname{Tr}\gamma^{(p)} \leqslant 1$.*

Proof. There is an orthonormal basis $(\varphi_i)_{i\in\mathbb{N}}$ and a sequence of nonnegative numbers $(\lambda_i)_{i\in\mathbb{N}}$ such that $\sum_i \lambda_i = 1$ and $\gamma = \sum_i \lambda_i |\varphi_i\rangle\langle\varphi_i|$. Therefore,

$$\gamma^{(p)} \;=\; \varepsilon_{i_1 \dots i_p}^{j_1 \dots j_p} \lambda_{i_1} \cdots \lambda_{i_p} |\varphi_{i_1} \otimes \cdots \otimes \varphi_{i_p}\rangle\langle\varphi_{j_1} \otimes \cdots \otimes \varphi_{j_p}|$$

This yields

$$\begin{aligned} \operatorname{Tr}\gamma^{(p)} \;&=\; \varepsilon_{i_1 \dots i_p}^{j_1 \dots j_p} \lambda_{i_1} \cdots \lambda_{i_p} \delta_{i_1 k_1} \cdots \delta_{i_p k_p} \delta_{j_1 k_1} \cdots \delta_{j_p k_p} \\ &=\; \sum_{i_1, \dots, i_p \text{ disjoint}} \lambda_{i_1} \cdots \lambda_{i_p} \\ &\leqslant\; \sum_{i_1, \dots, i_p} \lambda_{i_1} \cdots \lambda_{i_p} \;=\; 1 \,. \end{aligned}$$

□

Next, we introduce a special class of quasi-free states, described by *Slater determinants*. Take an orthonormal sequence of orbitals $\Phi = (\varphi_i)_{i\in\mathbb{N}}$ and denote by $\Phi^{(N)}$ the truncated sequence $(\varphi_1, \dots, \varphi_N, 0, \dots)$. We define the N-particle Slater determinant as

$$S(\Phi^{(N)}) \;:=\; \varphi_1 \wedge \cdots \wedge \varphi_N \;=\; \frac{1}{\sqrt{N!}} a^*(\varphi_N) \cdots a^*(\varphi_1)\Omega \;=\; \sqrt{N!}\, P_-^{(N)}\, \varphi_1 \otimes \cdots \otimes \varphi_N \;\in\; \mathcal{H}_-^{(N)} \,.$$

Note that the normalization is chosen so that $\|S(\Phi^{(N)})\| = 1$. The corresponding N-particle density matrix is

$$\Gamma_N \;:=\; |S(\Phi^{(N)})\rangle\langle S(\Phi^{(N)})| \,.$$

The p-particle marginals of Γ_N are given by

$$\begin{aligned}\Gamma_N^{(p)} &:= \operatorname{Tr}_{p+1\dots N}\Gamma_N \\ &= \operatorname{Tr}_{p+1\dots N}\frac{1}{N!}\,\varepsilon_{i_1\dots i_N}\varepsilon_{j_1\dots j_N}\left|\varphi_{i_1}\otimes\cdots\otimes\varphi_{i_N}\right\rangle\left\langle\varphi_{j_1}\otimes\cdots\otimes\varphi_{j_N}\right| \\ &= \frac{(N-p)!}{N!}\,\varepsilon_{i_1\dots i_p}^{j_1\dots j_p}\left|\varphi_{i_1}\otimes\cdots\otimes\varphi_{i_p}\right\rangle\left\langle\varphi_{j_1}\otimes\cdots\otimes\varphi_{j_p}\right|. \end{aligned} \tag{5.2}$$

In particular,

$$\Gamma_N^{(1)} \;=\; \frac{1}{N}\sum_{i=1}^{N}|\varphi_i\rangle\langle\varphi_i| \;=\; \gamma_N\,, \tag{5.3}$$

where γ_N is the one-particle density matrix associated (by (3.1)) with the normalized truncated sequence

$$\tilde{\Phi}^{(N)} \;:=\; \frac{1}{\sqrt{N}}\Phi^{(N)}\,.$$

Thus, the explicit forms (5.1) and (5.2) imply a relation between the reduced density matrices and the marginals:

$$\gamma_N^{(p)} \;=\; \frac{1}{N^p}\,\varepsilon_{i_1\dots i_p}^{j_1\dots j_p}\left|\varphi_{i_1}\otimes\cdots\otimes\varphi_{i_p}\right\rangle\left\langle\varphi_{j_1}\otimes\cdots\otimes\varphi_{j_p}\right| \;=\; \frac{p!}{N^p}\binom{N}{p}\Gamma_N^{(p)}\,. \tag{5.4}$$

In other words, Slater determinants determine quasi-free states by their p-particle marginals. The normalization $\frac{p!}{N^p}\binom{N}{p}$ differs slightly from the usual normalization 1 of quasi-free states, but in the limit $N\to\infty$ this difference vanishes. Recalling (4.1), we see from (5.4) that

$$\left\langle S(\Phi^{(N)}), \widehat{\mathbb{A}}_N(a^{(p)})S(\Phi^{(N)})\right\rangle \;=\; \operatorname{Tr}\big(a^{(p)}\gamma_N^{(p)}\big)\,. \tag{5.5}$$

We also note that

$$\|\gamma_N\| \;=\; \frac{1}{N}\,. \tag{5.6}$$

This is a special case of the well-known statement (see e.g. [12]) that $\left\|\operatorname{Tr}_{2\dots N}\Gamma\right\| \leqslant N^{-1}$, for any fermionic N-particle density matrix Γ [2]. The estimate (5.6) will play a fundamental role in our analysis.

Finally, we remark that the sequence $\Phi^{(N)}(t)$ satisfies the rescaled Hartree-Fock equation (1.3) if and only if the normalized sequence $\tilde{\Phi}^{(N)}(t)$ satisfies the unrescaled Hartree-Fock equation (2.3). Similarly, $\tilde{\Phi}^{(N)}(t)$ is a solution of the integral equation (2.6) if and only if $\Phi^{(N)}(t)$ is a solution of the rescaled integral equation

$$\varphi_i(t) \;=\; \mathrm{e}^{-\mathrm{i}th}\varphi_i - \frac{\mathrm{i}}{N}\int_0^t \mathrm{d}s\;\mathrm{e}^{-\mathrm{i}(t-s)h}\sum_{j=1}^{N}\big((w*|\varphi_j(s)|^2)\varphi_i(s) - (w*(\varphi_i(s)\bar{\varphi}_j(s)))\,\varphi_j(s)\big)\,. \tag{5.7}$$

6. The limit and main result

We may now state our main result. Take an infinite sequence $\Phi=(\varphi_i)_{i\in\mathbb{N}}$ of orthonormal orbitals, and denote the truncated sequences by $\Phi^{(N)}$. Let $\Phi^{(N)}(t)$ be the solution of the rescaled integral Hartree-Fock equation (5.7) with initial data $\Phi^{(N)}$.

[2] This can also be inferred from (5.6) by writing Γ as a linear combination of projectors.

THEOREM 6.1. *Let $p \in \mathbb{N}$ and $a^{(p)} \in \mathcal{L}(\mathcal{H}_-^{(p)})$. Then, for any $t \in \mathbb{R}$, we have*

$$\left\langle \mathrm{e}^{-\mathrm{i}tH_N} S(\Phi^{(N)}) \,,\, \widehat{\mathbb{A}}_N(a^{(p)})\, \mathrm{e}^{-\mathrm{i}tH_N} S(\Phi^{(N)}) \right\rangle - \left\langle S\big(\Phi^{(N)}(t)\big) \,,\, \widehat{\mathbb{A}}_N(a^{(p)}) S\big(\Phi^{(N)}(t)\big) \right\rangle \;\longrightarrow\; 0$$

as $N \to \infty$.

We may also express our main result in terms of density matrices. Denote by

$$\Gamma_N(t) \;:=\; \mathrm{e}^{-\mathrm{i}tH_N} \left|S(\Phi^{(N)})\right\rangle\!\left\langle S(\Phi^{(N)})\right| \mathrm{e}^{\mathrm{i}tH_N}$$

the N-particle density matrix evolved in time using the N-body dynamics. Similarly, denote by

$$\tilde{\Gamma}_N(t) \;:=\; \left|S\big(\Phi^{(N)}(t)\big)\right\rangle\!\left\langle S\big(\Phi^{(N)}(t)\big)\right|$$

the N-particle density matrix evolved in time using the Hartree-Fock dynamics. Denote by $\Gamma_N^{(p)}(t)$ and $\tilde{\Gamma}_N^{(p)}(t)$ their respective p-particle marginals.

THEOREM 6.2. *Let $p \in \mathbb{N}$. Then, for any $t \in \mathbb{R}$, we have*

$$\lim_{N\to\infty} \left\| \Gamma_N^{(p)}(t) - \tilde{\Gamma}_N^{(p)}(t) \right\|_1 \;=\; 0\,.$$

REMARK 6.3. *The limit $N \to \infty$ of $\Gamma_N^{(p)}(t)$ does not exist in $\|\cdot\|_1$. Indeed, $\lim_{N\to\infty} \|\Gamma_N^{(p)}(t)\| = 0$ but $\operatorname{Tr} \Gamma_N^{(p)}(t) = 1$ (similarly for $\tilde{\Gamma}_N^{(p)}(t)$).*

REMARK 6.4. *As mentioned in the beginning of Section 2, both Theorems 6.1 and 6.2 extend trivially to the case of spin-s fermions. In that case, we replace the space $\tilde{\mathcal{H}}$ from Section 2 with the space $l^2(\mathbb{N}) \otimes L^2(\mathbb{R}^3; \mathbb{C}^{2s+1})$. Thus, $\alpha = (x, \sigma, i)$ where $\sigma = -s, -s+1, \ldots, s$ denotes the spin index. Vectors $\Phi = (\varphi_i) \in \tilde{\mathcal{H}}$ are now sequences of wave functions $\varphi_i \equiv \varphi_i(x, \sigma)$ which also depend on the spin index σ. The exchange operator E acts in the natural way: $(E\Psi)(x_1, \sigma_1; x_2, \sigma_2) = \Psi(x_2, \sigma_2; x_1, \sigma_1)$. With these minor modifications, the statements and proofs of Theorems 6.1 and 6.2 may be taken over verbatim.*

REMARK 6.5. *As in [10], one can show that the rate of convergence in Theorems 6.1 and 6.2 is a power law $N^{-\beta(t)}$, with $\beta(t) > 0$ for all t. However, $\beta(t) \to 0$ as $t \to \infty$. Our bound on the rate of convergence is therefore far from the expected optimal rate $\beta(t) = 1$, which we only obtain for short times.*

7. Proof of Theorems 6.1 and 6.2

The main tool of our proof is the graph expansion scheme developed in [10].

