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Bernard Ducomet

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WEAK INTERACTION LIMIT FOR NUCLEAR MATTER AND THE TIME-DEPENDENT HARTREE-FOCK EQUATION

Bernard Ducomet, Bruyères le Châtel

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Abstract. We consider an effective model of nuclear matter including spin and isospin degrees of freedom, described by an N-body Hamiltonian with suitably renormalized two-body and three-body interaction potentials. We show that the corresponding mean-field theory (the time-dependent Hartree-Fock approximation) is "exact" as N tends to infinity.

Keywords: time-dependent Hartree-Fock equation, nuclear matter

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1. Introduction

The time-dependent Hartree Fock (TDHF) approximation, used in various quantum situations, is based on the hope that one can describe an interacting fermion system in terms of an effective single-particle problem. The many-body wave-function of the system with Hamiltonian H is approximated by a single (Slater) determinant $|\Psi(t)\rangle$ by using a variational criterion: at any $t > 0$, the deviation between $|\Psi(t)\rangle$ and the true wave-function is minimized. In other words, the variation $\delta(\langle\Psi(t)|\mathrm{i}\hbar\partial_t - H|\Psi(t)\rangle)$ equals zero with the constraint that at each time the trial function is a single Slater determinant $\Psi(t) = (1/\sqrt{N!})\det\{\varphi_i(x_j,t)\}$, where $\varphi_i(x_j,t)$ are single-particle functions.

In order to have a more precise idea of this deviation, a natural way to proceed is to build a quantum hierarchy (analogous to the BBGKY (Bogoliubov-Born-Green-Kirkwood-Yvon) hierarchy of classical statistical mechanics) having the TDHF equation as a "weak interacting" limit in a sense to be defined (see [23]). This strategy has been recently elaborated in a series of works (see [16] and the references therein).

In nuclear physics involving nucleons (spin $\frac{1}{2}$ and isospin $\frac{1}{2}$ particles), the mean field computed with the TDHF approximation is especially interesting: it is a natural candidate to get collective information in large amplitude dynamics, while its static limit accurately predicts energies and charge density distributions for most of nuclei throughout the Periodic table [19]; moreover, in the small amplitude limit, TDHF reduces to the Random Phase Approximation (RPA) which qualitatively describes the excitation energies and transition charge densities for appropriate low-lying collective states [21].

In this article we consider a model of nuclear matter including two-body and three-body interactions and we derive the time-dependent Hartree-Fock equation as a mean field dynamical equation for this system. The corresponding mean field limit is conveniently investigated in terms of a density operator $D_N(t)$, in the Schrödinger picture, where $D_N(t)$ obeys the von Neumann equation

$$
\begin{aligned}
\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}D_N(t) = \sum_{1\leqslant j\leqslant N}[L_j, D_N(t)] + \frac{1}{N-1}\sum_{1\leqslant i<j\leqslant N}[V_{ij}, D_N(t)] \\
+ \frac{1}{(N-1)(N-2)}\sum_{1\leqslant i<j<k\leqslant N}[W_{ijk}, D_N(t)]
\end{aligned}
\tag{1.1}
$$

with V_{ij} denoting the two-body potential V acting between the ith and jth particles ($[\,,]$ denoting the commutator) and W_{ijk} denoting the three-body potential W acting between the ith, the jth and the kth particles.

The physical situation described by (1.1) is a weak interaction limit in the following sense: each term on the right-hand side is supposed to act on an equal footing which implies renormalization coefficients of order N^{-1} for the two-body potential and N^{-2} for the three-body potential.

The limit as $N \to \infty$ of the n-body density operator, denoted by $D_{N:n}(t)$, is shown to converge to the suitably antisymmetrized version of $D(t)^{\otimes n}$, where $D(t)$ obeys the so-called time-dependent Hartree-Fock equation.

As in [3], the initial state is chosen to be a Slater determinant which is a suitably factorized state consistent with Fermi-Dirac statistics. Assuming that $\{D_N(0)\}$ is a sequence of initial states for (1.1) that are close to Slater determinants (this property described below will be called the Slater closure), we can prove that $\{D_N(t)\}$ has the Slater closure for all $t > 0$. Since $\{D_N(t)\}$ has Slater closure, the two-body density operator $D_{N:2}(t)$ and the three-body density operator $D_{N:3}(t)$ are approximately equal to $(D_{N:1}(t) \otimes D_{N:1}(t))\Sigma_2$, and $(D_{N:1}(t) \otimes D_{N:1}(t) \otimes D_{N:1}(t))\Sigma_3$ when N is large.

Substituting $(D_{N:1}(t)\otimes D_{N:1}(t))\Sigma_2$ for $D_{N:2}(t)$ and $(D_{N:1}(t)\otimes D_{N:1}(t)\otimes D_{N:1}(t))\Sigma_3$ for $D_{N:2}(t)$ and $D_{N:3}(t)$ in the hierarchy, one may guess that for large N, the single-body density operator should nearly obey the time-dependent Hartree-Fock (TDHF) equation

$$i\hbar \frac{\mathrm{d}}{\mathrm{d}t} F(t) = [L, F(t)] + [V, (F(t) \otimes F(t))\Sigma_2]_{:1} + [W, (F(t) \otimes F(t) \otimes F(t))\Sigma_3]_{:1},$$
$$F(0) = D_{N:1}(0).$$

In fact, according to our result (Theorem 3.1), the distance in the trace norm between $D_{N:1}(t)$ and the corresponding solution to the TDHF equation tends to 0 as N tends to infinity.

In this article, we assume that the two-body potential V and the three-body potential W are bounded operators in a suitable Hilbert space. For technical reasons, which are commented from a physical point of view in Section 2, our results are limited to non charged fermions. However, recent works [5], [18] suggest that it may be possible to prove a theorem similar to our Theorem 3.1 for the case, where V is the Coulomb potential.

The plan of the paper is as follows: in Section 2 we briefly review some specific aspects of effective nuclear interactions, then we state and prove (Section 3) our convergence result, finally we comment in the last section on the Hartree approximation and the main difficulties one has to face in order to consider more realistic models.

2. The nuclear N-body problem

Low energy nuclear physics considers nucleons (neutrons and protons) as the elementary constituents of nuclei. In fact nucleons may be considered as bound states of quarks, themselves strongly interacting through gluons, but one (presently) does not know how to derive qualitatively the nucleon-nucleon interaction from the corresponding gauge field theory (Quantum Chromodynamics or QCD). As far as low energy nuclear physics is concerned the quark-gluons degrees of freedom are not directly observed and nucleons are the physically relevant objects. However, even in this context, properties of nuclei cannot directly be derived from a possible "bare" interaction between nucleons, which is too singular to be treated through perturbative methods and one is forced to derive "dressed" (effective) interactions, modelling the "nuclear medium" in a phenomenological way, the so-called effective phenomenological interactions, for which the many body methods such as Hartree-Fock approximation may be used. These effective forces include a number of parameters which have to be adjusted in order to fit experimental data.

In various contexts such as dynamics of heavy nuclei or neutron stars astrophysics, one deals with a large number of particles and it is natural to consider an idealized situation consisting of an infinite collection of nucleons. However, this simple model leads to some conceptual difficulties: contrary to the "atomic" situation, where negative charges of electrons are neutralized by the positively charged ionic background, such a neutralization cannot exist in the nuclear case.

One observes that, for light nuclei, the numbers of protons and neutrons tend to be equal for the more stable configurations. As the mass of the nucleus increases, the number of neutrons exceeds the number of protons, due to the Coulomb repulsion between the protons: it is precisely this Coulomb force which prevents nuclei of arbitrary mass from being stable.

