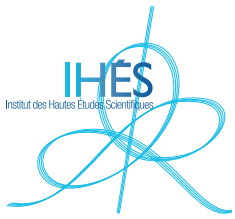

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Mean-field evolution of fermionic systems

Marcello Porta

Abstract

We study the dynamics of interacting fermionic systems, in the mean-field regime. We consider initial states which are close to quasi-free states and prove that, under suitable assumptions on the inital data and on the many-body interaction, the quantum evolution of the system is approximated by a time-dependent quasi-free state. In particular we prove that the evolution of the reduced one-particle density matrix converges, as the number of particles goes to infinity, to the solution of the time-dependent Hartree-Fock equation. Our theorems allow to describe the dynamics of both pure states (zero temperature states) and mixed states (positive temperature states). Our results hold for all times, and give effective estimates on the rate of convergence towards the Hartree-Fock evolution. The results on pure states are based on joint works with N. Benedikter and B. Schlein, [5, 6]; while those on mixed states are based on a joint work with N. Benedikter, V. Jaksic, C. Saffirio and B. Schlein, [7].

1 Introduction

Systems composed by many interacting particles are often too difficult to describe mathematically starting from first principles. A major goal of statistical mechanics is to provide effective models to describe complex systems, that capture the main features of the system under investigation and at that the same time can be studied explicitly. For instance, concerning the dynamics of classical particles, two well-known examples of effective models are the Boltzmann equation, for an interacting gas in the low density regime, or the Vlasov equation, for particles interacting in the mean-field scaling. For quantum systems, examples of effective theories are the Thomas-Fermi theory for the ground state of large atoms, or the Gross-Pitaevskii theory, for the ground-state and the dynamics of Bose-Einstein condensates. Physically, these models are widely accepted as good effective descriptions of complex interacting particle systems. The question of rigorously proving their validity is, however, not at all an easy one. Nevertheless, after decades of intense research, the above mentioned effective theories have been rigorously justified starting from microscopic principles; see, for instance, [16, 8, 18, 17, 11].

Here I will focus on *fermionic* systems. Compared to bosonic systems, the mathematical understanding of the validity of fermionic effective theories is at a much earlier stage. I will focus on the dynamics of interacting fermionic systems in the mean-field regime. In particular, I will present two theorems: one concerns the rigorous derivation of the time-dependent Hartree-Fock equation for pure states (*i.e.* zero temperature states), while the other concerns the analogous result for fermionic mixed states (*i.e.* positive temperature states).

This note is organized as follows. In Section 2 I will introduce fermionic mean-field scaling, and I will recall the definitions of two effective models for the ground state of fermionic systems in the mean-field regime: Thomas-Fermi theory and Hartree-Fock theory. In Section 3 I will discuss fermionic dynamics in the mean-field limit, which turns out to be naturally coupled with a semiclassical scaling. In particular, I will recall two well-known

effective evolution equations, that are expected to provide a good description of the dynamics of fermionic systems in this scaling regime: namely, the Vlasov equation and the time-dependent Hartree-Fock equation. Finally, in Sections 4, 5 I will present our results.

2 Fermionic mean field scaling

We consider a system of $N \gg 1$ quantum particles in $\mathbb{R}^3$, with wave function $\psi_N \in L^2(\mathbb{R}^{3N})$, $\|\psi_N\|_2 = 1$. We assume the particles to be *fermions*; that is

$$\psi_N \in L^2_{\mathrm{a}}(\mathbb{R}^{3N}) := \Big\{ \psi \in L^2(\mathbb{R}^{3N}) \mid \psi(x_1, \dots, x_n) = \sigma_\pi \psi(x_{\pi(1)}, \dots, x_{\pi(N)}) \Big\} , \tag{2.1}$$

where π is a permutation of $\{1, 2, \dots, N\}$ with sign $\sigma_\pi \in \{-1, +1\}$. The Hamiltonian of the system has the form

$$H_N^{\mathrm{trap}} = \sum_{j=1}^N \big[-\Delta_j + V_{\mathrm{ext}}(x_j) \big] + \lambda \sum_{i<j}^N V(x_i - x_j) , \tag{2.2}$$

where V_{ext} confines the system in a region $\Lambda \subset \mathbb{R}^3$, with volume $|\Lambda| = O(1)$. That is, we are considering a *high density regime*: $\rho = N/|\Lambda| = O(N)$. The interaction potential V is supposed to vary on the scale of Λ: each particle interacts with the remaining $N - 1$. We will choose the coupling constant $\lambda \equiv \lambda(N)$ in such a way that the interaction energy per particle is not negligible with respect to the kinetic energy per particle. This choice defines the *mean-field regime*.