7.1. The Schwinger-Dyson graph expansion. For the convenience of the reader we summarize the relevant results of the graph expansion in [10]. For details and proofs we refer to [10].

Let $a^{(p)} \in \mathcal{L}(\mathcal{H}_-^{(p)})$. From now on, we restrict all operators on $\mathcal{F}$ to $\mathcal{H}_-^{(N)}$; in particular, we understand expressions of the form $\widehat{\mathbb{A}}_N(a^{(p)})$ to mean $\widehat{\mathbb{A}}_N(a^{(p)})\big|_{\mathcal{H}_-^{(N)}}$. We start with the Schwinger-Dyson series for the time-evolved operator $\mathrm{e}^{\mathrm{i}tH_N} \widehat{\mathbb{A}}_N(a^{(p)}) \mathrm{e}^{-\mathrm{i}tH_N}$. We write

$$H_N \;=\; N\left[\widehat{\mathbb{A}}_N(h) + \frac{1}{2}\widehat{\mathbb{A}}_N(W)\right],$$

and regard the second term as a perturbation. Thus we get the series expansion

$$\mathrm{e}^{\mathrm{i}tH_N}\,\widehat{\mathbb{A}}_N(a^{(p)})\,\mathrm{e}^{-\mathrm{i}tH_N} \;=\; \sum_{k=0}^{\infty}\int_{\Delta^k(t)}\mathrm{d}\underline{t}\;\frac{(\mathrm{i}N)^k}{2^k}\Big[\widehat{\mathbb{A}}_N(W_{t_k}),\ldots\Big[\widehat{\mathbb{A}}_N(W_{t_1}),\widehat{\mathbb{A}}_N(a_t^{(p)})\Big]\ldots\Big]\,, \tag{7.1}$$

where $\underline{t}=(t_1,\ldots,t_k)$ and $\Delta^k(t)$ is the k-simplex $\{(t_1,\ldots,t_k):0<t_k<\cdots<t_1<t\}$. Here, as before, a time subscript refers to free time evolution:

$$a_t^{(p)} \;:=\; \mathrm{e}^{\mathrm{i}\sum_i h_i t}\,a^{(p)}\,\mathrm{e}^{-\mathrm{i}\sum_i h_i t}\,.$$

In [10] it was shown how the normal ordering of the multiple commutators in (7.1) gives rise to terms that can be classified graphically. The graph expansion reads

$$\mathrm{e}^{\mathrm{i}tH_N}\,\widehat{\mathbb{A}}_N(a^{(p)})\,\mathrm{e}^{-\mathrm{i}tH_N} \;=\; \sum_{k=0}^{\infty}\sum_{l=0}^{k}\frac{1}{N^l}\,\widehat{\mathbb{A}}_N\big(G_t^{(k,l)}(a^{(p)})\big)\,. \tag{7.2}$$

The $(p+k-l)$-particle operator $G_t^{(k,l)}(a^{(p)})$ corresponds to the sum of all l-loop graphs contributing to the multiple commutator of order k. Explicitly, it is given by

$$G_t^{(k,l)}(a^{(p)}) \;:=\; \int_{\Delta^k(t)}\mathrm{d}\underline{t}\;G_{t,\underline{t}}^{(k,l)}(a^{(p)})\,, \tag{7.3}$$

where the operators $G_{t,\underline{t}}^{(k,l)}(a^{(p)})$ are recursively defined by

$$\begin{aligned}G_{t,t_1,\ldots,t_k}^{(k,l)}(a^{(p)}) \;&=\; \mathrm{i}P_-\sum_{i=1}^{p+k-l-1}\Big[W_{i\,p+k-l,t_k},G_{t,t_1,\ldots,t_{k-1}}^{(k-1,l)}(a^{(p)})\otimes\mathbb{1}\Big]P_-\\ &\quad+\mathrm{i}P_-\sum_{1\leqslant i<j\leqslant p+k-l}\Big[W_{ij,t_k},G_{t,t_1,\ldots,t_{k-1}}^{(k-1,l-1)}(a^{(p)})\Big]P_-\,,\end{aligned} \tag{7.4}$$

as well as $G_t^{(0,0)}(a^{(p)}):=a_t^{(p)}$. If $l<0$ or $l>k$ then $G_{t,t_1,\ldots,t_k}^{(k,l)}(a^{(p)})=0$.

As a sum over graphs[3], $G_t^{(k,l)}(a^{(p)})$ reads

$$G_t^{(k,l)}(a^{(p)}) \;=\; \frac{\mathrm{i}^k}{2^k}\sum_{\mathcal{Q}\in\mathscr{Q}(p,k,l)}i_{\mathcal{Q}}\int_{\Delta_{\mathcal{Q}}^k(t)}\mathrm{d}\underline{t}\;G_{t,t_1,\ldots,t_k}^{(k,l)(\mathcal{Q})}(a^{(p)})\,, \tag{7.5}$$

where $i_{\mathcal{Q}}\in\{0,1\}$, $\Delta_{\mathcal{Q}}^k(t)\subset[0,t]^k$, and $\mathscr{Q}(p,k,l)$ is a set of graphs whose cardinality satisfies

$$|\mathscr{Q}(p,k,l)| \;\leqslant\; 2^k\binom{k}{l}\binom{2p+3k}{k}\,(p+k-l)^l\,. \tag{7.6}$$

The operator $G_{t,t_1,\ldots,t_k}^{(k,l)(\mathcal{Q})}(a^{(p)})$ is an *elementary term*, indexed by the graph $\mathcal{Q}$, of the form

$$P_-\,W_{i_1j_1,t_{v_1}}\cdots W_{i_rj_r,t_{v_r}}\,\big(a_t^{(p)}\otimes\mathbb{1}^{(k-l)}\big)\,W_{i_{r+1}j_{r+1},t_{v_{r+1}}}\cdots W_{i_kj_k,t_{v_k}}P_-\,, \tag{7.7}$$

[3]called graph structures in [10]

where $r = 0, \dots, k$ and $(t_{v_1}, \dots, t_{v_k})$ is some permutation of $(t_1, \dots, t_k)$.

The operator norm of $G_t^{(k,l)}(a^{(p)})$ may now be bounded using the dispersive estimate

$$\int \mathrm{d}t \, \big\| |x|^{-1} \mathrm{e}^{\mathrm{i}t\Delta} \psi \big\|^2 \;\leqslant\; \pi \|\psi\|^2 \,. \tag{7.8}$$

Going to centre of mass coordinates and using Cauchy-Schwarz, one sees that (7.8) implies

$$\int_0^t \mathrm{d}s \, \big\| W_{ij,s} \, \varphi \big\| \;\leqslant\; \sqrt{\frac{\pi\kappa^2 t}{2}} \, \|\varphi\| \,. \tag{7.9}$$

Recalling the estimate (7.6), it is now easy to argue, as in [10], that (7.2) converges uniformly in N for small times t. Moreover, the large-N asymptotics of the Schwinger-Dyson series (7.2) is given by the tree terms: for small times t we have

$$\mathrm{e}^{\mathrm{i}tH_N} \, \widehat{\mathbb{A}}_N(a^{(p)}) \, \mathrm{e}^{-\mathrm{i}tH_N} \;=\; \sum_{k=0}^{\infty} \widehat{\mathbb{A}}_N\big(G_t^{(k,0)}(a^{(p)})\big) + L_N(t) \,, \tag{7.10}$$

where $L_N(t)$, corresponding to the sum of all terms with at least one loop ($l \geqslant 1$), satisfies the estimate

$$\|L_N(t)\| \;\leqslant\; C(p, \kappa, t) \|a^{(p)}\| N^{-1} \,, \tag{7.11}$$

for small times t.

7.2. Convergence of the Hartree-Fock time evolution to the tree terms. We now give the main argument of our proof. We show that the Hartree-Fock time evolution is asymptotically ($N \to \infty$) given by the tree terms (i.e. the terms $l = 0$) of the Schwinger-Dyson series (7.2). This result is summarized in Lemma 7.2 below.

The main idea of the proof is to iterate the integral Hartree-Fock equation so as to obtain a Schwinger-Dyson-type series. If iterated, the Hartree-Fock evolution of the observable $\widehat{\mathbb{A}}_N(a^{(p)})$ yields a power series expansion that *differs* from the tree expansion

$$\sum_{k=0}^{\infty} \widehat{\mathbb{A}}_N\big(G_t^{(k,0)}(a^{(p)})\big) \,.$$

Thus, at each step of the iteration we extract an error term, and continue the iteration on what remains. This is done in such a way that the resulting power series is equal to the tree expansion. The main work is to estimate the error terms arising at each step of the iteration. This is done by using a tree expansion combined with the dispersive estimate (7.9).