In fact, despite Coulomb repulsion, the fact that nucleons can be brought together to form stable nuclei shows that the specifically nuclear forces are much stronger that the Coulomb forces. To study the effect of these nuclear forces, it is therefore convenient to think of the Coulomb force switched off.

Finally, we adopt the following definition of nuclear matter: a large but equal number of protons and neutrons held together only by the strong nuclear forces, which is physically relevant as one expects that the cores of large nuclei that exist in nature will bear some resemblance to chunks of this idealized matter.

In the rest of this section, we briefly review the main models used by physicists to model nuclear interactions and we show that a mean-field result applies to an important class of effective interactions including the D1S model [12].

2.1. The Hamiltonian for nuclear matter: a short review

To describe particles with spin and isospin degrees of freedom (see [1]), the appropriate one-particle Hilbert space is $\mathfrak{H} = L^2(\mathbb{R}^3 \times \{-1/2, 1/2\} \times \{-1/2, 1/2\}) \sim L^2(\mathbb{R}^3, \mathbb{C}^2 \otimes \mathbb{C}^2)$, corresponding to the discrete spin (spin up $\sigma = 1/2$ and spin down $\sigma = -1/2$) and isospin (neutron $\tau = -1/2$ and proton $\tau = 1/2$) degrees of freedom.

Denoting collectively by $x := (r, \sigma, \tau)$ the space-spin-isospin degree of freedom, the scalar product on $\mathfrak{H}$ is

$$(\varphi, \psi) := \sum_{\sigma=-1/2,1/2} \sum_{\tau=-1/2,1/2} \int_{\mathbb{R}^3} \varphi(r, \sigma, \tau) \overline{\psi}(r, \sigma, \tau) \, \mathrm{d}r.$$

If one wants to stress the spinor character of the wave function [1], a convenient and global notation for the wave function of a particle j is

$$\psi_j(x) = \varphi_j(r) \chi_\sigma(j) \zeta_\tau(j),$$

where x denotes the set (r, σ, τ), $\varphi_j(r)$ is the spatial part of the wave function, $\chi_\sigma(j)$ is the spin wave-function, and $\zeta_\tau(j)$ is the isospin wave-function.

The angular momentum operator $\mathbf{L}$ with components $\mathbf{L}_\alpha$ for $\alpha = 1, 2, 3$ is defined by

$$\mathbf{L}_\alpha := -\mathrm{i}\Big(r_\beta \frac{\partial}{\partial r_\gamma} - r_\gamma \frac{\partial}{\partial r_\beta}\Big),$$

where (α, β, γ) is a cyclic permutation of $(1, 2, 3)$.

The spin operators $\mathbf{S}_3$, $\mathbf{S}_+$, and $\mathbf{S}_-$ are defined by

$$(\mathbf{S}_3\varphi)(r,\sigma,\tau) := \hbar\sigma\varphi(r,\sigma,\tau) \quad \text{for } \sigma \in \{-1/2, 1/2\},$$
$$(\mathbf{S}_+\varphi)(r,\sigma,\tau) := \hbar\sqrt{(1/2+\sigma)(3/2-\sigma)}\varphi(r,\sigma-1,\tau) \quad \text{for } \sigma \in \{-1/2, 1/2\},$$

and

$$(\mathbf{S}_-\varphi)(r,\sigma,\tau) := \hbar\sqrt{(1/2-\sigma)(3/2+\sigma)}\varphi(r,\sigma+1,\tau) \quad \text{for } \sigma \in \{-1/2, 1/2\},$$

where one checks that $(\mathbf{S}_+\varphi)(r,\sigma = -1/2,\tau) = (\mathbf{S}_-\varphi)(r,\sigma = 1/2,\tau) = 0$, and the three components $\mathbf{S}_\alpha$, for $\alpha = 1, 2, 3$, of the spin operator $\vec{\mathbf{S}}$ used in the spin-orbit interaction are defined by $\mathbf{S}_1 = \mathrm{i}^{-1}(\mathbf{S}_+ + \mathbf{S}_-)$, $\mathbf{S}_2 = -\mathrm{i}^{-1}(\mathbf{S}_+ - \mathbf{S}_-)$, and $\mathbf{S}_3$.

The isospin operators $\mathbf{T}_1$, $\mathbf{T}_2$, and $\mathbf{T}_3$ are defined exactly by the same expressions, just by exchanging the respective roles of the spin σ and the isospin τ.

For a two nucleons system (1,2), one also defines the two-body spin exchange operator $\mathbf{P}_\sigma$ acting on simple states by

$$\mathbf{P}_\sigma\varphi(r_1,\sigma_1,\tau_1)\varphi(r_2,\sigma_2,\tau_2) = \varphi(r_1,\sigma_2,\tau_1)\varphi(r_2,\sigma_1,\tau_2),$$

the two-body isospin exchange operator $\mathbf{P}_\tau$ by

$$\mathbf{P}_\tau\varphi(r_1,\sigma_1,\tau_1)\varphi(r_2,\sigma_2,\tau_2) = \varphi(r_1,\sigma_1,\tau_2)\varphi(r_2,\sigma_2,\tau_1),$$

and the Majorana operator

$$\mathbf{P}_M = -\mathbf{P}_\sigma\mathbf{P}_\tau.$$

For the one-body contribution we take the kinetic operator together with the intrinsic spin-orbit contribution

$$\mathcal{L} := -\frac{\hbar^2}{2m}\Delta + w_{ls}\mathbf{L}\cdot\mathbf{S}, \tag{2.1}$$

where one can take (see below) $w_{ls} = 115\ \ \mathrm{MeV\,fm}^5$.

Concerning the N-body contributions with $N > 1$, a lot of models have been proposed, suitable for different physical contexts: a *bare interaction* successful to describe nucleon-nucleon scattering is often not convenient to describe static properties of large nuclei. In this last case, *effective interactions* taking into account the medium effects are better, however they do not give correct agreement with experiments in scattering processes.

From a general point of view, the best way to go ahead is first to discuss the general properties an interaction should have in order to satisfy general symmetry requirements[1], then to specialize to either the bare interactions or the effective ones.

2.1.1. General properties of nucleon-nucleon interaction. Let us postulate the following general form for the nucleon-nucleon potential

$$V = V(r_1, r_2, p_1, p_2, \sigma_1, \sigma_2, \tau_1, \tau_2),$$

where $(r_1, p_1, \sigma_1, \tau_1)$ and $(r_2, p_2, \sigma_2, \tau_2)$ are the position, momentum, spin and isospin of the first and the second particle, respectively.

According to the first principles of quantum mechanics, the functional form of V is restricted by the symmetries acting on the system: due to *translational invariance*, V depends only on $r := r_1 - r_2$, then by *Galilei invariance*, V depends only on the relative momentum $p := p_1 - p_2$, by *rotational invariance*, any contribution in V must have a zero total momentum; by *isospin invariance*, as only contributions scalar under rotation in the isospin space are allowed, V must include only powers of $\tau_1 \cdot \tau_2$. Finally, *parity invariance* requires that $V(r, p, \sigma_1, \sigma_2, \tau_1, \tau_2) = V(-r, -p, \sigma_1, \sigma_2, \tau_1, \tau_2)$ (only even powers of r and p are allowed) and *time reversal invariance* requires that $V(r, p, \sigma_1, \sigma_2, \tau_1, \tau_2) = V(r, -p, -\sigma_1, -\sigma_2, \tau_1, \tau_2)$ (only an even number of p and σ combined are allowed in each term).

Even after these restrictions a lot of models may be constructed, starting with the lowest order terms such as $\mathbf{S}_1 \cdot \mathbf{S}_2$, $(\mathbf{r} \cdot \mathbf{S}_1)(\mathbf{r} \cdot \mathbf{S}_2)$ or $-i\hbar(\mathbf{r} \times \mathbf{p}) \cdot (\mathbf{S}_1 + \mathbf{S}_2)$, where $\mathbf{S}_j$ and $\mathbf{T}_j$ are the previous spin and isospin operators corresponding to the nucleon j for $j = 1, 2$.