To properly define fermionic mean-field scaling, it is useful to recall the typical sizes of kinetic and of interaction energy for the kind of system under study. Let us start with the interaction energy. For a bounded potential V we have, independently of the statistics of the particles:

$$\langle \psi_N, \lambda \sum_{i<j} V(x_i - x_j) \psi_N \rangle = O(\lambda N^2) ; \tag{2.3}$$

the total interaction energy grows quadratically in the particle number, simply because the sum involves $O(N^2)$ terms. The size of the interaction energy is independent of the fermionic nature of the wave function. Instead, the antisymmetry of the wave function plays a crucial role in estimating the size of the kinetic energy. A general way to see that is by the *Lieb-Thirring kinetic energy inequality*. This inequality states that for any $\psi \in L^2_{\mathrm{a}}(\mathbb{R}^{3N})$:

$$\langle \psi_N, \sum_{i=1}^N -\Delta_i \, \psi_N \rangle \geq C \int dx \, \rho_\psi(x)^{5/3} , \tag{2.4}$$

for a suitable constant $C > 0$ independent of N and ψ. The *density* ρ_ψ is defined as follows:

$$\rho_\psi(x) := N \int dx_2 \dots dx_N \, |\psi_N(x, x_2, \dots, x_N)|^2 , \tag{2.5}$$

and the normalization is chosen so that $\|\rho\|_1 = N$. Thus, under reasonable assumptions on the density of the system we have

$$\langle \psi_N, \sum_{i=1}^N -\Delta_j \, \psi_N \rangle \gtrsim N^{5/3} . \tag{2.6}$$

Eqs. (2.3), (2.6) show that in order to define a nontrivial mean-field scaling one is led to the choice $\lambda = N^{-1/3}$. That is, the mean-field Hamiltonian is:

$$H_N^{\rm trap} = \sum_{j=1}^N \big[-\Delta_j + V_{\rm ext}(x_j)\big] + N^{-1/3} \sum_{i<j}^N V(x_i - x_j) \; . \tag{2.7}$$

One is typically interested in the ground state properties of this Hamiltonian (*e.g.*, the ground state energy). Another interesting question, which is the one we will investigate here, is to describe the time evolution of the low energy states of $H_N^{\rm trap}$, once the trapping potential has been modified (otherwise the dynamics is trivial). Of course, the mean-field scaling simplifies the analysis; but still, these problems are far from being trivial. We will start by rewieving two well-known effective theories for the ground state of $H_N^{\rm trap}$, Thomas-Fermi theory and Hartree-Fock theory, which capture important features of the model as $N \to \infty$. After this introductory part, we will focus on the dynamical properties of the system.

2.1 Thomas-Fermi theory

The simplest effective theory for the ground state of $H_N^{\rm trap}$ is *Thomas-Fermi theory*. This theory only depends on the density of the system. More precisely, given a density profile $\rho \in \mathcal{T} := \{\rho \mid \rho(x) \geq 0,\, \|\rho\|_1 = N,\, \|\rho\|_{5/3} < \infty\}$, its Thomas-Fermi energy is:

$$\begin{aligned} \mathcal{E}_{\rm TF}(\rho) &= \frac{3}{5} c_{\rm TF} \int dx\, \rho(x)^{5/3} + \int dx\, V_{\rm ext}(x)\rho(x) + D(\rho,\rho) \; , \\ D(\rho,\rho) &= \frac{1}{2N^{1/3}} \int dxdy\, V(x-y)\rho(x)\rho(y) \; . \end{aligned} \tag{2.8}$$

with $c_{\rm TF} = (6\pi^2)^{2/3}$. The first term in (2.8) approximates the kinetic energy of the system, while the last two describe the interaction of the particles with the external trap and among each other.

In the limit $N \to \infty$, Thomas-Fermi theory provides a good approximation of the full ground state energy. For example, for a bounded potential such that $\widehat{V} \geq 0$:

$$\inf_{\psi \in L^2_{\rm a}(\mathbb{R}^{3N})} \frac{\langle \psi, H_N^{\rm trap} \psi\rangle}{\langle \psi, \psi\rangle} = \inf_{\rho \in \mathcal{T}} \mathcal{E}_{TF}(\rho) + o(N^{5/3}) \; . \tag{2.9}$$

Notice that the Thomas-Fermi energy is $O(N^{5/3})$, hence it captures the leading behavior of the ground state energy as $N \to \infty$. In Eq. (2.9), the main source of error comes from approximating the kinetic energy with $\|\rho\|_{5/3}^{5/3}$.

Concerning rigorous results, the validity of Thomas-Fermi theory has been first proved by Lieb-Simon for large atoms (which can be thought as mean-field systems) in [18].

2.2 Hartree-Fock theory

Hartree-Fock theory provides a better approximation of the ground state of $H_N^{\rm trap}$. It depends on the *reduced one-particle density matrix* γ. Given a fermionic wave function $\psi_N \in L^2_{\rm a}(\mathbb{R}^{3N})$, we define its reduced one-particle density matrix as:

$$\gamma_\psi^{(1)} := N \, {\rm tr}_{2,\dots,N} \, |\psi_N\rangle\langle\psi_N| \; , \tag{2.10}$$

where the trace is over $N-1$ particle labels. The normalization is chosen so that ${\rm tr}\, \gamma_\psi^{(1)} = N$. Notice that the density of ψ is just the diagonal of $\gamma_\psi^{(1)}$: $\rho_\psi(x) = \gamma_\psi^{(1)}(x;x)$. More generally,

k-particle reduced densities are obtained by tracing out $N-k$ particles (and replacing the normalization factor N by $\binom{N}{k}$). Fermionic one-particle densities satisfy the important property $0 \leq \gamma_\psi^{(1)} \leq 1$. We denote by $\mathcal{D}$ the set of admissible fermionic density matrices: $\mathcal{D} := \{\gamma \mid 0 \leq \gamma \leq 1, \operatorname{tr}\gamma = N\}$.