We work with the density matrix formulation (3.4) of the Hartree-Fock equation. We seek an expansion for the quantity

$$\big\langle S(\Phi^{(N)}(t)) \,, \widehat{\mathbb{A}}_N(a^{(p)}) S(\Phi^{(N)}(t)) \big\rangle \;=\; \mathrm{Tr}\big(a^{(p)} \gamma_N^{(p)}(t)\big) \,; \tag{7.12}$$

see (5.5). In this subsection, the special form (5.3) of γ_N is unimportant. We therefore assume that we have an arbitrary orthogonal sequence $\Phi = (\varphi_i)_{i \in \mathbb{N}} \in \mathcal{K}$, and denote by $\Phi(t)$ the solution of the Hartree-Fock equation (2.6) with initial data Φ. Let $\gamma(t) := \gamma_{\Phi(t)}$ be the associated one-particle density matrix.

By choosing $A = \mathbb{A}(\tilde{a}^{(p)})$, $a^{(p)} \in \mathcal{L}(\mathcal{H}_-^{(p)})$, in Lemma 2.2 and mimicking the proof of Lemma 3.1 one finds that

$$\mathrm{Tr}\big(a^{(p)} \, \gamma(t)^{\otimes p}\big) \;=\; \mathrm{Tr}\big(a_t^{(p)} \gamma^{\otimes p}\big) - \mathrm{i} \int_0^t \mathrm{d}s \sum_{i=1}^{p} \mathrm{Tr}\Big(a_{t-s}^{(p)} \, \mathrm{Tr}_{p+1}\big[\mathcal{W}_{i \; p+1}, \gamma(s)^{\otimes (p+1)}\big]\Big) \,. \tag{7.13}$$

It is convenient to use the representation $\tilde{\gamma}(t)$ defined in (3.5). Using the substitution $a^{(p)} \mapsto a^{(p)}_{-t}$ in (7.13), we get

$$\mathrm{Tr}\big(a^{(p)}\,\tilde{\gamma}(t)^{\otimes p}\big) \;=\; \mathrm{Tr}\big(a^{(p)}\gamma^{\otimes p}\big) - \mathrm{i}\int_0^t \mathrm{d}s \sum_{i=1}^{p} \mathrm{Tr}\Big(a^{(p)}\,\mathrm{Tr}_{p+1}\big[\mathcal{W}_{i\;p+1,s}, \tilde{\gamma}(s)^{\otimes(p+1)}\big]\Big)\,,$$

where, we recall,

$$\tilde{\gamma}(t) \;:=\; \mathrm{e}^{\mathrm{i}th}\,\gamma(t)\,\mathrm{e}^{-\mathrm{i}th}\,.$$

Recall that $\mathcal{W}_{ij} = W_{ij}(\mathbb{1} - E_{ij})$. Also, E_{ij} commutes with W_{ij} and with $\tilde{\gamma}(s)^{\otimes(p+1)}$. Thus $\Sigma_-^{(p)} a^{(p)} = p!\,a^{(p)}$, together with the fact that $a^{(p)}$ was arbitrary, implies the integral equation

$$\tilde{\gamma}(t)^{\otimes p}\,\Sigma_-^{(p)} \;=\; \gamma^{\otimes p}\,\Sigma_-^{(p)} - \mathrm{i}\int_0^t \mathrm{d}s\;\mathrm{Tr}_{p+1}\left[\sum_{i=1}^{p} W_{i\;p+1,s}, \tilde{\gamma}(s)^{\otimes(p+1)}(\mathbb{1} - E_{i\;p+1})\right]\Sigma_-^{(p)}. \tag{7.14}$$

The tree expansion would be obtained by iterating the somewhat different integral equation

$$\tilde{\gamma}(t)^{\otimes p}\,\Sigma_-^{(p)} \;=\; \gamma^{\otimes p}\,\Sigma_-^{(p)} - \mathrm{i}\int_0^t \mathrm{d}s\;\mathrm{Tr}_{p+1}\left[\sum_{i=1}^{p} W_{i\;p+1,s}, \tilde{\gamma}(s)^{\otimes(p+1)}\,\Sigma_-^{(p+1)}\right]. \tag{7.15}$$

In order to compare (7.14) with (7.15), we use the elementary identity

$$\Sigma_-^{(p+1)} \;=\; \Big(\mathbb{1} - \sum_{j=1}^{p} E_{j\;p+1}\Big)\Sigma_-^{(p)}\,.$$

Thus we find

$$\begin{aligned}\mathrm{Tr}_{p+1}\left[\sum_{i=1}^{p} W_{i\;p+1,s}, \tilde{\gamma}(s)^{\otimes(p+1)}\,\Sigma_-^{(p+1)}\right] \;&=\; \mathrm{Tr}_{p+1}\left[\sum_{i=1}^{p} W_{i\;p+1,s}, \tilde{\gamma}(s)^{\otimes(p+1)}\Big(\mathbb{1} - \sum_{j=1}^{p} E_{j\;p+1}\Big)\Sigma_-^{(p)}\right] \\ &=\; \mathrm{Tr}_{p+1}\left[\sum_{i=1}^{p} W_{i\;p+1,s}, \tilde{\gamma}(s)^{\otimes(p+1)}\Big(\mathbb{1} - \sum_{j=1}^{p} E_{j\;p+1}\Big)\right]\Sigma_-^{(p)}\,.\end{aligned}$$

Together with (7.14) this yields

$$\tilde{\gamma}(t)^{\otimes p}\,\Sigma_-^{(p)} \;=\; \gamma^{\otimes p}\,\Sigma_-^{(p)} - \mathrm{i}\int_0^t \mathrm{d}s\;\mathrm{Tr}_{p+1}\left[\sum_{i=1}^{p} W_{i\;p+1,s}, \tilde{\gamma}(s)^{\otimes(p+1)}\,\Sigma_-^{(p+1)}\right] + R_p(t)\,, \tag{7.16}$$

with an error term

$$R_p(t) \;:=\; -\mathrm{i}\sum_{1\leqslant i\neq j\leqslant p}\int_0^t \mathrm{d}s\;\mathrm{Tr}_{p+1}\Big[W_{i\;p+1,s}, \tilde{\gamma}(s)^{\otimes(p+1)}E_{j\;p+1}\Big]\,\Sigma_-^{(p)}. \tag{7.17}$$

The partial trace is most conveniently computed using operator kernels. We find

$$\begin{aligned}&\Big(W_{i\;p+1,s}\tilde{\gamma}(s)^{\otimes(p+1)}E_{j\;p+1}\Big)\,(x_1,\ldots,x_{p+1};y_1,\ldots,y_{p+1}) \\ &\qquad=\; \int \mathrm{d}z_1\,\mathrm{d}z_2\;\left[\prod_{r\neq i,j}\tilde{\gamma}(s)(x_r;y_r)\right]\,W_s(x_i,x_{p+1};z_1,z_2)\,\tilde{\gamma}(s)(z_1;y_i)\,\tilde{\gamma}(s)(x_j;y_{p+1})\,\tilde{\gamma}(s)(z_2;y_j)\,,\end{aligned}$$

so that

$$\begin{aligned}
&\mathrm{Tr}_{p+1}\left(W_{i\,p+1,s}\tilde{\gamma}(s)^{\otimes(p+1)}E_{j\,p+1}\right)(x_1,\ldots,x_p;y_1,\ldots,y_p)\\
&= \int \mathrm{d}z_1\,\mathrm{d}z_2\,\mathrm{d}z_3\,\left[\prod_{r\neq i,j}\tilde{\gamma}(s)(x_r;y_r)\right]W_s(x_i,z_3;z_1,z_2)\,\tilde{\gamma}(s)(z_1;y_i)\,\tilde{\gamma}(s)(x_j;z_3)\,\tilde{\gamma}(s)(z_2;y_j)\\
&= \left(\tilde{\gamma}_j(s)W_{ij,s}\tilde{\gamma}(s)^{\otimes p}\right)(x_1,\ldots,x_p;y_1,\ldots,y_p)\,. \qquad (7.18)
\end{aligned}$$

The second term of the commutator in (7.17) is the adjoint of the first and we get

$$\begin{aligned}
R_p(t) &= -\mathrm{i}\sum_{1\leqslant i\neq j\leqslant p}\int_0^t \mathrm{d}s\,\left(\tilde{\gamma}_j(s)W_{ij,s}\tilde{\gamma}(s)^{\otimes p}-\tilde{\gamma}(s)^{\otimes p}W_{ij,s}\tilde{\gamma}_j(s)\right)\Sigma_-^{(p)}\\
&= -\mathrm{i}\sum_{1\leqslant i\neq j\leqslant p}\int_0^t \mathrm{d}s\,\left(\tilde{\gamma}_j(s)W_{ij,s}\tilde{\gamma}(s)^{\otimes p}\Sigma_-^{(p)}-\tilde{\gamma}(s)^{\otimes p}\Sigma_-^{(p)}W_{ij,s}\tilde{\gamma}_j(s)\right).
\end{aligned}$$

We remark at this point that the formula (7.18) is the key identity behind our proof. From it our strategy is already apparent: the factor $\tilde{\gamma}_j(s)$ multiplies a trace class operator, so that the trace norm of the right-hand side of (7.18) may eventually (after the smoothing effect of the free time evolution has been exploited) be estimated using the *operator norm* of $\tilde{\gamma}_j(s)$, which is bounded by N^{-1}. Moreover, it is also apparent why it is crucial to keep the exchange term in (7.14) for our argument to work. Indeed, if the exchange term in (7.14) were dropped, the restriction $i\neq j$ in (7.17) would no longer hold. In that case we would have to estimate the term

$$\mathrm{Tr}_{p+1}\left[W_{i\,p+1,s},\tilde{\gamma}(s)^{\otimes(p+1)}E_{i\,p+1}\right],$$

for which the computation of (7.18) does not hold.