The simplest form of V is the central momentum-independent force:

$$V = V_0(r) + V_\sigma(r)\, \mathbf{S}_1 \cdot \mathbf{S}_2 + V_\tau(r)\, \mathbf{T}_1 \cdot \mathbf{T}_2 + V_{\sigma\tau}(r)\, (\mathbf{S}_1 \cdot \mathbf{S}_2)(\mathbf{S}_1 \cdot \mathbf{S}_2),$$

which one rewrites, using the previous exchange operators, as

$$V = V_W(r) + V_M(r)\mathbf{P}_r + V_B(r)\mathbf{P}_\sigma + V_H(r)\mathbf{P}_\tau, \tag{2.2}$$

where the indices stand for Wigner, Majorana, Barlett, and Heisenberg.

[1] This is the strategy commonly used in mechanics of continuous media, where symmetries give restrictions on the state functions.

2.1.2. “Bare” interactions from nucleon-nucleon scattering. From low-energy nucleon-nucleon scattering, some basic features emerge: the interaction is short range (about 1 fm), within this range it is attractive at “large distance” and strongly repulsive at “short distance” ($\leqslant 0.5$ fm), and it depends both on the spin and isospin of the two nucleons. Starting from the idea that the nucleon-nucleon interaction is mediated by pions as Coulomb interaction is mediated by photons, one gets the OPEP (One Pion Exchange Potential)

$$\mathbf{V}_{\mathrm{OPEP}}(r_1 - r_2, \sigma_1, \sigma_2, \tau_1, \tau_2) = -\frac{f^2}{4\pi\mu}(\mathbf{T}_1 \cdot \mathbf{T}_2)(\mathbf{S}_1 \cdot \nabla_1)(\mathbf{S}_2 \cdot \nabla_2)\frac{\mathrm{e}^{-\mu|r_1 - r_2|}}{|r_1 - r_2|}, \tag{2.3}$$

where f is a coupling constant and μ the mass of the pion.

A second popular version of nucleon-nucleon interaction is the Hamada-Johnston potential, which has the general form

$$\mathbf{V}_{HJ} = \mathbf{V}_C(r) + V_T(r)\mathbf{S}_{12} + V_{LS}(r)\mathbf{L} \cdot \mathbf{S} + V_{LL}(r)\mathbf{L}_{12}, \tag{2.4}$$

where

$$\mathbf{S}_{12} := (V_0(r) + V_1(r)(\mathbf{T}_1 \cdot \mathbf{T}_2))\Big[\frac{(r \cdot \mathbf{S}_1)(r \cdot \mathbf{S}_2)}{r^2} - \frac{1}{3}\mathbf{S}_1 \cdot \mathbf{S}_2\Big]$$

is a tensor term taking into account the quadrupole moment of the deuteron (two-nucleon state), and

$$\mathbf{L}_{12} := \mathbf{L}^2(\mathbf{S}_1 \cdot \mathbf{S}_2) - \frac{1}{2}[(\mathbf{S}_1 \cdot \mathbf{L})(\mathbf{S}_2 \cdot \mathbf{L}) + (\mathbf{S}_2 \cdot \mathbf{L})(\mathbf{S}_1 \cdot \mathbf{L})],$$

and the radial parts are inspired by the meson exchange potentials

$$\mathbf{V}_C(r) = c_0\mu c^2(\mathbf{T}_1 \cdot \mathbf{T}_2)(\mathbf{S}_1 \cdot \mathbf{S}_2)\frac{\mathrm{e}^{-\mu r}}{\mu r}\Big(1 + a_C\frac{\mathrm{e}^{-\mu r}}{\mu r} + b_C\frac{\mathrm{e}^{-2\mu r}}{\mu r^2}\Big)$$

and similar expressions for V_T, V_{LS}, and V_{LL}.

While the models discussed previously describe successfully scattering experiments, they are rarely used in typical nuclear structure calculations. It seems that in nuclei the interaction is strongly modified by complicated many-body effects and it becomes more profitable to design effective interactions, which include many-body correlations, and accordingly are especially suitable for mean-field calculations.

2.1.3. Effective interactions. The simplest effective interactions correspond to contact forces (Dirac distributions)

$$\mathbf{V}_{ij} = V_0\delta(r)\mathbf{I} + V_1(\mathbf{p}_i^2\delta(r) + \delta(r)\mathbf{p}_j^2) + V_2\mathbf{p}_i \cdot \delta(r)\mathbf{p}_j, \tag{2.5}$$

where $\mathbf{p}_j$ is the momentum operator for the nucleon j.

The radial parts may be chosen as gaussian $V(r) = -V_0 \mathrm{e}^{-r^2/r_0^2}$, or of Hulthén type $V(r) = -V_0\,\mathrm{e}^{-r/r_0}/(1-\mathrm{e}^{-r/r_0})$, or of contact type $V(r) = -V_0\delta(r/r_0)$, where $V_0 \sim 50\,\mathrm{MeV}$ and $1 \leqslant r_0 \leqslant 2\,\mathrm{fm}$.

However, the most widely used interactions in Hartree-Fock calculations are the forces of Skyrme type [21], which also include a three-body contribution. The total interaction is then

$$V = \sum_{i<j}^{N} V_{ij} + \sum_{i<j<k} V_{ijk}.$$

The two-body term contains the momentum dependence and the spin-exchange contribution and a spin-orbit term

$$\begin{aligned}\mathbf{V}_{ij} &= t_0(1 + x_0\mathbf{P}_\sigma)\delta(r_i - r_j) + \frac{1}{2}t_2\big(\delta(r_i - r_j)\mathbf{k}^2 + \mathbf{k}'^2\delta(r_i - r_j)\big)\\ &\quad + t_2\mathbf{k}'\cdot\delta(r_i - r_j)\mathbf{k} + \mathrm{i}w_0(\mathbf{S}_i + \mathbf{S}_j)\cdot\mathbf{k}'\times\delta(r_i - r_j)\mathbf{k},\end{aligned} \tag{2.6}$$

where the relative momenta operators $\mathbf{k} := \frac{1}{2}\mathrm{i}^{-1}(\nabla_i - \nabla_j)$ and $\mathbf{k}' := -\frac{1}{2}\mathrm{i}^{-1}(\nabla_i - \nabla_j)$ are supposed to obey the convention that $\mathbf{k}$ and $\mathbf{k}'$ act on the wave function at its right and left, respectively.

The three-body interaction is purely local:

$$\mathbf{W}_{ijk} = t_3\delta(r_i - r_j)\delta(r_j - r_k)\mathbf{I}. \tag{2.7}$$

The six parameters t_0, t_1, t_2, t_3, x_0, and w_0 are chosen in order to reproduce the properties of some fixed finite nuclei (for the so-called "Skyrme III" interaction [7], one takes for example $t_0 = -1128.75\,\mathrm{MeV\,fm}^3$, $t_1 = 395.0\,\mathrm{MeV\,fm}^5$, $t_2 = -95.0\,\mathrm{MeV\,fm}^5$, $t_3 = 14000.0\,\mathrm{MeV\,fm}^6$, $w_0 = 120\,\mathrm{MeV\,fm}^5$, $x_0 = 0.45$, where $1\,\mathrm{fm}$ (fermi) $= 10^{-15}\,\mathrm{m}$ and $1\,\mathrm{MeV} = 1.602\cdot 10^{-13}\,\mathrm{J}$ are the standard nuclear units).