Given a fermionic density matrix γ, its Hartree-Fock energy is:

$$\mathcal{E}_{\mathrm{HF}}(\gamma) = \operatorname{tr} h\gamma + \frac{1}{2N^{1/3}} \int dxdy\, V(x-y)\big[\gamma(x;x)\gamma(y;y) - |\gamma(x;y)|^2\big] \tag{2.11}$$

where $h = -\Delta + V_{\mathrm{ext}}$. The second term in Eq. (2.11) is called the *direct term*, while the last one is called the *exchange term*. It is not difficult to see that the exchange term is always smaller than the direct term.

One expects the infimum of $\mathcal{E}_{\mathrm{HF}}$ to be a good approximation of the ground state energy of H_N^{trap}. For example, for a bounded potential V such that $\widehat{V} \geq 0$:

$$\inf_{\psi \in L^2_{\mathrm{a}}(\mathbb{R}^{3N})} \frac{\langle \psi, H_N^{\mathrm{trap}} \psi\rangle}{\langle \psi, \psi\rangle} = \inf_{\gamma \in \mathcal{D}} \mathcal{E}_{\mathrm{HF}}(\gamma) + O(N^{2/3})\,; \tag{2.12}$$

the error terms are bounded proportionally to $N^{2/3}$, which is better than what one would get comparing with Thomas-Fermi theory.

Concerning the structure of the Hartree-Fock minimizer in the right hand side of (2.12), *Lieb's variational principle* implies that it is an orthogonal projection: $\omega = \omega^2$. In other words, the optimal Hartree-Fock energy is the energy of a suitable *Slater determinant*. Given N orthonormal functions $f_i \in L^2(\mathbb{R}^3)$, also called *orbitals*, the corresponding Slater determinant is:

$$\psi_{\mathrm{Slater}}(x_1, \dots, x_N) := \frac{1}{\sqrt{N!}} \sum_{\pi \in S_N} \sigma_\pi f_{\pi(1)}(x_1) \cdots f_{\pi(N)}(x_N)\,, \tag{2.13}$$

where S_N is the set of permutations of $\{1, 2, \dots, N\}$, with sign $\sigma_\pi = \pm 1$. The reduced one-particle density matrix of ψ_{Slater} is:

$$\omega = N \operatorname{tr}_{2,\dots,N} |\psi_{\mathrm{Slater}}\rangle\langle\psi_{\mathrm{Slater}}| = \sum_{j=1}^N |f_j\rangle\langle f_j|\,. \tag{2.14}$$

Slater determinants are examples of *quasi-free states*; these are states for which all k-particle marginals can be computed starting from the reduced one-particle density matrix, in a well-defined way (using the *Wick rule*). In particular, their energy only depends on the reduced one-particle density (in presence of a two-body potential, the energy of a generic state would also depend on the two-particle density). The fact that ω is a projection is referred to by saying that Slater determinants are *pure* quasi-free states.

Semiclassical ideas can be used to approximate the minimizer of the Hartree-Fock enegy functional. Let us introduce

$$\begin{aligned} h(p,q) &= p^2 + \phi_{\mathrm{TF}}(q) \\ \phi_{\mathrm{TF}} &= V_{\mathrm{ext}} + N^{-1/3}\rho_{\mathrm{TF}} * V\,, \qquad p, q \in \mathbb{R}^3\,, \end{aligned} \tag{2.15}$$

where ρ_{TF} is the minimizer of the Thomas-Fermi energy functional. The function ϕ_{TF} is called the *Thomas-Fermi potential*. Let us define:

$$\omega_{\mathrm{sc}} := \int_{h(p,q)\leq\mu} |f_{pq}\rangle\langle f_{pq}|\,, \qquad f_{pq}(x) = e^{ip\cdot x} g(x-q) \tag{2.16}$$

for a suitable $g \in L^2(\mathbb{R}^3)$. The parameter μ is called *chemical potential*, and it is chosen so that $\mathrm{tr}\,\omega_{\rm sc} = N$. The functions f_{pq} are called *coherent states*; roughly, f_{pq} is the wave function of one particle localized around q, with momentum p. Following [14], it is possible to show that for $N \gg 1$ the minimizer ω of $\mathcal{E}_{\rm HF}$ is well approximated by $\omega_{\rm sc}$:

$$\mathrm{tr}\ |\omega_{\rm sc} - \omega|^2 \leq CN^{5/6}\ . \tag{2.17}$$

Recall that the trivial estimate would be N. The operator $\omega_{\rm sc}$ is called the *semiclassical approximation* of ω.

The validity of Hartree-Fock theory has been first proven by Bach for large atoms, [3]; later, a simpler and more general proof has been given by Graf-Solovej, [14]. Notice that in the case of a bounded potential the estimate of the error term in (3.22) is not negligible with respect to the exchange term. However, the exchange term becomes larger in presence of an unbounded interaction potential. In particular, in [3, 14] the Authors considered particles interacting via a Coulomb interaction, and they proved that the error term is subleading with respect to the exchange term.