We are now ready to iterate (7.16). Multiplying (7.16) by $a^{(p)}\in\mathcal{L}(\mathcal{H}_-^{(p)})$ yields

$$\begin{aligned}
\mathrm{Tr}\left(a_t^{(p)}\,\tilde{\gamma}(t)^{\otimes p}\,\Sigma_-^{(p)}\right) &= \mathrm{Tr}\left(a_t^{(p)}\,\gamma^{\otimes p}\,\Sigma_-^{(p)}\right)\\
&\quad+\mathrm{i}\int_0^t \mathrm{d}s\,\sum_{i=1}^{p}\mathrm{Tr}\left(\left[W_{i\,p+1,s},a_t^{(p)}\otimes\mathbb{1}\right]\,\tilde{\gamma}(s)^{\otimes(p+1)}\,\Sigma_-^{(p+1)}\right)+\mathrm{Tr}\left(a_t^{(p)}\,R_p(t)\right).
\end{aligned}$$

Iterating this K times yields our main expansion

$$\begin{aligned}
\mathrm{Tr}\left(a_t^{(p)}\,\tilde{\gamma}(t)^{\otimes p}\,\Sigma_-^{(p)}\right) &= \sum_{k=0}^{K-1}\int_{\Delta^k(t)}\mathrm{d}\underline{t}\;\mathrm{Tr}\left(G_{t,\underline{t}}^{(k,0)}(a^{(p)})\,\gamma^{\otimes(p+k)}\Sigma_-^{(p+k)}\right)\\
&\quad+\int_{\Delta^K(t)}\mathrm{d}\underline{t}\;\mathrm{Tr}\left(G_{t,\underline{t}}^{(K,0)}(a^{(p)})\,\tilde{\gamma}(t_K)^{\otimes(p+K)}\Sigma_-^{(p+K)}\right)\\
&\quad+\sum_{k=0}^{K-1}\sum_{1\leqslant i\neq j\leqslant p+k}R_{ij}^k(t)\,, \qquad (7.19)
\end{aligned}$$

where the error terms are given by

$$\begin{aligned}
R_{ij}^k(t) &:= -\mathrm{i}\int_{\Delta^{k+1}(t)}\mathrm{d}\underline{t}\;\mathrm{Tr}\Big(G_{t,t_1,\ldots,t_k}^{(k,0)}(a^{(p)})\,\tilde{\gamma}_j(t_{k+1})\,W_{ij,t_{k+1}}\,\tilde{\gamma}(t_{k+1})^{\otimes(p+k)}\,\Sigma_-^{(p+k)}\\
&\qquad\qquad-W_{ij,t_{k+1}}\,\tilde{\gamma}_j(t_{k+1})\,G_{t,t_1,\ldots,t_k}^{(k,0)}(a^{(p)})\,\tilde{\gamma}(t_{k+1})^{\otimes(p+k)}\,\Sigma_-^{(p+k)}\Big).
\end{aligned}$$

Next, we estimate $R^k_{ij}(t)$. Let us concentrate on the first term, which we rewrite using the renaming $t_{k+1} \to s$ as

$$\int_{\Delta^k(t)} \mathrm{d}\underline{t} \int_0^{\wedge \underline{t}} \mathrm{d}s \ \mathrm{Tr}\left(G^{(k,0)}_{t,t_1,\ldots,t_k}(a^{(p)})\, \tilde{\gamma}_j(s)\, W_{ij,s}\, \tilde{\gamma}(s)^{\otimes(p+k)}\, \Sigma_-^{(p+k)} \right), \tag{7.20}$$

where $\wedge \underline{t} := \min\{t_1, \ldots, t_k\}$. The outline of our strategy is as follows. We expand both $G^{(k,0)}_{t,t_1,\ldots,t_k}(a^{(p)})$ and $\tilde{\gamma}(s)^{\otimes(p+k)}$ using a graph expansion. The integral over s allows us to control the singularity in the potential $W_{ij,s}$ by invoking the dispersive estimate (7.9). The term $\tilde{\gamma}_j(s)$ is bounded by its operator norm.

We start by deriving a tree expansion for $\tilde{\gamma}(s)^{\otimes p}$.

LEMMA 7.1. *Let $a^{(p)} \in \mathcal{L}(\mathcal{H}_-^{(p)})$. For small times we have the tree expansion*

$$\mathrm{Tr}\big(a^{(p)} \tilde{\gamma}(t)^{\otimes p} \Sigma_-^{(p)}\big) \ = \ \sum_{k=0}^{\infty} \int_{\Delta^k(t)} \mathrm{d}\underline{t} \ \mathrm{Tr}\big(T^{(k)}_{\underline{t}}(a^{(p)}) \gamma^{\otimes(p+k)} \Sigma_-^{(p)}\big)\,, \tag{7.21}$$

where $T^{(k)}_{\underline{t}}$ is the linear operator defined by $T^{(0)}(a^{(p)}) := a^{(p)}$ and

$$T^{(k)}_{t_1 \ldots t_k}(a^{(p)}) \ = \ \mathrm{i} \sum_{i=1}^{p+k-1} \Big[\mathcal{W}_{i\, p+k, t_k}, T^{(k-1)}_{t_1 \ldots t_{k-1}}(a^{(p)}) \otimes \mathbb{1} \Big]\,.$$

PROOF. Lemma 2.2 applied to $A = \mathbb{A}(\tilde{a}^{(p)})$ yields

$$\mathrm{Tr}\big(a^{(p)} \tilde{\gamma}(t)^{\otimes p}\big) \ = \ \sum_{k=0}^{\infty} \int_{\Delta^k(t)} \mathrm{d}\underline{t} \ \mathrm{Tr}\big(T^{(k)}_{\underline{t}}(a^{(p)}) \gamma^{\otimes(p+k)}\big)\,.$$

The claim then follows by noting that $\Sigma_-^{(p)} a^{(p)} = p! a^{(p)}$ and that $\sum_{i=1}^{p+k-1} \mathcal{W}_{i\, p+k, t_k}$ commutes with $\Sigma_-^{(p)}$. The proof of convergence of the series is the same as the proof of convergence of the series (7.2) outlined in Section 7.1. □

We use Lemma 7.1 to expand $\tilde{\gamma}(s)^{\otimes(p+k)}$ in (7.20). The result is that (7.20) equals

$$\sum_{k'=0}^{\infty} \int_{\Delta^k(t)} \mathrm{d}\underline{t} \int_0^{\wedge \underline{t}} \mathrm{d}s \int_{\Delta^{k'}(s)} \mathrm{d}\underline{t}' \ \mathrm{Tr}\Big\{ T^{(k')}_{\underline{t}'}\Big(G^{(k,0)}_{t,\underline{t}}(a^{(p)}) \tilde{\gamma}_j(s) W_{ij,s} \Big) \gamma^{\otimes(p+k+k')} \Sigma_-^{(p+k)} \Big\}\,.$$

Next, we recall from (7.5) that $G^{(k,0)}_{t,t_1,\ldots,t_k}(a^{(p)})$ can be written as a sum over tree graphs $\mathcal{Q} \in \mathscr{Q}(p,k,0)$ of elementary terms of the form (7.7). Also, since the definition of $T^{(k)}_{t_1,\ldots,t_k}(a^{(p)})$ is the same as the definition of $G^{(k,0)}_{0,t_1,\ldots,t_k}(a^{(p)})$ with W replaced by $\mathcal{W}$, we immediately get that $T^{(k)}_{t_1,\ldots,t_k}(a^{(p)})$ is equal to a sum over tree graphs $\mathcal{Q} \in \mathscr{Q}(p,k,0)$ of elementary terms of the form

$$P_- \, \mathcal{W}_{i_1 j_1, t_{v_1}} \cdots \mathcal{W}_{i_r j_r, t_{v_r}} \left(a_t^{(p)} \otimes \mathbb{1}^{(k-l)} \right) \mathcal{W}_{i_{r+1} j_{r+1}, t_{v_{r+1}}} \cdots \mathcal{W}_{i_k j_k, t_{v_k}} P_-\,.$$

In particular, using the dispersive estimate (7.9) and the bound (7.6), one readily sees that the tree expansion (7.21) converges for small times.

Applying the tree expansion to both $G^{(k,0)}_{t,t_1,\dots,t_k}(a^{(p)})$ and $\tilde\gamma(s)^{\otimes(p+k)}$ in (7.20), we see that (7.20) is equal to

$$\sum_{k'=0}^{\infty} \frac{\mathrm{i}^{k+k'}}{2^{k+k'}} \sum_{\mathcal{Q}\in\mathscr{Q}(p,k,0)} \sum_{\mathcal{Q}'\in\mathscr{Q}(p+k,k',0)} i_{\mathcal{Q}} i_{\mathcal{Q}'} \int_{\Delta^k_{\mathcal{Q}}(t)} \mathrm{d}\underline{t} \int_0^{\wedge\underline{t}} \mathrm{d}s \int_{\Delta^{k'}_{\mathcal{Q}'}(s)} \mathrm{d}\underline{t}' \\ \mathrm{Tr}\Big\{ A\, a^{(p)}_{1\dots p,t}\, B P_-^{(p+k)} \tilde\gamma_j(s) W_{ij,s}\, C\, \gamma^{\otimes(p+k+k')} \Sigma_-^{(p+k)} \Big\}, \quad (7.22)$$

where A, B, and C are operators with the following properties:

(i) A, B, and C depend on the variables $(\mathcal{Q}, \mathcal{Q}', k, k', \underline{t}, \underline{t}')$;

(ii) A, B, and C are each a product of operators of the form $W_{i'j',r}$, or $\mathcal{W}_{i'j',r}$, where r stands for a time variable in $\{t_1,\dots,t_k,t'_1,\dots,t'_{k'}\}$;

(iii) the product ABC contains k factors W and k' factors $\mathcal{W}$;

(iv) each time variable in $t_1,\dots,t_k,t_1,\dots,t_{k'}$ appears exactly once in the product ABC.