One observes that, from the mathematical point of view, the above Skyrme interaction does not lead to a well behaved Hamiltonian, due to the presence of Dirac distributions. Moreover, from the physical point of view, although this model is able to reproduce a number of physical quantities (nuclear binding energies, nuclei radii) over the whole periodic table with a reasonable set of parameters, it leads to "physical divergences", where pairing properties (illustrating superfluid properties of the main part of nuclei) are involved.

In order to avoid these drawbacks, a finite-range interaction has been devised by J. Dechargé and D. Gogny in the seventies, which is free of all these divergences [12], which may be considered as a smeared version of the Skyrme interaction.

For the two-body operator $\mathbf{V}_{ij}$, one considers the short range model [21], [12]

$$\mathbf{V}_{ij} = \sum_{n=1}^{2} \mathrm{e}^{-(|r_i - r_j|)^2/\mu_n}(w_n + b_n\mathbf{P}_\sigma - h_n\mathbf{P}_\tau - m_n\mathbf{P}_\sigma\mathbf{P}_\tau), \tag{2.8}$$

where the sum involves the operators $\mathbf{P}_\sigma$, which exchanges spins σ_i and σ_j, and $\mathbf{P}_\tau$, which exchanges isospins τ_i and τ_j.

We consider finally a purely spatial smeared contribution to the three-body operator $\mathbf{W}_{ijk}$:

$$\mathbf{W}_{ijk} = t_3 \mathrm{e}^{-(|r_i - r_j|^2 + |r_j - r_k|^2)/\mu_2} \mathbf{I}. \tag{2.9}$$

In these expressions w_n, b_n, h_n, m_n are the so-called Wigner, Bartlett, Majorana, and Heisenberg coefficients. Together with the spin-orbit coefficient w_{ls}, the three-body coefficient t_3 and the nuclear ranges μ_n are adjusted to experimental data with precise values (see [12]) given by $\mu_1 = 0.7\,\mathrm{fm}$, $w_1 = -402.4\,\mathrm{MeV}$, $b_1 = -100\,\mathrm{MeV}$, $h_1 = -496.2\,\mathrm{MeV}$, $m_1 = -23.56\,\mathrm{MeV}$, $\mu_2 = 1.2\,\mathrm{fm}$, $w_2 = -21.3\,\mathrm{MeV}$, $b_2 = -11.77\,\mathrm{MeV}$, $h_2 = 37.27\,\mathrm{MeV}$, $m_2 = -68.81\,\mathrm{MeV}$, $w_{ls} = 115\,\mathrm{MeV\,fm}^5$, and $t_3 = 1350\,\mathrm{MeV\,fm}^4$.

We have the following result.

Proposition 1. *Assume that the one body operator is given by* (2.1),

$$\mathcal{L}_i := -\frac{\hbar^2}{2m}\Delta_{r_i} + w_{ls}\mathbf{L}_i \cdot \mathbf{S}_i,$$

and that the interacting operators $\mathbf{V}_{ij}$ and $\mathbf{W}_{ijk}$ satisfy, for any $x = (r, \sigma, \tau) \in \mathbb{R}^3 \times \{-1/2, 1/2\} \times \{-1/2, 1/2\}$, the conditions

$$\mathbf{V}_{ij} := \sum_{l=1}^{4} a_l V_l(|r_i - r_j|)\mathbf{T}_l,$$

where a_l are real constants, $\mathbf{T}_l$ are the spin-isospin exchange operators defined above with $\mathbf{T}_1 = \mathbf{1}$, $\mathbf{T}_2 = \mathbf{P}_\sigma$, $\mathbf{T}_3 = \mathbf{P}_\tau$ and $\mathbf{T}_4 = \mathbf{P}_\sigma\mathbf{P}_\tau$, and such that

$$V_l \in L^2(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$$

for $l = 1, 2, 3, 4$, and

$$\mathbf{W}_{ijk} := W(|r_i - r_j|, |r_j - r_k|)\mathbf{T}_1$$

with

$$W \in L^2(\mathbb{R}^3 \times \mathbb{R}^3) + L^\infty(\mathbb{R}^3 \times \mathbb{R}^3).$$

Then the Hamiltonian $\mathbf{H}_N$ defined in $\mathfrak{H}^N$ by

$$\mathbf{H}_N := \sum_{i=1}^{N} \mathcal{L}_i + \frac{1}{N-1} \sum_{1 \leqslant i < j \leqslant N} \mathbf{V}_{ij} + \frac{1}{(N-1)(N-2)} \sum_{1 \leqslant i < j < k \leqslant N} \mathbf{W}_{ijk}, \tag{2.10}$$

with the domain $\mathcal{D}(\mathbf{H}_N) = (H^2(\mathbb{R}^3, \mathbb{C}^2 \otimes \mathbb{C}^2))^N$, is essentially self-adjoint.

P r o o f. As the spin-isospin dependence of the interaction is present only through the spin-isospin exchange operators $\mathbf{P}_\sigma$ and $\mathbf{P}_\tau$ which are clearly bounded operators, and as the spin-orbit contribution defines a self-adjoint operator by virtue of classical results (see [1], p. 470, and [25]), the above proposition is a direct consequence of Kato's self adjointness criterion [17] for operators $\mathbf{H}_N = \mathbf{H}_0 + \mathbf{H}_I$, where $\mathbf{H}_0 := \sum\limits_{i=1}^{N} \mathcal{L}_i$ is essentially self-adjoint, $\mathbf{H}_I := (N-1)^{-1} \sum\limits_{1\leqslant i<j\leqslant N} \mathbf{V}_{ij} + (N-1)^{-1}(N-2)^{-1} \sum\limits_{1\leqslant i<j<k\leqslant N} \mathbf{W}_{ijk}$ is symmetric and H_0-bounded with H_0-bound less than 1. □

This result implies that Proposition 1 holds for the finite-range model ("D1S Gogny interaction") of nuclear matter introduced in [12], given by (2.8) and (2.9).

Just note that the more singular Skyrme model (2.6)–(2.7) does not satisfy the requirements of Theorem 1, due to the presence of delta distributions.

Moreover, we observe that the two-body and three-body interactions given by (2.8), (2.9) are bounded operators, which will be crucial for applying the machinery of [4].

3. The time-dependent Hartree-Fock approximation

Let us briefly recall some notation from [3]. For nucleons (protons and neutrons) the appropriate N-particle Hilbert space of wavefunctions is the antisymmetric subspace $\mathcal{A}_N \subset \mathfrak{H}_N$ defined by using unitary permutation operators on $\mathfrak{H}_N$. For any π in the group $\mathfrak{G}_N$ of permutations of $\{1,2,\ldots,N\}$, one considers the permutation operator U_π as $U_\pi(\xi_1 \otimes \ldots \otimes \xi_n) = \xi_{\pi^{-1}(1)} \otimes \ldots \otimes \xi_{\pi^{-1}(n)}$. Then $\mathcal{A}_N = \{\psi \in \mathfrak{H}_N \colon\ U_\pi\psi = \operatorname{sgn}(\pi)\psi\ \forall\, \pi \in \mathfrak{G}_N\}$.