3 Fermionic mean-field dynamics

We are interested in the dynamics of interacting fermionic systems in the mean-field scaling. In order to observe a nontrivial evolution, let us assume that at the time $t = 0$ the trapping potential $V_{\rm ext}$ is modified, or switched off for simplicity. The Schrödinger dynamics is:

$$i\partial_t \psi_{N,t} = \Big[\sum_{j=1}^N -\Delta_j + N^{-1/3}\sum_{i<j} V(x_i - x_j)\Big]\psi_{N,t}\ , \qquad \psi_{N,0} \equiv \psi_N\ . \tag{3.18}$$

It is important to identify the relevant time scale, on which the system undergoes a macroscopic change. The typical kinetic energy per particle is $O(N^{2/3})$; hence, the "classical" velocity of one particle is $N^{1/3}$. That is, a particle covers a distance of order 1 in a time of order $N^{-1/3}$; thus, on this time scale the system undergoes a macroscopic change, since the initial data was initially confined in a region $\Lambda \subset \mathbb{R}^3$ with volume $|\Lambda| = O(1)$. It is convenient to rescale time, so that a particle covers a distance $O(1)$ in a time $O(1)$. After rescaling time, the Schrödinger equation becomes:

$$iN^{1/3}\partial_t \psi_{N,t} = \Big[\sum_{j=1}^N -\Delta_j + N^{-1/3}\sum_{i<j} V(x_i - x_j)\Big]\psi_{N,t}\ . \tag{3.19}$$

Let us introduce the parameter $\varepsilon = N^{-1/3}$. Multiplying left hand side and right hand side of (3.19) by ε^2 we get:

$$\begin{aligned} i\varepsilon\partial_t \psi_{N,t} &= \Big[\sum_{j=1}^N -\varepsilon^2\Delta_j + N^{-1}\sum_{i<j} V(x_i - x_j)\Big]\psi_{N,t} \\ &\equiv H_N \psi_{N,t}\ . \end{aligned} \tag{3.20}$$

That is, *fermionic mean–field scaling is naturally coupled with a semiclassical scaling.*

3.1 Hartree-Fock and Vlasov dynamics

Given the solution at time t of the Schrödinger equation (3.20), $\psi_{N,t} = e^{-iH_N t/\varepsilon}\psi_N$, we define the time-evolved reduced one-particle density matrix as

$$\gamma^{(1)}_{N,t} := N \operatorname{tr}_{2,\dots,N} |\psi_{N,t}\rangle\langle\psi_{N,t}| \,. \tag{3.21}$$

At the time $t = 0$ the state of the system is well approximated by a Slater determinant, with reduced one-particle density matrix given by the minimizer of $\mathcal{E}_{\mathrm{HF}}$. At time $t > 0$, one expects that state of the system to be *still* described by a suitable Slater determinant; its reduced one-particle density matrix $\omega_{N,t} = \omega^2_{N,t}$ is the solution of the *time-dependent Hartree-Fock equation*:

$$\begin{aligned} i\varepsilon\partial_t\omega_{N,t} &= \big[h_{\mathrm{HF}}(t), \omega_{N,t}\big] \\ h_{\mathrm{HF}}(t) &= -\varepsilon^2\Delta + \rho_t * V - X_t \,, \end{aligned} \tag{3.22}$$

where $\rho_t(x) = N^{-1}\omega_{N,t}(x;x)$ and X_t is an operator on $L^2(\mathbb{R}^3)$ with kernel $X_t(x;y) = N^{-1}V(x-y)\omega_{N,t}(x;y)$.

As $N \to \infty$, the next degree of approximation is provided by the *Vlasov equation*. Let us define the *Wigner transform* of the solution at time t of (3.22) as

$$W_{N,t}(x,p) := \frac{\varepsilon^3}{(2\pi)^3}\int dy\, e^{-ip\cdot y}\omega_{N,t}(x+\varepsilon y/2; x-\varepsilon y/2) \,. \tag{3.23}$$

As $N \to \infty$, we expect the "phase-space density" $W_{\infty,t}(x,p)$ to evolve according to the Vlasov equation:

$$\partial_t W_{\infty,t}(x,p) + p\cdot\nabla_x W_{\infty,t}(x,p) = \big(\nabla V * \rho_t\big)(x)\cdot\nabla_p W_{\infty,t}(x,p) \,. \tag{3.24}$$

The Vlasov equation describes a classical effective dynamics; it can be derived directly from classical mechanics, for particles interacting in the mean-field scaling. The emergence of a classical effective dynamics is not surprising, and it is due to the presence of the semiclassical limit $\varepsilon \to 0$ in (3.22).

3.2 Rigorous results

In the *mean-field plus semiclassical scaling*, the first rigorous derivation of the Vlasov equation is the one of Narnhofer-Sewell [21], for analytic interaction potentials. Shortly after, the result has been generalized to a much larger class of potentials by Spohn [24], who considered twice differentiable interactions. Concerning the time-dependent Hartree-Fock equation, the first rigorous derivation in this scaling regime is the one of Elgart-Erdős-Schlein-Yau [10], for short times and for analytic interaction potentials. Recently, this resut has been generalized by Benedikter-Porta-Schlein [5] to a much larger class of interactions (essentially, twice differentiable); convergence was proven for all times, with effective estimates on the rate of convergence. Later, the same result has been obtained by Petrat-Pickl [22], with a different method. The result of [5] applies to initial data describing *pure states* (*e.g.*, approximate Slater determinants); very recently a similar result has been proven for *mixed states* (describing positive temperature states) by Benedikter-Jaksic-Porta-Saffirio-Schlein [7].

Concerning other scaling regimes, different groups studied the case of mean-field ($1/N$ coupling) *without* semiclassical scaling. The first derivation of the time-dependent Hartree-Fock equation is the one of Bardos-Golse-Gottlieb-Mauser [4], for bounded interaction potentials.