Next, we estimate the operator norm of the operator multiplying $\gamma^{\otimes(p+k+k')}$ in (7.22). Let $\varphi\in\mathcal{H}^{\otimes(p+k+k')}$ and estimate

$$I := \Big\| \sum_{\mathcal{Q}\in\mathscr{Q}(p,k,0)} \sum_{\mathcal{Q}'\in\mathscr{Q}(p+k,k',0)} i_{\mathcal{Q}} i_{\mathcal{Q}'} \int_{\Delta^k_{\mathcal{Q}}(t)} \mathrm{d}\underline{t} \int_0^{\wedge\underline{t}} \mathrm{d}s \int_{\Delta^{k'}_{\mathcal{Q}'}(s)} \mathrm{d}\underline{t}'\; A\, a^{(p)}_{1\dots p,t}\, B P_-^{(p+k)} \tilde\gamma_j(s) W_{ij,s}\, C\, \varphi \Big\| \\ \leqslant \sum_{\mathcal{Q}\in\mathscr{Q}(p,k,0)} \sum_{\mathcal{Q}'\in\mathscr{Q}(p+k,k',0)} \int_{[0,t]^k} \mathrm{d}\underline{t} \int_0^t \mathrm{d}s \int_{[0,t]^{k'}} \mathrm{d}\underline{t}' \, \Big\| A\, a^{(p)}_{1\dots p,t}\, B P_-^{(p+k)} \tilde\gamma_j(s) W_{ij,s}\, C\, \varphi \Big\|$$

We now perform all time integrations, starting from the left, and using at each step the estimate (7.9) as well as

$$\int_0^t \mathrm{d}r \, \big\| \mathcal{W}_{i'j',r}\varphi \big\| \;\leqslant\; \sqrt{2\pi\kappa^2 t}\, \|\varphi\|\,,$$

which follows trivially from (7.9). Also, Lemma 2.1 implies that $\|\tilde\gamma(s)\| = \|\gamma\|$. Thus we find that

$$I \;\leqslant\; \sum_{\mathcal{Q}\in\mathscr{Q}(p,k,0)} \sum_{\mathcal{Q}'\in\mathscr{Q}(p+k,k',0)} \left(\frac{\pi\kappa^2 t}{2}\right)^{(k+1)/2} \big(2\pi\kappa^2 t\big)^{k'/2} \|a^{(p)}\| \|\gamma\| \|\varphi\|$$

Using the bound

$$|\mathscr{Q}(p,k,0)| \;\leqslant\; 4^p\, 16^k\,,$$

which can be inferred from (7.6), we find

$$I \;\leqslant\; 4^p\, 16^k\, 4^{p+k} 16^{k'} \left(\frac{\pi\kappa^2 t}{2}\right)^{(k+1)/2} \big(2\pi\kappa^2 t\big)^{k'/2} \|a^{(p)}\| \|\gamma\| \|\varphi\| \\ \leqslant\; 16^p \sqrt{2\pi\kappa^2 t}\, \big(32\sqrt{2\pi\kappa^2 t}\big)^k \, \big(16\sqrt{2\pi\kappa^2 t}\big)^{k'} \, \|a^{(p)}\| \|\gamma\| \|\varphi\|\,.$$

Let $t < (2^{11}\pi\kappa^2)^{-1}$. Now Lemma 5.1 implies that $\|\gamma^{\otimes(p+k+k')}\Sigma_-^{(p+k)}\|_1 \leqslant 1$. Using the inequality $\mathrm{Tr}(A\Gamma) \leqslant \|A\|\|\Gamma\|_1$ we therefore find that (7.20) is bounded by

$$16^p \sum_{k'=0}^{\infty} \big(32\sqrt{2\pi\kappa^2 t}\big)^k \big(16\sqrt{2\pi\kappa^2 t}\big)^{k'} \|a^{(p)}\|\|\gamma\| \;=\; 16^p \frac{\big(32\sqrt{2\pi\kappa^2 t}\big)^k}{1-16\sqrt{2\pi\kappa^2 t}} \|a^{(p)}\|\|\gamma\|\,.$$

The second term of $R_{ij}^k(t)$ is equal to the complex conjugate of the first. We thus arrive at the desired bound

$$|R_{ij}^k(t)| \;\leqslant\; 2\cdot 16^p \frac{\big(32\sqrt{2\pi\kappa^2 t}\big)^k}{1-16\sqrt{2\pi\kappa^2 t}} \|a^{(p)}\|\|\gamma\|\,. \tag{7.23}$$

Therefore the last line of (7.19) is bounded by

$$2\cdot 16^p \frac{1}{1-16\sqrt{2\pi\kappa^2 t}} \|a^{(p)}\|\|\gamma\| \sum_{k=0}^{\infty} (p+k)^2 \big(32\sqrt{2\pi\kappa^2 t}\big)^k$$
$$\leqslant\; 4\cdot 16^p\, \mathrm{e}^p \frac{1}{1-16\sqrt{2\pi\kappa^2 t}} \frac{1}{\big(1-32\sqrt{2\pi\kappa^2 t}\big)^3} \|a^{(p)}\|\|\gamma\|\,,$$

where we used the estimate $\sum_{k=0}^{\infty}(p+k)^L x^k \leqslant \frac{\mathrm{e}^p\, L!}{(1-x)^{L+1}}$.

Next, we note that the second line of (7.19), i.e. the rest term, vanishes in the limit $K\to\infty$. The procedure is almost identical to (in fact easier than) the above estimation of $|R_{ij}^k(t)|$. The result is

$$\left|\int_{\Delta^K(t)} \mathrm{d}\underline{t}\; \mathrm{Tr}\left(G_{t,\underline{t}}^{(K,0)}(a^{(p)})\,\tilde\gamma(t_K)^{\otimes(p+K)}\Sigma_-^{(p+K)}\right)\right| \;\leqslant\; 2\cdot 16^p \frac{\big(32\sqrt{2\pi\kappa^2 t}\big)^K}{1-16\sqrt{2\pi\kappa^2 t}} \|a^{(p)}\| \;\longrightarrow\; 0\,,$$

as $K\to\infty$.

We summarize what we have proven: For small times the Hartree-Fock time evolution is equal to the tree expansion plus an error term of order $\|\gamma\|$.

LEMMA 7.2. *Let $a^{(p)} \in \mathcal{L}(\mathcal{H}_-^{(p)})$. Then, for small times, we have*

$$\left|\mathrm{Tr}\Big(a^{(p)}\,\gamma(t)^{\otimes p}\,\Sigma_-^{(p)}\Big) - \sum_{k=0}^{\infty} \mathrm{Tr}\Big(G_t^{(k,0)}(a^{(p)})\,\gamma^{\otimes(p+k)}\Sigma_-^{(p+k)}\Big)\right| \;\leqslant\; \|a^{(p)}\|\,\|\gamma\|\,C(p,\kappa,t)\,,$$

for some constant $C(p,\kappa,t)$.

7.3. Conclusion of the proof. We now have all the necessary ingredients to prove our main result. Take an infinite sequence $\Phi = (\varphi_i)_{i\in\mathbb{N}}$ of orthonormal orbitals, and denote by $\Phi^{(N)}(t)$ the solution of the rescaled integral Hartree-Fock equation (5.7) with initial data $\Phi^{(N)}$.

Then, for small times, we find from (7.10) and (7.12) that

$$\begin{aligned}
&\Big\langle \mathrm{e}^{-\mathrm{i}tH_N} S(\Phi^{(N)})\,,\, \widehat{\mathbb{A}}_N(a^{(p)})\,\mathrm{e}^{-\mathrm{i}tH_N} S(\Phi^{(N)})\Big\rangle - \Big\langle S\big(\Phi^{(N)}(t)\big)\,,\, \widehat{\mathbb{A}}_N(a^{(p)}) S\big(\Phi^{(N)}(t)\big)\Big\rangle \\
&= \sum_{k=0}^{\infty} \Big\langle S(\Phi^{(N)})\,,\, \widehat{\mathbb{A}}_N\big(G_t^{(k,0)}(a^{(p)})\big) S(\Phi^{(N)})\Big\rangle + \big\langle S(\Phi^{(N)}), L_N(t) S(\Phi^{(N)})\big\rangle - \mathrm{Tr}\big(a^{(p)}\gamma_N^{(p)}(t)\big) \\
&= \sum_{k=0}^{\infty} \mathrm{Tr}\Big(G_t^{(k,0)}(a^{(p)})\,\gamma_N^{(p+k)}\Big) - \mathrm{Tr}\big(a^{(p)}\gamma_N^{(p)}(t)\big) + \big\langle S(\Phi^{(N)}), L_N(t) S(\Phi^{(N)})\big\rangle\,.
\end{aligned}$$

Thus, Lemma 7.2 and (7.11) imply

$$\left|\left\langle \mathrm{e}^{-\mathrm{i}tH_N} S(\Phi^{(N)}) \,,\, \widehat{\mathbb{A}}_N(a^{(p)})\, \mathrm{e}^{-\mathrm{i}tH_N} S(\Phi^{(N)})\right\rangle - \left\langle S\big(\Phi^{(N)}(t)\big) \,,\, \widehat{\mathbb{A}}_N(a^{(p)}) S\big(\Phi^{(N)}(t)\big)\right\rangle\right| \\ \leqslant\; C(p,\kappa,t)\|a^{(p)}\|\big(\|\gamma_N\| + N^{-1}\big) \;\leqslant\; \frac{2C(p,\kappa,t)}{N}\|a^{(p)}\|\,, \quad (7.24)$$

by (5.6).