We denote in the sequel $\Sigma_n := n! P_{\mathcal{A}_N}$, where $P_{\mathcal{A}_N} = N!^{-1} \sum\limits_{\pi\in\mathfrak{G}_N} \operatorname{sgn}(\pi) U_\pi$ 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 $\mathcal{A}_N$ and the statistical states of the N-fermion system are the positive trace class operators of trace 1 (density operators) D on $\mathcal{A}_N$. These fermionic densities are those density operators that satisfy

$$DU_\pi = U_\pi D = \operatorname{sgn}(\pi) D \quad \forall\, \pi \in \mathfrak{G}_N. \tag{3.1}$$

It is proved in [3] that the operator norm $\|D\|$ of a fermionic density operator on $\mathfrak{H}_N$ is bounded by $1/N$. If $\{e_j\}_{j\in J}$ is an orthonormal basis of $\mathfrak{H}$ then the family

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

is an orthonormal basis of $\mathfrak{H}_N$. Since $\mathcal{A}_N$ is the range of $P_{\mathcal{A}_N}$ and since $P_{\mathcal{A}_N}(e_{j_1} \otimes e_{j_2} \otimes \ldots \otimes e_{j_N}) = 0$, unless all of the indices j_i are distinct, the set

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

is a spanning set for $\mathcal{A}_N$ and the basis vectors for $\mathcal{A}_N$ built in this way are called the *Slater determinants.*

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

$$\langle T_{:n} w, x\rangle = \sum_{j=1}^{N-n} \sum_{y_j \in \mathcal{O}} \langle T(w \otimes y_1 \otimes \ldots \otimes y_{N-n}), (x \otimes y_1 \otimes \ldots \otimes y_{N-n})\rangle \tag{3.2}$$

for any $w, x \in \mathfrak{H}^{\otimes n}$. If a trace class operator $T \in \mathcal{T}(\mathfrak{H}^{\otimes N})$ satisfies (3.1) then so does $T_{:n}$; the partial trace defines a positive contraction from $\mathcal{T}(\mathfrak{H}^{\otimes N})$ to $\mathcal{T}(\mathfrak{H}^{\otimes n})$ that carries fermionic densities to fermionic densities. Finally, if a density operator D on $\mathfrak{H}_N$ commutes with every permutation operator U_π then it is *symmetric.*

Observing that if P_{Ψ_N} denotes the orthogonal projector onto the span of $\Psi_N \in \mathcal{A}_N$ then

$$(P_{\Psi_N})_{:n} = \frac{N^n(N-n)!}{N!}(P_{\Psi_N})_{:1}^{\otimes n} \sum_{\pi \in \Pi_n} \operatorname{sgn}(\pi) U_\pi, \tag{3.3}$$

we introduce the following definition.

Definition 3.1. For each N, let D_N be a symmetric density operator on $\mathfrak{H}_N$. The sequence $\{D_N\}$ has *Slater closure* if, for each fixed n,

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

The N-particle dynamics is described by a self-adjoint operator $\mathrm{i}L^{(N)}$ on $\mathfrak{H}$, where $L^{(N)}$ is the one body potential acting on a single particle; in addition to the kinetic term $-\hbar^2(2m)^{-1}\Delta$, it may also include an external field and the (intrinsic) spin-orbit interaction (see below for a precise definition). Then the free motion of the jth particle will be given by

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

where I denotes the identity operator on $\mathfrak{H}$.

The two-body interaction between the particles will have 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 $\mathfrak{H}\otimes\mathfrak{H}$ that commutes with the transposition operator $U_{(12)}$. Define the operator V_{12} on $\mathfrak{H}_N$ by

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

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 $\pi(j)=2$.

Analogously, the three-body interaction between the particles will have the form $1/(N-1)(N-2)$ times the sum over triples of distinct particles of a three-body potential W. Let W be a bounded Hermitian operator on $\mathfrak{H}\otimes\mathfrak{H}\otimes\mathfrak{H}$ that commutes with the transposition operator U_π for $\pi\in\Pi_3$.

Define also the operator W_{123} on $\mathfrak{H}_N$ by

$$W_{123}(x_1\otimes x_2\otimes x_3\otimes\ldots\otimes x_N)=W(x_1\otimes x_2\otimes x_3)\otimes x_4\otimes\ldots\otimes x_N$$

and for each $1\leqslant i<j<k\leqslant N$ define $W_{ijk}=U_{\pi'}^*W_{123}U_{\pi'}$, where π' is any permutation with $\pi'(i)=1$, $\pi'(j)=2$, and $\pi'(k)=3$.

Let

$$H_N=\sum_{1\leqslant j\leqslant N}L_j^{(N)}+\frac{1}{N-1}\sum_{1\leqslant i<j\leqslant N}V_{ij}+\frac{1}{(N-1)(N-2)}\sum_{1\leqslant i<j<k\leqslant N}W_{ijk}\tag{3.4}$$

be the *N-particle Hamiltonian* operator on $\mathfrak{H}_N$.

The von Neumann equation for the N-particle density operator $D_N(t)$ is

$$\begin{aligned}\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}D_N(t)=&\sum_{1\leqslant j\leqslant N}[L_j^{(N)},D_N(t)]+\frac{1}{N-1}\sum_{1\leqslant i<j\leqslant N}[V_{ij},D_N(t)]\\&+\frac{1}{(N-1)(N-2)}\sum_{1\leqslant i<j<k\leqslant N}[W_{ijk},D_N(t)].\end{aligned}\tag{3.5}$$

Next we define the time-dependent Hartree-Fock equation. Let $L^{(N)}$, V, and W be as above. The time-dependent Hartree-Fock (TDHF) equation for a density operator $F(t)$ on $\mathfrak{H}$ is

$$\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}F(t)=[L^{(N)},F(t)]+[V,F_2^-(t)]_{:1}+[W,F_3^-(t)]_{:1},\tag{3.6}$$

where

$$F_2^-(t) = (F(t) \otimes F(t)) \sum_{\pi \in \Pi_2} \operatorname{sgn}(\pi) U_\pi = F(t)^{\otimes 2}(I - U_{(12)}) = F(t)^{\otimes 2} \Sigma_2$$

and

$$\begin{aligned} F_3^-(t) &= (F(t) \otimes F(t) \otimes F(t)) \sum_{\pi \in \Pi_3} \operatorname{sgn}(\pi) U_\pi \\ &= F(t)^{\otimes 3}(I - U_{(12)} - U_{(13)} - U_{(23)} + U_{(12)}U_{(13)} + U_{(12)}U_{(23)}) = F(t)^{\otimes 3}\Sigma_3 \end{aligned}$$

(the subscript $_{:1}$ on the last two commutators denotes partial contraction). Following [9], we define a strong solution of equation (3.6) as a continuously differentiable function $F(t)$ from $[0, \infty)$ to the real Banach space of Hermitian trace class operators such that the domain of A is invariant under $F(t)$ for all $t \geqslant 0$ and

$$\mathrm{i}\hbar \frac{\mathrm{d}F(t)}{\mathrm{d}t} x = [L^{(N)}, F(t)]x + [V, F_2^-(t)]_{:1} x + [W, F_3^-(t)]_{:1} x$$

for all x in the domain of A. A straightforward extension of the results proved in [9] including the three-body bounded potentials show that (3.6) has a strong solution if the domain of A contains the range of the initial condition $F(0)$. Furthermore, $F(t) = U^* F(0) U$ for some unitary operator depending on t and $F^{(N)}(0)$. In particular, the operator norm of $F(t)$ is constant.

The relationship between the N-particle system and the TDHF equation is described by the following result.

Theorem 3.1. *For each N, let $D_N(t)$ be a solution to (3.5) whose initial value $D_N(0)$ is a symmetric density. Let $F^{(N)}(t)$ be the solution of the TDHF equation (3.6) whose initial value is $F^{(N)}(0) = D_{N:1}(0)$.*

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

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

for all $t > 0$.