The result has been extended by Fröhlich-Knowles [12] to the case of a Coulomb interaction. Finally, a regularized Coulomb interaction with a $N^{-2/3}$ coupling constant has been studied by Petrat-Pickl [22].

The above results concern the derivation of the Hartree-Fock or of the Vlasov equation starting from many-body quantum dynamics. It is also interesting to study the derivation of the Vlasov equation starting from the Hartree-Fock equation. This problem has been investigated by Lions-Paul [19] and Markovich-Mauser [20], for a Coulomb interaction. In these works, the Authors proved the convergence of the Hartree-Fock equation to the Vlasov equation in a weak sense, for mixed states. More recently, Athanassoulis-Paul-Pezzotti-Pulvirenti [2] gave a derivation of the Vlasov equation from the Hartree-Fock equation with estimates on the rate of convergence, for bounded interaction potentials and for mixed states.

4 Hartree-Fock dynamics of pure states

Here we discuss our result about the derivation of the time-dependent Hartree-Fock equation for the dynamics of pure states, [5].

4.1 Main result

We present the theorem in a simplified form. We refer the reader to [5, 6] for more details.

Theorem 4.1. *Let $V \in L^1(\mathbb{R}^3)$, such that $\int dp\, |\widehat{V}(p)|(1+|p|^2) < \infty$. Let $\psi_N \in L^2_a(\mathbb{R}^{3N})$ such that $\mathrm{tr}\, |\gamma_N^{(1)} - \omega_N| \leq C$, with $\omega_N = \omega_N^2$, $\mathrm{tr}\, \omega_N = N$ and*

$$\mathrm{tr}\ |[x, \omega_N]| \leq CN\varepsilon\ , \qquad \mathrm{tr}\ |[\varepsilon\nabla, \omega_N]| \leq CN\varepsilon\ , \qquad \varepsilon = N^{-1/3}\ . \tag{4.25}$$

Let $\gamma_{N,t}^{(1)}$ be the reduced one-particle density matrix of $\psi_{N,t} = e^{-iH_N t/\varepsilon}\psi_N$, the solution of (3.18). Let $\omega_{N,t}$ be the solution of the time-dependent Hartree-Fock equation:

$$i\varepsilon\partial_t \omega_{N,t} = [-\varepsilon^2\Delta + V * \rho_t - X_t, \omega_{N,t}]\ , \qquad \omega_{N,0} \equiv \omega_N\ .$$

Then, for some constant $c > 0$ and for all $t \in \mathbb{R}$:

$$\mathrm{tr}\, |\gamma_{N,t}^{(1)} - \omega_{N,t}|^2 \leq \exp(c\exp(c|t|)) \quad \mathrm{tr}\, |\gamma_{N,t}^{(1)} - \omega_{N,t}| \leq N^{1/2}\exp(c\exp(c|t|)) \tag{4.26}$$

Remark.

(i) Recall that $\mathrm{tr}\, |\omega_{N,t}| = \mathrm{tr}\, |\omega_{N,t}|^2 = N$. Thus, the above theorem proves convergence of many-body quantum dynamics towards Hartree-Fock dynamics with rate $1/N^{1/2}$ in both Hilbert-Schmidt[1] and trace norms.

(ii) It is well known that in Hartree-Fock theory the exchange term is subleading with respect to the direct term. This fact is evident in our result, too: dropping X_t does not deteriorate the rate of convergence. Thus, the theorem does not distinguish between Hartree and Hartree-Fock evolutions. In analogy with the study of the ground state of large atoms [3, 14], one expects the exchange term to become more relevant for more singular potentials (*e.g.* Coulomb).

[1] The Hilbert-Schmidt norm is defined as $\|A\|_{\mathrm{HS}} = \sqrt{\mathrm{tr}\, |A|^2}$.

(iii) The result has been extended in [6] to the dynamics of pseudorelativistic fermions. That is, the Laplacian is replaced by $\sqrt{-\varepsilon^2\Delta + m^2}$, with $m = O(1)$. Being the typical momentum of order $N^{1/3}$, this case is not a trivial modification of the one discussed above. Under similar assumptions, we proved the convergence of the quantum many-body dynamics to the pseudorelativistic Hartree-Fock evolution:

$$i\varepsilon\partial_t\omega_{N,t} = [\sqrt{-\varepsilon^2\Delta + m^2} + \rho_t * V - X_t, \omega_{N,t}] \,. \tag{4.27}$$

(iv) The estimates (4.25) are crucial for our result; without them, the result is not expected to hold. These estimates encode the *s*emiclassical structure of the initial data, which is expected to hold for the Hartree-Fock approximation of the ground state of H_N^{trap}. For instance, it is possible to see that they are true for the semiclassical approximation of the ground state, given by ω_{sc} in Eq. (2.16).

(v) A similar result holds for $k-$particle densities, with $k > 1$.