Next, we observe that the quantum-mechanical and the Hartree-Fock time-evolutions are norm-preserving. We may therefore iterate (7.24), as in [10], to extend it to all times. Thus we find, for all times $t \in \mathbb{R}$,

$$\left|\left\langle \mathrm{e}^{-\mathrm{i}tH_N} S(\Phi^{(N)}) \,,\, \widehat{\mathbb{A}}_N(a^{(p)})\, \mathrm{e}^{-\mathrm{i}tH_N} S(\Phi^{(N)})\right\rangle - \left\langle S\big(\Phi^{(N)}(t)\big) \,,\, \widehat{\mathbb{A}}_N(a^{(p)}) S\big(\Phi^{(N)}(t)\big)\right\rangle\right| \\ \leqslant\; C(p,\kappa,t)\|a^{(p)}\|\big(\|\gamma_N\| + N^{-1}\big) \;\leqslant\; C(p,\kappa,t) f(t,N)\|a^{(p)}\|\,, \quad (7.25)$$

where $f(t,N)$ is some function satisfying $\lim_N f(t,N) = 0$ for all $t \in \mathbb{R}$. Theorem 6.1 follows immediately.

Finally, we prove Theorem 6.2. Let $\Gamma_N^{(p)}(t)$ and $\tilde{\Gamma}_N^{(p)}(t)$ be defined as in Section 6. Thus, plugging (5.4) and (5.5) into (7.25) yields

$$\frac{p!}{N^p}\binom{N}{p}\left|\mathrm{Tr}\Big[\Big(\Gamma_N^{(p)}(t) - \tilde{\Gamma}_N^{(p)}(t)\Big)a^{(p)}\Big]\right| \;\leqslant\; C(p,\kappa,t) f(t,N)\|a^{(p)}\|\,.$$

Thus, by the duality $(\mathcal{L}^1)^* = \mathcal{L}$, we find

$$\big\|\Gamma_N^{(p)}(t) - \tilde{\Gamma}_N^{(p)}(t)\big\|_1 \;\leqslant\; C(p,\kappa,t) f(t,N)\,.$$

Theorem 6.2 follows.

8. A Egorov-type result for small times

In this section we describe how the many-body dynamics of fermions may be seen as the quantization of a classical "superhamiltonian" system, whose dynamics is approximately described by the Hartree-Fock equation.

8.1. A graded algebra of observables. We start by defining a Grassmann algebra of anticommuting variables over the one-particle space $\mathcal{H} = L^2(\mathbb{R}^3)$, and equip it with a suitable norm. Formally, we consider the infinite-dimensional Grassmann algebra generated by $\{\overline{\psi(x)}, \psi(x)\}_{x\in\mathbb{R}^3}$. As it turns out, this algebra can be made into a Banach algebra under a natural choice of norm. This norm is most conveniently formulated by identifying elements of the Grassmann algebra with bounded operators between L^2-spaces.

Let

$$a \;=\; (a^{(p,q)})_{p,q\in\mathbb{N}}\,, \qquad a^{(p,q)} \in \mathcal{L}(\mathcal{H}_-^{(q)}; \mathcal{H}_-^{(p)}), \quad (8.1)$$

be a family of bounded operators. Such objects will play the role of observables in the following. By a slight abuse of notation we identify $a^{(p,q)}$ with the family obtained by adjoining zeroes to it.

Define

$$\mathfrak{B}^G \;:=\; \{a = (a^{(p,q)}) \,:\, a^{(p,q)} = 0 \text{ for all but finitely many } (p,q)\}\,.$$

We introduce a norm on $\mathfrak{B}^G$ through

$$\|a\|_{\mathfrak{B}^G} \;:=\; \sum_{p,q\in\mathbb{N}} \|a^{(p,q)}\|\,, \tag{8.2}$$

and define $\overline{\mathfrak{B}}^G$ as the completion of $\mathfrak{B}^G$.

We also introduce a multiplication on $\overline{\mathfrak{B}}^G$ defined by

$$(ab)^{(p,q)} \;:=\; \sum_{\substack{p_1+p_2=p\\ q_1+q_2=q}} (-1)^{p_2(p_1+q_1)}\, P_-(a^{(p_1,q_1)}\otimes b^{(p_2,q_2)})P_-\,. \tag{8.3}$$

The seemingly odd choice of sign will soon become clear. It is now easy to check that $\overline{\mathfrak{B}}^G$ is an associative Banach algebra with identity

$$\mathbb{1}^{(p,q)} \;=\; \delta_{p0}\,\delta_{q0}\,.$$

Note that $\overline{\mathfrak{B}}^G$ bears a $\mathbb{Z}$-grading, with degree map

$$\deg a^{(p,q)} \;:=\; p-q\,.$$

An observable is gauge invariant when its degree is equal to 0. One readily sees that

$$ab = (-1)^{\deg a\,\deg b} ba\,.$$

We now identify $\overline{\mathfrak{B}}^G$ with a Grassmann algebra of anticommuting variables. For $f\in\mathcal{H}$ define $\psi(f)\in\mathcal{L}(\mathcal{H};\mathbb{C})\subset\overline{\mathfrak{B}}^G$ through

$$\psi(f)\,g \;:=\; \langle f\,,g\rangle \tag{8.4}$$

and $\overline{\psi}(f)\in\mathcal{L}(\mathbb{C};\mathcal{H})\subset\overline{\mathfrak{B}}^G$ through

$$\overline{\psi}(f)z \;:=\; fz\,. \tag{8.5}$$

We may now consider arbitrary polynomials in the variables $\{\overline{\psi}(f),\psi(f)\,:\,f\in\mathcal{H}\}$. It is a simple matter to check that

$$\psi(f)\,\psi(g)+\psi(g)\,\psi(f) \;=\; \psi(f)\overline{\psi}(g)+\overline{\psi}(g)\,\psi(f) \;=\; \overline{\psi}(f)\,\overline{\psi}(g)+\overline{\psi}(g)\,\overline{\psi}(f) \;=\; 0\,,$$

for all $f,g\in\mathcal{H}$. Furthermore, we have that

$$\overline{\psi}(f_p)\cdots\overline{\psi}(f_1)\psi(g_1)\cdots\psi(g_q) \;=\; P_-^{(p)}\,|f_1\otimes\cdots\otimes f_p\rangle\langle g_1\otimes\cdots\otimes g_q|\,P_-^{(q)}\,. \tag{8.6}$$

Linear combinations of expressions of the form (8.6) are dense in $\overline{\mathfrak{B}}^G$ (in the strong operator topology). It is often convenient to write a family a of bounded operators using the "Grassmann generators" $\{\overline{\psi},\psi\}$. To this end we set

$$\psi(x) \;:=\; \psi(\delta_x)\,,\qquad \overline{\psi}(x) \;:=\; \overline{\psi}(\delta_x)\,,$$

where δ_x is Dirac's delta mass at x. Expressions of the form (8.6) are now understood as densely defined quadratic forms. One immediately finds

$$\begin{aligned} a \;\equiv\; \mathbb{A}^G(a) \;:=\; \sum_{p,q}\int \mathrm{d}x_1\ldots\mathrm{d}x_p\,\mathrm{d}y_1\ldots\mathrm{d}y_q \\ \times\,\overline{\psi}(x_p)\cdots\overline{\psi}(x_1)\,a^{(p,q)}(x_1,\ldots,x_p;y_1,\ldots,y_q)\,\psi(y_1)\cdots\psi(y_q)\,. \end{aligned} \tag{8.7}$$

We use the notation $\mathbb{A}^G(a)$ to emphasize that the family a is represented using Grassmann generators.

8.2. A graded Poisson bracket. Next, we note that $\mathfrak{B}^G$ carries the graded Poisson bracket

$$\{a,b\} \;:=\; \mathrm{i}\int \mathrm{d}x\,\left[a\,\frac{\overleftarrow{\delta}}{\delta\overline{\psi}(x)}\,\frac{\overrightarrow{\delta}}{\delta\psi(x)}\,b + a\,\frac{\overleftarrow{\delta}}{\delta\psi(x)}\,\frac{\overrightarrow{\delta}}{\delta\overline{\psi}(x)}\,b\right], \tag{8.8}$$

where $a,b\in\mathfrak{B}^G$. Here we use the usual conventions for derivatives with respect to Grassmann variables (see e.g. [17], Appendix B). In terms of kernels the graded Poisson bracket can be expressed as

$$\{\psi(x),\overline{\psi}(y)\} \;=\; \mathrm{i}\delta(x-y) \qquad \{\psi(x),\psi(y)\} \;=\; \{\overline{\psi}(x),\overline{\psi}(y)\} \;=\; 0\,. \tag{8.9}$$

We now list the important properties of the graded Poisson bracket.