P r o o f. Following [3] and [4] the proof is based on a study of the deviation between two suitable hierarchies. We consider first the N-particle von Neumann equation (3.5) with symmetric initial data. From the symmetry of the Hamiltonian (3.4) $D_N(t)$ remains symmetric for all t and by virtue of (3.5) the partial trace $D_{N:n}(t)$

satisfies

$$
\begin{aligned}
\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}D_{N:n}(t) = &\sum_{1\leqslant j\leqslant n}[L_j^{(N)}, D_{N:n}(t)] + \frac{1}{N-1}\sum_{1\leqslant i<j\leqslant n}[V_{ij}, D_{N:n}(t)] \\
&+ \frac{1}{(N-1)(N-2)}\sum_{1\leqslant i<j<k\leqslant n}[W_{ijk}, D_{N:n}(t)] \\
&+ \frac{N-n}{N-1}\sum_{1\leqslant j\leqslant n}[V_{j,n+1}, D_{N:n+1}(t)]_{:n} \\
&+ \frac{N-n}{(N-1)(N-2)}\sum_{1\leqslant i<j\leqslant n}[W_{i,j,n+1}, D_{N:n+1}(t)]_{:n} \\
&+ \frac{(N-n)(N-n-1)}{(N-1)(N-2)}\sum_{1\leqslant j\leqslant n}[W_{j,n+1,n+2}, D_{N:n+2}(t)]_{:n}.
\end{aligned}
$$

This system for $D_{N:1}, D_{N:2}, \ldots, D_{N:N-1}$ together with the equation (3.5) for D_N is called the *N-particle hierarchy* and we rewrite it as

$$
\begin{aligned}
\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}D_{N:n}(t) = &\,\mathcal{L}_{N,n}(D_{N:n}(t)) \\
&+ \sum_{1\leqslant i\leqslant n}[V_{i,n+1}, D_{N:n+1}(t)]_{:n} \\
&+ \sum_{1\leqslant i\leqslant n}[W_{i,n+1,n+2}, D_{N:n+2}(t)]_{:n} + \mathcal{E}_n(t, N, D_N(0))
\end{aligned}
\tag{3.7}
$$

with

$$
\begin{aligned}
\mathcal{L}_{N,n}(\cdot) &= \sum_{1\leqslant j\leqslant n}[L_j^{(N)}, \cdot], \\
\mathcal{E}_n(t, N, D_N(0)) &= \frac{1}{N-1}\sum_{1\leqslant i<j\leqslant n}[V_{ij}, \cdot] \\
&\quad + \frac{1}{(N-1)(N-2)}\sum_{1\leqslant i<j<k\leqslant n}[W_{ijk}, \cdot] \\
&\quad + \frac{N-n}{(N-1)(N-2)}\sum_{1\leqslant i<j\leqslant n}[W_{ij,n+1}, D_{N:n+1}(t)]_{:n} \\
&\quad - \frac{n-1}{N-1}\sum_{1\leqslant i\leqslant n}[V_{i,n+1}, D_{N:n+1}(t)]_{:n} \\
&\quad - \frac{(n-1)(2N-n-2)}{(N-1)(N-2)}\sum_{1\leqslant i\leqslant n}[W_{i,n+1,n+2}, D_{N:n+2}(t)]_{:n}.
\end{aligned}
\tag{3.8}
$$

Now following [3] we consider another hierarchy built from the solutions to the TDHF equation. If F is a trace class operator, define $F_1^- = F$ and $F_n^- = F^{\otimes n}\Sigma_n$ for $n > 1$.

Simply iterating the formula $\Sigma_{n+1} = \Big(I - \sum\limits_{k=1}^{n} U_{(k,n+1)}\Big)\Sigma_n \otimes I_{\mathcal{B}(\mathfrak{H})}$ one checks now that if $F(t)$ is a strong solution of the TDHF equation (3.6) then

$$\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}F_n^-(t) = \sum_{j=1}^{n}[L_j^{(N)}, F_n^-(t)] + \sum_{j=1}^{n}[V_{j,n+1},\ F_{n+1}^-(t)]_{:n} + \sum_{j=1}^{n}[W_{j,n+1,n+2}, F_{n+2}^-(t)]_{:n} + \mathcal{R}_n(F(t)),$$

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

$$\begin{aligned}(3.9)\ \mathcal{R}_n(X) &= \sum_{j=1}^{n}\Big[V_{j,n+1}, X^{\otimes n+1}\sum_{k\neq j}U_{(k,n+1)}\Big]_{:n}\Sigma_n \\ &+ \sum_{j=1}^{n}\Big[W_{j,n+1,n+2}, X^{\otimes n+2}\Big(\sum_{k\neq l}U_{(k,n+1)}U_{(l,n+2)} \\ &+ \sum_{k\neq j}[U_{(k,n+1)}U_{(n+1,n+2)} + U_{(k,n+2)}U_{(k,n+1)} - U_{(k,n+2)} - U_{(k,n+1)}]\Big)\Big]_{:n}\Sigma_n\end{aligned}$$

for $n > 1$. Now let $D_N(t)$ be a solution of the N-particle von Neumann equation (3.5) and let $F(t)$ be a solution of the TDHF equation (3.6). For $1 \leqslant n \leqslant N$ define the nth *difference*

$$E_{N,n}(t) = D_{N:n}(t) - F_n^-(t). \tag{3.10}$$

The N-particle hierarchy equations (3.7), (3.8), and (3.9) imply that

$$\begin{aligned}(3.11)\quad \mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}E_{N,n}(t) &= \mathcal{L}_{N,n}(E_{N,n}(t)) + \sum_{j=1}^{n}[V_{j,n+1}, E_{N,n+1}(t)]_{:n} \\ &+ \sum_{j=1}^{n}[W_{j,n+1,n+2}, E_{N,n+2}(t)]_{:n} + \mathcal{E}_n(t,N,D_N(0)) - \mathcal{R}_n(F(t))\end{aligned}$$

for $n = 1, 2, \ldots, N-1$. Let us define the error

$$\mathrm{Err}(t,N,n) = \mathcal{E}_n(t,N,D_N(0)) - \mathcal{R}_n(F(t)), \tag{3.12}$$

let $U_{n,t}^{(N)}$ denote the unitary operator $\exp\Big((\mathrm{i}t/\hbar)\sum_{j=1}^{n} L_j^{(N)}\Big)$ on $\mathfrak{H}_n$ and define isometries $\mathcal{U}_{N,n,t}$ on the trace class operators by $\mathcal{U}_{N,n,t}(\cdot) = \mathrm{e}^{(\mathrm{i}t/\hbar)\mathcal{L}_{N,n}}(\cdot) = U_{n,t}^{(N)}(\cdot)U_{n,-t}^{(N)}$. Then $Z_{N,n}(t) = \mathcal{U}_{N,n,t}(E_{N,n}(t))$ has the same trace norm as $E_{N,n}(t)$ and satisfies

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}Z_{N,n}(t) = &-\frac{\mathrm{i}}{\hbar}\sum_{j=1}^{n}[V_{j,n+1}, Z_{N,n+1}(t)]_{:n}\\ &-\frac{\mathrm{i}}{\hbar}\sum_{j=1}^{n}[W_{j,n+1,n+2}, Z_{N,n+2}(t)]_{:n} - \frac{\mathrm{i}}{\hbar}\operatorname{Err}(t,N,n)\end{aligned}$$

for $n = 1, 2, \dots, N-1$. This yields that

$$\begin{aligned}\|E_{N,n}(t)\|_{\mathrm{tr}} &= \|Z_{N,n}(t)\|_{\mathrm{tr}}\\ &\leqslant \|Z_{N,n}(0)\|_{\mathrm{tr}} + \frac{2\|V\|n}{\hbar}\int_0^t \|Z_{N,n+1}(s)\|_{\mathrm{tr}}\,\mathrm{d}s\\ &\quad + \frac{2\|W\|n}{\hbar}\int_0^t \|Z_{N,n+2}(s)\|_{\mathrm{tr}}\,\mathrm{d}s + \frac{1}{\hbar}\int_0^t \|\operatorname{Err}(s,N,n)\|_{\mathrm{tr}}\,\mathrm{d}s\end{aligned}$$

for $n = 1, 2, \dots, N-1$, which implies that

$$\begin{aligned}\|E_{N,n}(t)\|_{\mathrm{tr}} \leqslant \varepsilon(N,n,t) &+ \frac{2\|V\|n}{\hbar}\int_0^t \|E_{N,n+1}(s)\|_{\mathrm{tr}}\,\mathrm{d}s\\ &+ \frac{2\|W\|n}{\hbar}\int_0^t \|E_{N,n+2}(s)\|_{\mathrm{tr}}\,\mathrm{d}s,\end{aligned}\tag{3.13}$$

where

$$\varepsilon(N,n,t) = \|E_{N,n}(0)\|_{\mathrm{tr}} + \frac{1}{\hbar}\int_0^t \|\operatorname{Err}(s,N,n)\|_{\mathrm{tr}}\,\mathrm{d}s.\tag{3.14}$$