4.2 Some elements of the proof

The proof of the theorem is based on a convenient representation of the quantum dynamics in *Fock space*. The fermionic Fock space is defined as:

$$\begin{aligned} \mathcal{F} &= \mathbb{C} \oplus \bigoplus_{n\geq 1} L^2_{\mathrm{a}}(\mathbb{R}^{3n}) \\ \mathcal{F} \ni \psi &= (\psi^{(0)}, \psi^{(1)}, \dots, \psi^{(n)}, \dots) \,, \qquad \psi^{(n)} \in L^2_{\mathrm{a}}(\mathbb{R}^{3n}) \,. \end{aligned} \tag{4.28}$$

Each entry of the infinite sequence ψ can be though as the (non-normalized, in general) wave function of n fermions. An important example of vector in the Fock space is the *vacuum*, $\Omega = (1, 0, \dots, 0, \dots)$. Physically, it describes the situation in which no particles are present.

It is convenient to introduce *creation/annihilation operators*, $a^*(f), a(f) : \mathcal{F} \to \mathcal{F}$, for $f \in L^2(\mathbb{R}^3)$. They act in the following way:

$$\begin{aligned} (a^*(f)\psi)^{(n)}(x_1, \dots, x_n) &= \frac{1}{\sqrt{n}} \sum_{j=1}^{n} (-1)^j f(x_j)\psi^{(n-1)}(x_1, \dots, x_{j-1}, x_{j+1}, \dots, x_n) \\ (a(f)\psi)^{(n)}(x_1, \dots, x_n) &= \sqrt{n+1} \int dx \overline{f}(x)\psi^{(n+1)}(x, x_1, \dots, x_n), \qquad \forall \psi \in \mathcal{F} \,. \end{aligned}$$

That is, they formally create or annihilate a fermionic particle with wave function f. They satisfy the *canonical anticommutation relations*:

$$\{a(f), a^*(g)\} = \langle f, g\rangle_{L^2} \,, \qquad \{a(f), a(g)\} = \{a^*(f), a^*(g)\} = 0 \,, \tag{4.29}$$

which in particular imply that fermionic operators are *bounded*: $\|a^*(f)\| = \|a(f)\| = \|f\|_2$.

Time evolution is generated in Fock space by $\mathcal{H}_N$, the second quantization of the Hamiltonian; it acts as $(\mathcal{H}_N\psi)^{(n)} = H_N^{(n)}\psi^{(n)}$, where:

$$H_N^{(n)} := \sum_{j=1}^{n} -\varepsilon^2\Delta_j + \frac{1}{N}\sum_{i<j}^{n} V(x_i - x_j) \tag{4.30}$$

is an operator on $L^2(\mathbb{R}^{3n})$. Thus, the time evolution of $\psi \in \mathcal{F}$ is $t \mapsto e^{-i\mathcal{H}_N t/\varepsilon}\psi$. Notice that the different sectors of the Fock space evolve independently.

A crucial role in our proof is played by *Bogoliubov transformations*, [23]. Let

$$\omega_N = \sum_{j=1}^{N} |f_j\rangle\langle f_j| \,, \tag{4.31}$$

with $\{f_j\}_{j=1}^N$ a family of N orthonormal functions. We complete this family to obtain an orthonormal basis of $L^2(\mathbb{R}^3)$, that we denote by $\{f_j\}_{j=1}^\infty$. A Bogoliubov transformation is a map $R_{\omega_N} : \mathcal{F} \to \mathcal{F}$ such that:

$$\begin{aligned} R_{\omega_N}\Omega &= (0, \dots, 0, \psi_{\text{Slater}}, 0, \dots) \\ R_{\omega_N} a(f_i) R^*_{\omega_N} &= a(f_i)\chi(i > N) + a^*(f_i)\chi(i \leq N) \,, \end{aligned} \tag{4.32}$$

where $\chi(\cdot)$ is the characteristic function. In Eq. (4.32), ψ_{Slater} is the Slater determinant with reduced one-particle density given by ω_N, and it appears in the N-particle component of $R_{\omega_N}\Omega$. Bogoliubov transformations are unitary maps, $R^*_{\omega_N} R_{\omega_N} = 1$. More generally, it is possible to define a time-dependent Bogoliubov transformation $R_{\omega_{N,t}} \equiv R_t$, where $\omega_{N,t}$ is the solution at time t of the time-dependent Hartree-Fock equation.

These notions allow to give a very clear interpretation of the convergence of the quantum many-body dynamics to the effective evolution. Assuming for simplicity the initial data to be a Slater determinant, it turns out that:

$$\operatorname{tr} |\gamma^{(1)}_{N,t} - \omega_{N,t}|^2 \leq C\langle \mathcal{U}_N(t)\Omega, \mathcal{N}\mathcal{U}_N(t)\Omega\rangle \,, \tag{4.33}$$

where: $\mathcal{N}$ is the number operator, $\mathcal{N} := \sum_{j=1}^\infty a^*(f_f)a(f_j)$, acting as $(\mathcal{N}\psi)^{(n)} = n\psi^{(n)}$; and $\mathcal{U}_N(t)$ is the *fluctuation dynamics*:

$$\mathcal{U}_N(t) := R^*_t e^{-i\mathcal{H}_N t/\varepsilon} R_0 \,. \tag{4.34}$$

This dynamics *does not* commute with the number operator. Physically, the expectation value of $\mathcal{N}$ over the state $\mathcal{U}_N(t)\Omega$ is the *number of fluctuations* of the many-body dynamics with respect to the effective evolution.