(i) $\{a,b\} \;=\; (-1)^{1+\deg a\,\deg b}\{b,a\}\,.$

(ii) $(-1)^{\deg b\,(\deg a+\deg c)}\{a,\{b,c\}\}+\text{cyclic permutations} \;=\; 0\,.$

(iii) $\{a,bc\} \;=\; \{a,b\}c+(-1)^{\deg a\,\deg b}b\{a,c\}\,.$

Proof. Let us start with (i):

$$\begin{aligned}\{a,b\} \;&=\; \mathrm{i}\int \mathrm{d}x\,\left[(-1)^{\deg a+1}\frac{\delta a}{\delta\overline{\psi}(x)}\frac{\delta b}{\delta\psi(x)}+(-1)^{\deg a+1}\frac{\delta a}{\delta\psi(x)}\frac{\delta b}{\delta\overline{\psi}(x)}\right]\\ &=\; \mathrm{i}\int \mathrm{d}x\,\left[(-1)^{\deg a\,\deg b+\deg b}\frac{\delta b}{\delta\psi(x)}\frac{\delta a}{\delta\overline{\psi}(x)}+(-1)^{\deg a\,\deg b+\deg b}\frac{\delta b}{\delta\overline{\psi}(x)}\frac{\delta a}{\delta\psi(x)}\right]\\ &=\; (-1)^{1+\deg a\,\deg b}\{b,a\}\,.\end{aligned}$$

In order to show (ii), we note that the left-hand side can be written as a sum of three terms, the first of which contains second derivatives of a, the second second derivatives of b and the third second derivatives of c. Let us consider the third one. It is equal to the terms containing second derivatives of c of

$$\begin{aligned}&(-1)^{\deg b(\deg a+\deg c)}\{a,\{b,c\}\}+(-1)^{\deg c(\deg b+\deg a)}\{b,\{c,a\}\}\\ &\qquad=\; (-1)^{\deg b(\deg a+\deg c)}\{a,\{b,c\}\}+(-1)^{\deg c(\deg b+\deg a)+1+\deg c\,\deg a}\{b,\{a,c\}\}\,,\end{aligned}$$

where (i) was used. Define the derivation $L_a b := \{a,b\}$. Thus we need to compute the terms containing second derivatives of c of

$$(-1)^{\deg a\,\deg b+\deg b\,\deg c}L_aL_bc-(-1)^{\deg b\,\deg c}L_bL_ac\,.$$

Since we are only considering terms containing second derivatives of c, both derivations L_a and L_b must act only on c, and one finds

$$(-1)^{\deg a\,\deg b+\deg b\,\deg c}L_aL_bc-(-1)^{\deg a\,\deg b+\deg b\,\deg c}L_aL_bc \;=\; 0\,.$$

We omit the straightforward proof of (iii). □

Furthermore, one finds by explicit calculation

$$\begin{aligned}\{\mathbb{A}^G(a^{(p_1,q_1)}),\mathbb{A}^G(b^{(p_2,q_2)})\} \;&=\; \mathrm{i}\,(-1)^{(p_2+1)(p_1+q_1)}q_1p_2\,\mathbb{A}^G\Big[\big(a^{(p_1,q_1)}\otimes\mathbb{1}^{(p_2-1)}\big)\,\big(\mathbb{1}^{(q_1-1)}\otimes b^{(p_2,q_2)}\big)\Big]\\ &\quad-\mathrm{i}\,(-1)^{(q_1+1)(p_2+q_2)}p_1q_2\,\mathbb{A}^G\Big[\big(b^{(p_2,q_2)}\otimes\mathbb{1}^{(p_1-1)}\big)\,\big(\mathbb{1}^{(q_2-1)}\otimes a^{(p_1,q_1)}\big)\Big]\,.\end{aligned} \tag{8.10}$$

8.3. States. We now introduce a space of states $\mathfrak{R} \subset \big(\overline{\mathfrak{B}}^G\big)^*$ on the algebra $(\overline{\mathfrak{B}}^G, \|\cdot\|_{\mathfrak{B}^G})$. A convenient choice is

$$\mathfrak{R} \;:=\; \big\{\rho = (\rho^{(p,q)})_{p,q\in\mathbb{N}} \,:\, \rho^{(p,q)} \in \mathcal{L}(\mathcal{H}_-^{(q)}; \mathcal{H}_-^{(p)})\,,\; \|\rho\|_{\mathfrak{R}} < \infty\big\}\,,$$

where

$$\|\rho\|_{\mathfrak{R}} \;:=\; \sup_{p,q\in\mathbb{N}} \|\rho^{(p,q)}\|_1$$

and

$$\|\rho^{(p,q)}\|_1 \;:=\; \sup\big\{\big|\mathrm{Tr}(\rho^{(p,q)} a^{(q,p)})\big| \,:\, a^{(q,p)} \in \mathcal{L}(\mathcal{H}_-^{(p)}, \mathcal{H}_-^{(q)})\,,\; \|a^{(q,p)}\| \leqslant 1\big\}\,.$$

Note that if $p = q$ then $\|\cdot\|_1$ is the usual trace norm. The dual action is given by

$$\langle \rho, a\rangle \;:=\; \sum_{p,q\in\mathbb{N}} \mathrm{Tr}(\rho^{(p,q)} a^{(q,p)})\,.$$

We abbreviate $\rho^{(p,p)} \equiv \rho^{(p)}$ in the case of gauge invariant states. Next, we note that (8.6) implies that the operator kernel of $\rho^{(p,q)}$ may be expressed as

$$\rho^{(p,q)}(x_1,\ldots,x_p;y_1,\ldots,y_q) \;=\; \big\langle \rho, \overline{\psi}(y_q)\cdots\overline{\psi}(y_1)\psi(x_1)\cdots\psi(x_p)\big\rangle\,. \tag{8.11}$$

There is a particular subset of gauge invariant states that is of interest for studying the Hartree-Fock dynamics. Let $\gamma \in \mathcal{D}$ be a one-particle density matrix. Define the state ρ_γ through $\rho_\gamma^{(p,q)} = 0$ if $p \neq q$ and

$$\rho_\gamma^{(p,p)} \;:=\; \gamma^{(p)}\,, \tag{8.12}$$

where $\gamma^{(p)}$ is defined in (5.1). One immediately finds $\|\rho_\gamma\|_1 = \|\gamma\|_1$.

8.4. Hamilton function and dynamics. Let h be the one-particle Hamiltonian and w the two-body interaction potential. We define a Hamilton function on (a dense subset of) the phase space $\mathfrak{R}$ through

$$\begin{aligned} H \;&:=\; \mathbb{A}^G(h) + \frac{1}{2}\mathbb{A}^G(W) \\ &=\; \int \mathrm{d}x\,\mathrm{d}y\; \overline{\psi}(x)\, h(x;y)\, \psi(y) + \frac{1}{2}\int \mathrm{d}x\,\mathrm{d}y\; \overline{\psi}(y)\overline{\psi}(x)\, w(w-y)\, \psi(x)\psi(y)\,. \end{aligned} \tag{8.13}$$

The Hamiltonian equations of motion read

$$\dot{a} \;=\; \{H, a\}\,,$$

where $a \in \mathfrak{B}^G$. Instead of the "Heisenberg" evolution of a we consider the dual "Schrödinger" evolution of states:

$$\langle \rho(t)\,, a\rangle \;:=\; \langle \rho\,, a(t)\rangle\,.$$

The equation of motion for states reads

$$\begin{aligned} \mathrm{i}\partial_t \rho^{(p,q)}(x_1,\ldots,x_p;y_1,\ldots,y_q) \;&=\; \Bigg(\sum_{i=1}^p h_{x_i} - \sum_{i=1}^q h_{y_i}\Bigg)\rho^{(p,q)}(x_1,\ldots,x_p;y_1,\ldots,y_q) \\ &\quad + \int \mathrm{d}u\, \Bigg(\sum_{i=1}^p w(u-x_i) - \sum_{i=1}^q w(u-y_i)\Bigg)\rho^{(p+1,q+1)}(x_1,\ldots,x_p,u;y_1,\ldots,y_q,u)\,. \end{aligned} \tag{8.14}$$

This has the form of an infinite hierarchy, which decouples over subspaces of different degree. In order to show (8.14) we compute

$$\begin{aligned}\mathrm{i}\big\{H,\overline{\psi}(y_q)\cdots\overline{\psi}(y_1)\psi(x_1)\cdots\psi(x_p)\big\} \;&=\; \left(\sum_{i=1}^{p}h_{x_i}-\sum_{i=1}^{q}h_{y_i}\right)\overline{\psi}(y_q)\cdots\overline{\psi}(y_1)\psi(x_1)\cdots\psi(x_p)\\ &+\int\mathrm{d}u\left(\sum_{i=1}^{p}w(u-x_i)-\sum_{i=1}^{q}w(u-y_i)\right)\overline{\psi}(u)\overline{\psi}(y_q)\cdots\overline{\psi}(y_1)\psi(x_1)\cdots\psi(x_p)\psi(u)\,.\end{aligned}$$

Then (8.14) follows from (8.11) and

$$\begin{aligned}\mathrm{i}\partial_t\rho^{(p,q)}(x_1,\ldots,x_p;y_1,\ldots,y_q) \;&=\; \mathrm{i}\partial_t\big\langle\rho,\overline{\psi}(y_q)\cdots\overline{\psi}(y_1)\psi(x_1)\cdots\psi(x_p)\big\rangle\\ &=\; \big\langle\rho,\mathrm{i}\big\{H,\overline{\psi}(y_q)\cdots\overline{\psi}(y_1)\psi(x_1)\cdots\psi(x_p)\big\}\big\rangle\,.\end{aligned}$$

Next, we outline how to solve the equation of motion (8.14). Let us first rewrite it as

$$\begin{aligned}\mathrm{i}\partial_t\rho^{(p,q)} \;=\; &\sum_{i=1}^{p}h_i\rho^{(p,q)}-\sum_{i=1}^{q}\rho^{(p,q)}h_i\\ &+\sum_{i=1}^{p}\mathrm{Tr}_{p+1,q+1}\big(W_{i\;p+1}\rho^{(p+1,q+1)}\big)-\sum_{i=1}^{q}\mathrm{Tr}_{p+1,q+1}\big(\rho^{(p+1,q+1)}W_{i\;q+1}\big)\,.\end{aligned}$$

We may now proceed exactly as with the density matrix Hartree-Fock equation (3.3), i.e. express it as an integral equation in the interaction picture. This yields a tree expansion for the quantity $\mathrm{Tr}\big(\rho^{(p,q)}(t)\,a^{(q,p)}\big)$, where $\rho(0)\in\mathfrak{R}$. We omit the uninteresting details. As above, the tree expansion converges if $t<T$, where

$$T \;:=\; (2^{11}\pi\kappa^2)^{-1}\,. \tag{8.15}$$

Unfortunately, the time evolution (8.14) does not preserve the norm of ρ, which means that we cannot iterate the short-time result.