Iterating the inequality (3.13) m times (for some $m \leqslant N-n-1$), we obtain the following bound on the trace norm of $E_{N,n}(t)$:

$$\begin{aligned}&\|E_{N,n}(t)\|_{\mathrm{tr}}\\ &\quad\leqslant \sum_{k=0}^{m}\frac{n(n+1)\dots(n+k-1)}{k!}\\ &\qquad\times\sum_{j=0}^{k}\Big(\frac{2\|V\|t}{\hbar}\Big)^j\Big(\frac{2\|W\|t}{\hbar}\Big)^{k-j}\binom{k}{j}\varepsilon(N,n+j,t)\\ &\qquad+\frac{n(n+1)\dots(n+m-1)}{m!}\Big(\frac{2(\|V\|+\|W\|)t}{\hbar}\Big)^m\\ &\qquad\qquad\times\sup_{s\in[0,t]}\Big\{\sup_{j\leqslant m}\|E_{N,n+j+1}(s)\|_{\mathrm{tr}}\Big\}.\end{aligned}\tag{3.15}$$

Now, if $D_N(0)$ is a density operator, it is clear from (3.8) that

$$\|\mathcal{E}_n(t, N, D_N(0))\|_{\mathrm{tr}} \leqslant \frac{4n(n-1)}{N-1}\|V\| + \frac{2n(n-1)(3N-n-2)}{(N-1)(N-2)}\|W\| \tag{3.16}$$

for all t. From [3] we know that if $\{D_N\}$ has the Slater closure then

$$\lim_{N\to\infty} \|D_{N:1}\| = 0, \tag{3.17}$$

and that for any density operator F

$$\|F_n^-\|_{\mathrm{tr}} \leqslant 1 \quad \text{for all } \ n. \tag{3.18}$$

Let $\mathcal{R}_n$ be as in (3.9) and let F be a density operator. Then in the same way as in [3] we get the bound

$$\|\mathcal{R}_n(F)\|_{\mathrm{tr}} \leqslant [2n(n-1)\|V\| + 8n(n-1)(n+4)\|W\|]\|F\|. \tag{3.19}$$

Let $F(t)$ be a solution of the TDHF equation (3.6). Since the (operator) norm of $F(t)$ is constant, it follows from (3.19) that $\|\mathcal{R}_n(F(t))\|_{\mathrm{tr}} \leqslant [2n(n-1)\|V\| + 8n(n-1)(n+4)\|W\|]\|F(0)\|$ for all $t \geqslant 0$. Thus by (3.16) the error $\mathrm{Err}(t, N, n)$ of equation (3.12) satisfies

$$\begin{aligned}\| \mathrm{Err}(t, N, n)\|_{\mathrm{tr}} \leqslant 2n(n-1)\|V\|\Big(\frac{2}{N-1} + \|F(0)\|\Big) \\ + 8n(n-1)(n+4)\|W\|\Big(\frac{3N-n-2}{4(n+4)(N-1)(N-2)} + \|F(0)\|\Big),\end{aligned}$$

so $\varepsilon(N, n, t)$ of equation (3.14) satisfies

$$\begin{aligned}&\varepsilon(N, n, t) \\ &\quad\leqslant 2n(n-1)\|V\|\frac{t}{\hbar}\Big(\frac{2}{N-1} + \|F(0)\|\Big) \\ &\qquad + 8n(n-1)(n+4)\|W\|\frac{t}{\hbar}\Big(\frac{3N-n-2}{4(n+4)(N-1)(N-2)} + \|F(0)\|\Big) \\ &\qquad + \|E_{N,n}(0)\|_{\mathrm{tr}}.\end{aligned} \tag{3.20}$$

Using the above estimates, we can complete the proof of Theorem 3.1. Let us assume that $D_N(0)$ is a symmetric density for each N and that the sequence $\{D_N(0)\}$ has the Slater closure. Let $D_N(t)$ be the solution of (3.5) with the initial value $D_N(0)$, and let $F^{(N)}(t)$ be the solution of the TDHF equation (3.6) 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 (3.15) for the trace norm of $E_{N,n}(t)$, into which we now substitute estimates (3.20). In the same way, majorizing $\binom{n+k-1}{n-1}$ by $(n+k)^n/n!$, using the fact that $\sup_{s\in[0,t]}\left\{\sup_{j\leqslant m}\|E_{N,n+j}(s)\|_{\mathrm{tr}}\right\}\leqslant 2$, by (3.18) together with (3.20) we obtain

$$
\begin{aligned}
&\|E_{N,n}(t)\|_{\mathrm{tr}}\\
&\leqslant \sum_{k=0}^{m}\frac{n(n+1)\dots(n+k-1)}{n!}\Big(\frac{2(\|V\|+\|W\|)t}{\hbar}\Big)^k\sum_{j=0}^{k}\binom{k}{j}\varepsilon(N,n+j,t)\\
&\quad+\frac{n(n+1)\dots(n+m-1)}{n!}\Big(\frac{2(\|V\|+\|W\|)t}{\hbar}\Big)^m\sum_{j=0}^{m}\binom{m}{j}\sup_{s\in[0,t]}\|E_{N,n+j+1}(s)\|_{\mathrm{tr}}\\
&\leqslant \sum_{k=0}^{m}\frac{(n+k)^k}{n!}\Big(\frac{2(\|V\|+\|W\|)t}{\hbar}\Big)^k\cdot 2^k\\
&\quad\times\left\{5n(n-1)(n+4)\Big(\frac{2(\|V\|+\|W\|)t}{\hbar}\Big)\Big[\frac{2}{N-1}+\|F^{(N)}(0)\|\Big]+\|E_{N,n}(0)\|_{\mathrm{tr}}\right\}\\
&\quad+\frac{(n+m)^m}{n!}\Big(\frac{2(\|V\|+\|W\|)}{\hbar}t\Big)^m\cdot 2^m\cdot 2.
\end{aligned}
$$

For $T=4(\|V\|+\|W\|)t/\hbar$ we get the bound

$$
\begin{aligned}
\text{(3.21)}\qquad \|E_{N,n}(t)\|_{\mathrm{tr}}\leqslant \frac{5}{2}\sum_{k=0}^{m}&\frac{(n+k)^{k+3}}{n!}T^{k+1}\Big[\frac{2}{N-1}+\|F^{(N)}(0)\|\Big]\\
&+\sum_{k=0}^{m}\frac{(n+k)^k}{n!}T^k\times\|E_{N,n}(0)\|_{\mathrm{tr}}+2\frac{(n+m)^m}{n!}T^m
\end{aligned}
$$

for $m\leqslant N-n-1$. Fix T to be less than 1, then $t<\hbar/(4(\|V\|+\|W\|))$. For fixed n, consider the limit of the right-hand side of (3.21) as N and m tend to infinity. The individual terms (fixed k) tend to 0, for $\|F^{(N)}(0)\|$ tends to 0 by (3.17) and $\|E_{N,n+k}(0)\|_{\mathrm{tr}}$ tends to 0 thanks to the hypothesis that $\{D_N(0)\}$ has the Slater closure. On the other hand, the series on the right-hand side of (3.21) are dominated, uniformly with respect to m, by a series that converges absolutely for $T<1$, so it follows that

$$\text{(3.22)}\qquad \lim_{N\to\infty}\|E_{N,n}(t)\|_{\mathrm{tr}}=0$$

if $t<\hbar/(4(\|V\|+\|W\|))$.