To control the growth of the fluctuations, we use a Gronwall-type strategy. Namely, the goal is to show that:

$$\left| i\varepsilon \frac{d}{dt} \langle \mathcal{U}_N(t)\Omega, (\mathcal{N}+1)\,\mathcal{U}_N(t)\Omega\rangle \right| \leq C(t)\varepsilon \langle \mathcal{U}_N(t)\Omega, (\mathcal{N}+1)\,\mathcal{U}_N(t)\Omega\rangle \,, \tag{4.35}$$

for a possibly time dependent $C(t)$, bounded uniformly in N for every fixed $t \in \mathbb{R}$. Then, if this estimate holds a standard application of Gronwall's lemma implies that the quantity $\langle \mathcal{U}_N(t)\Omega, \mathcal{N}\mathcal{U}_N(t)\Omega\rangle$ grows at most exponentially in time, uniformly in N. A crucial point is to extract the factor ε in the right hand side of (4.35). To do this, we rely on the semi-classical structure of the initial data, Eq. (4.25); in particular, we show that this structure is propagated along the flow of the Hartree-Fock equation. Namely, we prove that:

$$\operatorname{tr} |[x, \omega_{N,t}]| \leq CN\varepsilon \exp(c|t|) \,, \qquad \operatorname{tr} |[\varepsilon\nabla, \omega_{N,t}]| \leq CN\varepsilon \exp(c|t|) \,, \qquad \forall t \in \mathbb{R} \,. \tag{4.36}$$

These estimates can be used to extract the factor ε in the right hand side of Eq. (4.35) (where $C(t) = \exp(c|t|)$ now), and they allow to prove that for every fixed $t \in \mathbb{R}$ the number of fluctuations is bounded uniformly in N.

5 Hartree-Fock dynamics of mixed states

So far, we discussed the dynamics of pure states, which describe systems at zero temperature. Mathematically, pure states are described by vectors in Fock space. At positive temperature, however, this description does not apply: instead, one has to consider *mixed states*.

5.1 Araki-Wyss representation

A fermionic density matrix is an operator acting on the fermionic Fock space $\mathcal{F}$, of the following form:

$$\rho_N = \sum_n \lambda_n |\psi_n\rangle\langle\psi_n| \,, \qquad \psi_n \in \mathcal{F} \,, \qquad 0 \leq \lambda_n \leq 1 \,, \tag{5.37}$$

for $\{\psi_n\}$ orthonormal. The normalization condition is imposed by requiring $\sum_n \lambda_n = 1$. The coefficients $\{\lambda_n\}$ are the probabilities for finding the state in ψ_n. Pure states corresponds to the situation in which $\lambda_n \neq 0$ for only one value of n. If more than one λ_n is different from zero, we have a mixed state. As the expression (5.37) suggests, mixed states do not correspond to vectors in $\mathcal{F}$: their density matrix is not the projection over a $\psi_n \in \mathcal{F}$. However, it turns out that mixed states can be thought as vectors over a "larger" Fock space. This representation takes the name of *purification* (see [9] for an extensive review of the subject).

Let $\{\xi_n\}$ be a sequence of complex numbers, such that $|\xi_n|^2 = \lambda_n$, and let $\{\phi_n\}$ be an orthonormal basis on the Fock space $\mathcal{F}$. We define

$$\kappa_N = \sum_n \xi_n |\psi_n\rangle\langle\phi_n| \,, \qquad \kappa_N \kappa_N^* = \rho_N \,. \tag{5.38}$$

Being ρ_N trace-class in $\mathcal{F}$, κ_N is a Hilbert-Schmidt operator. As such, it is isomorphic to a vector in $\mathcal{F} \otimes \mathcal{F}$:

$$\kappa_N \simeq \sum_n \xi_n \psi_n \otimes \overline{\phi}_n \,. \tag{5.39}$$

This observation allows to represent the state of the system as a vector in $\mathcal{F} \otimes \mathcal{F}$. Let O be an observable, that is a self-adjoint operator on $\mathcal{F}$. Its expectation over the state ρ_N is:

$$\langle O \rangle_{\rho_N} = \operatorname{tr} O \rho_N = \langle \kappa_N, O \otimes 1 \kappa_N \rangle \,, \tag{5.40}$$

where $\langle \cdot, \cdot \rangle$ is the standard scalar product in $\mathcal{F} \otimes \mathcal{F}$.

It is useful to notice that the doubled Fock space $\mathcal{F} \otimes \mathcal{F}$ is unitarily equivalent to $\mathcal{F}(L^2 \oplus L^2)$, the Fock space built over $L^2(\mathbb{R}^3) \oplus L^2(\mathbb{R}^3)$. The unitary implementing the equivalence is called *exponential law*, and acts in the following way:

$$\begin{aligned} U\Omega \otimes \Omega &= \Omega_{\mathcal{F}(L^2 \oplus L^2)} \\ U \left[a(f) \otimes 1 \right] U^* &= a(f \oplus 0) \\ U \left[(-1)^{\mathcal{N}} \otimes a(f) \right] U^* &= a(0 \oplus f) \,. \end{aligned} \tag{5.41}$$

Thus, a mixed state corresponds to a vector in $\mathcal{F}(L^2 \oplus L^2)$. In particular, the *mixed quasi-free state* with reduced one-particle density matrix ω_N (and with zero pairing amplitude, [23]) is represented by a vector of the form:

$$\varphi_N = R_{\omega_N} \Omega_{\mathcal{F}(L^2 \oplus L^2)} \,, \tag{5.42}$$

with R_{ω_N} a suitable Bogoliubov transformation on $\mathcal{F}(L^2 \oplus L^2)$. Recall that ω_N satisfies $0 \leq \omega_N \leq 1$, $\mathrm{tr}\, \omega_N = N$; but, in general, $\omega_N \neq \omega_N^2$. This representation of mixed quasi-free states is an example of the *Araki-Wyss construction* [1, 9], a well-known tool in quantum statistical mechanics.