8.5. A Schwinger-Dyson series for the time evolution of observables. From now on, we only consider gauge invariant quantities. Take some gauge invariant state $\rho=(\rho^{(p)})_{p\in\mathbb{N}}\in\mathfrak{R}$. For simplicity, we assume that the sequence ρ is finite (as is the case if ρ is defined by a Slater determinant, see below). Let us denote the Hamiltonian flow on $\mathfrak{R}$ by ϕ^t. We have seen that ϕ^t is well-defined by its tree expansion for $t<T$. The solution of (8.14) with initial data ρ, $\rho(t)=\phi^t(\rho)$, satisfies the equation

$$\tilde{\rho}^{(p)}(t) \;=\; \rho^{(p)}-\mathrm{i}\int_0^t\mathrm{d}s\;\sum_{i=1}^{p}\mathrm{Tr}_{p+1}\big[W_{i\;p+1,s},\tilde{\rho}^{(p+1)}(s)\big]\,, \tag{8.16}$$

where $\tilde{\rho}^{(p)}(t):=\mathrm{e}^{\mathrm{i}\sum_i h_i t}\,\rho^{(p)}(t)\,\mathrm{e}^{-\mathrm{i}\sum_i h_i t}$. Let us take a gauge invariant observable $a^{(p,p)}\equiv a^{(p)}\in\mathfrak{A}^G$, where

$$\mathfrak{A}^G \;:=\; \{a\in\mathfrak{B}^G\,:\,a^{(p,q)}=0\text{ if }p\neq q\}$$

is the set of gauge invariant observables. Then (8.16) implies

$$\mathrm{Tr}\big(a^{(p)}\rho^{(p)}(t)\big) \;=\; \mathrm{Tr}\big(a_t^{(p)}\tilde{\rho}^{(p)}(t)\big) \;=\; \mathrm{Tr}\big(a_t^{(p)}\rho^{(p)}\big)+\mathrm{i}\int_0^t\mathrm{d}s\;\sum_{i=1}^{p}\mathrm{Tr}\Big(\Big[W_{i\;p+1,s},a_t^{(p)}\otimes\mathbb{1}\Big]\tilde{\rho}^{(p+1)}(s)\Big)\,.$$

Iteration of this identity gives

$$\mathrm{Tr}\big(a^{(p)}\rho^{(p)}(t)\big) \;=\; \sum_{k=0}^{\infty} \mathrm{Tr}\Big(G_t^{(k,0)}(a^{(p)})\,\rho^{(p+k)}\Big)\,.$$

Summarizing:

$$\begin{aligned}\big\langle a^{(p)}\circ\phi^t\,,\rho\big\rangle \;=\; \big\langle a^{(p)}\,,\rho(t)\big\rangle \;&=\; \mathrm{Tr}\big(a^{(p)}\rho^{(p)}(t)\big)\\ &=\; \sum_{k=0}^{\infty}\mathrm{Tr}\Big(G_t^{(k,0)}(a^{(p)})\,\rho^{(p+k)}\Big) \;=\; \left\langle \sum_{k=0}^{\infty} G_t^{(k,0)}(a^{(p)})\;,\;\rho\right\rangle.\end{aligned}$$

This series converges for $t<T$, uniformly for bounded $\|a^{(p)}\|_{\mathfrak{B}^G}$ and $\|\rho\|_{\mathfrak{R}}$. Therefore we get the norm-convergent series

$$\mathbb{A}^G(a^{(p)})\circ\phi^t \;=\; \sum_{k=0}^{\infty}\mathbb{A}^G\Big(G_t^{(k,0)}(a^{(p)})\Big)\,, \tag{8.17}$$

provided that $t<T$.

Finally, we discuss the relationship between the Hartree-Fock dynamics and the dynamics generated by (8.14). Take a density matrix $\gamma\in\mathcal{D}$ and consider the state $\rho=\rho_\gamma$ defined in (8.12). If one chooses a sequence γ_N such that $\|\gamma_N\|\to 0$ as $N\to\infty$ (e.g. a sequence of Slater determinants), then Lemma 7.2 implies that (8.14) and the Hartree-Fock equation describe the same dynamics for large N.

8.6. Quantization and a Egorov-type theorem. In this final section we introduce a Wick quantization of the above "superhamiltonian" system and formulate the mean-field limit as a Egorov-type theorem. It is advantageous to use the second quantized formulation of Section 4.

We define *quantization*, denoted by $\widehat{(\cdot)}_\nu$, as the linear map defined by the replacement $\psi(x)\mapsto a_\nu(x)$ and $\overline{\psi}(x)\mapsto a_\nu^*(x)$, followed by Wick ordering. Quantization $\widehat{(\cdot)}_\nu$ maps observables in $\mathfrak{B}^G$ to closed operators on $\mathcal{F}$. Moreover, we have

$$\widehat{(\cdot)}_\nu \;:\; \mathbb{A}^G(a^{(p)}) \;\mapsto\; \widehat{\mathbb{A}}_\nu(a^{(p)})\,.$$

Using (8.10), it is easy to see that, for $A,B\in\mathfrak{A}^G$,

$$\big[\widehat{A}_\nu,\widehat{B}_\nu\big] \;=\; \frac{\nu^{-1}}{\mathrm{i}}\widehat{\{A,B\}}_\nu + O(\nu^{-2})\,.$$

This identifies ν^{-1} as the deformation parameter of $\widehat{(\cdot)}_\nu$.

Extending the definition of $\widehat{(\cdot)}_\nu$ to unbounded operators in the obvious way, we define a Hamiltonian $\widehat{H}_\nu$ on $\mathcal{F}$ as the quantization of the Hamilton function H defined in (8.13). When restricted to $\mathcal{H}_-^{(N)}$, $N\widehat{H}_N$ is equal to the Hamiltonian with mean-field scaling (1.2).

Now (7.10), (7.11) and (8.17) yield the following Egorov-type theorem.

THEOREM 8.1. *Let $A\in\mathfrak{A}^G$ and $t<T$, with T defined in* (8.15). *Then*

$$\left\|\left(\mathrm{e}^{\mathrm{i}tN\widehat{H}_N}\,\widehat{A}_N\,\mathrm{e}^{-\mathrm{i}tN\widehat{H}_N} - \widehat{(A\circ\phi^t)}_N\right)\Big|_{\mathcal{H}_-^{(N)}}\right\| \;\leqslant\; \frac{C}{N}\,,$$

for some $C>0$.

A. Hamiltonian formulation for density matrices

In Section 2 we chose a Hamiltonian formulation of the Hartree-Fock equation (2.3) in terms of sequences of orbitals. Alternatively, we could just as well have used a Hamiltonian formulation in terms of density matrices. To see how the density matrix Hartree-Fock equation (3.3) can be written as a Hamiltonian equation of motion of a classical Hamiltonian system, consider the Hilbert space

$$\widehat{\mathcal{H}} \;=\; \mathcal{L}^2(\mathcal{H})\,,$$

the space of Hilbert-Schmidt operators, with scalar product

$$\langle \kappa\,,\rho\rangle \;:=\; \mathrm{Tr}(\kappa^*\rho)\,.$$

We write the density matrix $\gamma \in \mathcal{D}$ as $\gamma = \kappa\kappa^*$, where $\kappa \in \widehat{\mathcal{H}}$. The classical phase space is then given by a Sobolev-type space of Hilbert-Schmidt operators

$$\widehat{\Gamma} \;:=\; \big\{\kappa \in \widehat{\mathcal{H}} \,:\, \mathrm{Tr}(\kappa^*(\mathbb{1}-\Delta)\kappa) < \infty\big\}\,.$$

We define polynomial functions on $\widehat{\Gamma}$ through

$$\mathbb{B}(a^{(p)})(\kappa) \;:=\; \big\langle \kappa^{\otimes p}, a^{(p)}\kappa^{\otimes p}\big\rangle\,,$$

where $a^{(p)} \in \mathcal{L}(\mathcal{H}^{\otimes p})$.

The affine space $\widehat{\Gamma}$ carries a Symplectic form defined by

$$\omega \;=\; -\mathrm{i}\int \mathrm{d}x\,\mathrm{d}y\;\mathrm{d}\bar\kappa(x,y)\wedge \mathrm{d}\kappa(x,y)\,,$$

where $\kappa(x,y)$ is the operator kernel of κ. The Poisson bracket then reads

$$\begin{aligned}\big\{\kappa^{\#}(x,y),\kappa^{\#}(x',y')\big\} \;&=\; 0\\ \{\kappa(x,y),\bar\kappa(x',y')\} \;&=\; -\mathrm{i}\delta(x-x')\delta(y-y')\,.\end{aligned}$$

The Hamilton function is defined by

$$H \;:=\; \mathbb{B}(h) + \frac{1}{2}\mathbb{B}(\mathcal{W})\,.$$

By using Sobolev-type inequalities one readily sees that H is well-defined on $\widehat{\Gamma}$. After a short computation, one finds that the Hamiltonian equation of motion,

$$\mathrm{i}\partial_t\kappa(x,y) \;=\; \frac{\delta H}{\delta\bar\kappa(x,y)} \;=\; \mathrm{i}\,\{H,\kappa(x,y)\}\,,$$

reads

$$\mathrm{i}\partial_t\kappa \;=\; h\kappa + \mathrm{Tr}_2\big(\mathcal{W}\,\kappa\otimes(\kappa\kappa^*)\big)\,.$$

It follows that $\gamma = \kappa\kappa^*$ satisfies (3.3).

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