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

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

for $n > 1$ and $t < \hbar/(2\|V\|)$. Finally, from (3.22) it follows again that, for any n and any $t < \hbar/(4(\|V\| + \|W\|))$,

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

i.e., $\{D_N(t)\}$ has the Slater closure. This proves the theorem up to $t = \hbar/(4(\|V\| + \|W\|))$, and the argument may be repeated to establish the conclusion of the theorem for all $t > 0$, as in [3]. □

4. Final comments

Let us suppose that quantum statistics may be neglected in the above analysis (see below for physical motivations). Then, assuming that $\{D_N(0)\}$ is a sequence of initial states for (1.1) that has a simple factorized structure, we can prove, relying on the analysis in [2], that $\{D_N(t)\}$ has the same structure for all $t > 0$. In this case, the two-body density operator $D_{N:2}(t)$ and the three-body density operator $D_{N:3}(t)$ are approximately equal to $D_{N:1}(t)\otimes D_{N:1}(t)$ and $D_{N:1}(t)\otimes D_{N:1}(t)\otimes D_{N:1}(t)$ when N is large, and the single-body density operator nearly obeys the so-called time-dependent Hartree (TDH) equation

$$\begin{aligned} &\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}F(t) = [L, F(t)] + [V, F(t)\otimes F(t)]_{:1} + [W, F(t)\otimes F(t)\otimes F(t)]_{:1},\\ &F(0) = D_{N:1}(0). \end{aligned} \tag{4.1}$$

Then, the analogue of Theorem 3.1 asserts that the distance in the trace norm between $D_{N:1}(t)$ and the corresponding solution to the TDH equation tends to 0 as N tends to infinity.

Theorem 4.1. *For each N, let $D_N(t)$ be a solution to (3.5) whose initial value $D_N(0)$ is a factorized density. Let $F^{(N)}(t)$ be the solution of the TDH equation (4.1) whose initial value is $F^{(N)}(0) = D_{N:1}(0)$.*

If $\{D_N(0)\}$ is factorized then $\{D_N(t)\}$ is factorized too and

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

for all $t > 0$.

Proof. The proof of this result is a straightforward extension of the one given in [2] for the two-body case. □

Let us comment now on the physical meaning of this result. It is well known that the above Hartree ansatz is strictly speaking not appropriate for the treatment of identical particles which obey either Fermi or Bose statistics, except in the special case of Bose condensation. However, if one decomposes TDHF equation as follows

$$
\begin{aligned}
(4.2)\quad \mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}F(t) = [L, F(t)] &+ [V, (F(t)\otimes F(t))]_{:1} \\
&+ [W, (F(t)\otimes F(t)\otimes F(t))]_{:1} + [V, (F(t)\otimes F(t))(\Sigma_2 - I)]_{:1} \\
&+ [W, (F(t)\otimes F(t)\otimes F(t))(\Sigma_3 - I)]_{:1},
\end{aligned}
$$

one calls the second and third terms on the right-hand side of (4.2) the *direct contribution*, and the and the last two terms the *exchange contribution.* So one sees that it is possible to consider the Hartree equation as an approximation of the Hartree-Fock one, as soon as the exchange contribution is small with respect to the direct term.

It is known [15] that for long-range interparticle potentials (as in atomic physics) the exchange contribution is usually much smaller than the direct one: as the exclusion principle prevents two particle of the same spin from occupying the same particle state, the two-particle density correlation function for parallel spins vanishes throughout a region comparable to the interparticle spacing. As the potential extends far beyond the interparticle spacing, the exclusion principle plays a minor role.

However, in our case of short range potentials (nuclear physics), the range of the potential is less than the interparticle spacing, the exclusion principle is crucial (for example in determining the ground state energy), the direct and exchange terms are comparable in magnitude, and some extra argument must be given to justify Hartree's ansatz.

In fact one has to keep in mind that contrary to atomic potential (Coulomb), nuclear interaction is not completely known, and one can use various parametrizations corresponding to different physical situations. For example, in the particular case of transactinides and super-heavy elements (nuclei with proton number $Z \geqslant 102$) where Hartree-Fock computations are very hard, a suitable effective interaction can be devised [8] precisely in such a way that exchange contribution is very small and can be neglected in realistic computations, which justifies the use of Hartree-type wave functions.

Let us conclude by mentioning that even in the nuclear relativistic situation (which is beyond our scope in the present paper), Hartree formalism is also considered as a good approximation in relativistic nuclear many-body problems [22].

Let us briefly comment on two open ways in order to generalize our results to more realistic interactions.

Let us first emphasize that, in the same spirit as Coulomb interaction, we have neglected in the previous model (see [20] for such an approximation) the relative (two-body) spin-orbit contribution

$$w_{ls}\mathrm{e}^{-(|r_i-r_j|)^2/\mu_3}\vec{\mathbf{L}}_{ij}\cdot\vec{\mathbf{S}}_{ij},$$

where $\vec{\mathbf{S}}_{ij} := \vec{\mathbf{S}}_i + \vec{\mathbf{S}}_j$ is the total spin operator of the two-body system (i, j), and the relative angular momentum $\vec{\mathbf{L}}_{12}$ with components $\mathbf{L}_{12j}$ for $j = 1, 2, 3$ is

$$\mathbf{L}_{12j} := -\mathrm{i}\Big(r_{12k}\frac{\partial}{\partial r_{12l}} - r_{12l}\frac{\partial}{\partial r_{12k}}\Big),$$

where $r_{12} = r_1 - r_2$.

In fact, we have replaced this two-body contribution by its one-body intrinsic counterpart $W_{ls}\vec{\mathbf{L}}\cdot\vec{\mathbf{S}}$, which is reminiscent of the nuclear shell model [21]: each nucleon is only submitted to a self-coupling between its own spin and its own angular momentum.

The second remark is related to effective interactions. In various models (as the set of Skyrme interactions [11] or Gogny D1S force [12]) the three body term is replaced by a density-dependent two body non-local contribution

$$\mathbf{V}_\varrho = \frac{1}{6}t_3(1+\mathbf{P}_\sigma)\delta(r_i - r_j)\varrho^\lambda\Big(\frac{1}{2}(r_i + r_j)\Big),$$

where $0 \leqslant \lambda \leqslant 1$. For example in the Skyrme case the parameter $\lambda = 1$ and one can check directly at the formal level [24] that the three-body "contact" term

$$\mathbf{W}_{ijk} = t_3\delta(r_i - r_j)\delta(r_j - r_k)\mathbf{I}$$

is equivalent to the density-dependent two body contribution

$$\mathbf{V}_{ij}(\varrho) = \frac{1}{6}t_3(1+\mathbf{P}_\sigma)\delta(r_i - r_j)\varrho\Big(\frac{1}{2}(r_i + r_j)\Big).$$

Such density-dependent terms reflect phenomenologically the effect of the density of the surrounding medium on the pair i, j. Clearly a new difficulty occurs in this case as we start from a non-linear (and non-local) Hamiltonian and the TDHF procedure. Although some progresses have been achieved on the existence of solutions of the corresponding Hartree-Fock (or time-dependent Hartree-Fock) problems (see [19], [10]), the derivation of the TDHF equation from the hierarchy along the previous strategy is presently not clear from the mathematical point of view.

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Author's address: *B. Ducomet*, CEA, DAM, DIF, F-91297 Arpajon, France, e-mail: `bernard.ducomet@cea.fr`.