Finally, the time evolution $t \mapsto \psi_t$ of $\psi_0 \equiv \psi \in \mathcal{F}(L^2 \oplus L^2)$ is implemented by the *Liouvillian*:

$$\mathcal{L}_N := U\big[\mathcal{H}_N \otimes 1 - 1 \otimes \mathcal{H}_N\big]U^* \,, \tag{5.43}$$

with $\mathcal{H}_N$ the second quantized Hamiltonian (see Section 4.2). That is, $\psi_t = e^{-i\mathcal{L}_N t/\varepsilon}\psi$.

5.2 Main result

Here we present the main result of [7], in a simplified form. We refer the reader to [7] for more details.

Theorem 5.1. *Let $V \in L^1(\mathbb{R}^3)$, such that $\int dp\, |\widehat{V}(p)|(1+|p|^2) < \infty$. Let $\varphi_N = R_{\omega_N}\Omega_{\mathcal{F}(L^2\oplus L^2)}$, with $0 \leq \omega_N \leq 1$, $\mathrm{tr}\, \omega_N = N$ such that, for $\varepsilon = N^{-1/3}$:*

$$\begin{aligned} &\mathrm{tr}\ |[x, \sqrt{\omega_N}]|^2 \leq CN\varepsilon^2 \qquad &&\mathrm{tr}\ |[\varepsilon\nabla, \sqrt{\omega_N}]|^2 \leq CN\varepsilon^2 \\ &\mathrm{tr}\ |[x, \sqrt{1-\omega_N}]|^2 \leq CN\varepsilon^2 \qquad &&\mathrm{tr}\ |[\varepsilon\nabla, \sqrt{1-\omega_N}]|^2 \leq CN\varepsilon^2 \,. \end{aligned} \tag{5.44}$$

Let $\gamma^{(1)}_{N,t}$ be the reduced one-particle density matrix of $\varphi_{N,t} = e^{-i\mathcal{L}_N t/\varepsilon}\varphi_N$. Let $\omega_{N,t}$ be the solution of the time-dependent Hartree-Fock equation:

$$i\varepsilon\partial_t \omega_{N,t} = [-\varepsilon^2\Delta + \rho_t * V - X_t, \omega_{N,t}] \,, \qquad \omega_{N,0} \equiv \omega_N \,. \tag{5.45}$$

Then, for some $c > 0$ and for all $t \in \mathbb{R}$:

$$\mathrm{tr}\, |\gamma^{(1)}_{N,t} - \omega_{N,t}|^2 \leq \exp(c\exp(c|t|)) \,, \quad \mathrm{tr}\, |\gamma^{(1)}_{N,t} - \omega_{N,t}| \leq N^{1/2}\exp(c\exp(c|t|)) \,. \tag{5.46}$$

Remark.

(i) This theorem proves the convergence of quantum dynamics to the Hartree-Fock evolution, with rate $1/N^{1/2}$ in both Hilbert-Schmidt and trace norms.

(ii) The estimates (5.44) play a role analogous to the one of (4.25) in Theorem 4.1. They encode the semiclassical structure of the initial data, which is expected to hold for the thermal state of H_N^{trap} at positive temperature.

(iii) The result can be extended to approximate quasi-free states $R_{\omega_N}\xi_N$, under the assumptions:

$$\xi_N = \chi(\mathcal{N} \leq CN)\xi_N \,, \qquad \langle \xi_N, \mathcal{N}^{10}\xi_N\rangle \leq \widetilde{C} \,, \tag{5.47}$$

where $\mathcal{N}$ is the number operator on $\mathcal{F}(L^2 \oplus L^2)$, and C, $\widetilde{C}$ are N-independent constants.

(iv) As for Theorem 4.1, the exchange term is subleading: dropping it does not affect the estimates.

(v) A similar result holds for k-particle densities, with $k > 1$.

The proof is based on a strategy conceptually similar to the one followed in the proof of Theorem 4.1. We have

$$\operatorname{tr}|\gamma_{N,t}^{(1)}-\omega_{N,t}|^2\leq C\langle\mathcal{U}_N(t)\Omega,\mathcal{N}\,\mathcal{U}_N(t)\Omega\rangle\;, \tag{5.48}$$

where $\Omega\equiv\Omega_{\mathcal{F}(L^2\oplus L^2)}$, and $\mathcal{U}_N(t):=R^*_{\omega_{N,t}}e^{-i\mathcal{L}_N t/\varepsilon}R_{\omega_N}$ is the dynamics of the fluctuations in $\mathcal{F}(L^2\oplus L^2)$, an operator that *does not* commute with $\mathcal{N}$. We control the growth of the number of fluctuations using a Gronwall-type strategy (similar but not equal to the one of [5]); as in the proof of Theorem 4.1, the semiclassical structure of the initial data (encoded in Eqs. (5.44)) plays a crucial role in controlling the error on the physically relevant time scale $t=O(1)$.

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