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Derivation of effective evolution equations from many-body quantum mechanics

Abstract. In these notes, based on a mini-course held at the summer school "Methods and Models of Kinetic Theory" that took place in Porto Ercole in June 2016, we review some of the recent developments in the derivation of effective evolution equations starting from many-body quantum mechanics. We discuss the derivation of the Hartree equation in the bosonic mean-field limit, of the Gross-Pitaevskii equation describing the dynamics of initially trapped Bose-Einstein condensates and of the Hartree-Fock equation for fermions in a joint mean-field and semiclassical limit.

Keywords. Quantum dynamics, Bose-Einstein condensation, Gross-Pitaevskii dynamics, Hartree-Fock equation.

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Contents

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A quantum system of N particles can be described by a wave function $\psi_N \in L^2(\mathbb{R}^{3N})$, normalized so that $\|\psi_N\|_2 = 1$. Observable quantities are associated with self-adjoint operators on $L^2(\mathbb{R}^{3N})$. The expected values of an observable A in the state ψ_N is given by the inner product $\langle \psi_N, A\psi_N \rangle$. In particular, position observables are associated with multiplication operators and momenta are associated with differential operator. Hence, $|\psi_N(x_1, \dots, x_N)|^2$ is the probability density for finding particles close to $(x_1, \dots, x_N) \in \mathbb{R}^{3N}$ and $|\widehat{\psi}_N(p_1, \dots, p_N)|^2$ is the probability density for finding particles with momenta close to $(p_1, \dots, p_N) \in \mathbb{R}^{3N}$.

We distinguish two types of particles, bosons and fermions, whose wave functions behave differently with respect to permutations. For systems with bosonic statistics, ψ_N is symmetric with respect to permutation, i.e.

$$\psi_N(x_{\pi 1}, \dots, x_{\pi N}) = \psi_N(x_1, \dots, x_N)$$

for all $\pi \in S_N$ (the group of permutations of N objects). For systems with fermionic statistics, on the other hand, ψ_N is antisymmetric with respect to permutations, i.e.

$$\psi_N(x_{\pi 1}, \dots, x_{\pi N}) = \sigma_\pi \psi_N(x_1, \dots, x_N)$$

where $\sigma_\pi \in \{\pm 1\}$ is the sign of the permutation π.

The time-evolution is governed by the many-body Schrödinger equation

$$i\partial_t \psi_{N,t} = H_N \psi_{N,t} \tag{1}$$

where $\psi_{N,t} \in L^2(\mathbb{R}^{3N})$ denotes the wave function at time $t \in \mathbb{R}$ and, on the right hand side, H_N is a self-adjoint operator, known as the Hamilton operator of the system. We will restrict our attention to Hamilton operators of the form

$$H_N = \sum_{j=1}^N \left[-\Delta_{x_j} + V_{\text{ext}}(x_j) \right] + \lambda \sum_{i<j}^N V(x_i - x_j) \tag{2}$$

where $V_{\text{ext}}, V : \mathbb{R}^3 \to \mathbb{R}$ are an external and, respectively, an interaction potential and $\lambda \in \mathbb{R}$ is a coupling constant. We use units such that the mass of the particles is $m = 1/2$ and Planck's constant $\hbar = 1$. Notice that H_N is invariant with respect to permutation of the N particles; as a consequence, (1) preserves the statistics (bosonic or fermionic).

The Schrödinger equation (1) is linear and it can be solved by means of the unitary group generated by H_N. In other words, for any $\psi_N \in L^2(\mathbb{R}^{3N})$, the unique solution of (1) with initial data $\psi_{N,t=0} = \psi_N$ is given by $\psi_{N,t} =$

$e^{-iH_N t}\psi_N$. In physically interesting situations, however, the number of particles N involved in the dynamics is very large (ranging between values of the order $N \simeq 10^3$ for extremely dilute samples of Bose-Einstein condensates, up to values of the order $N \simeq 10^{23}$ in chemistry). It is therefore very difficult to extract useful information, beyond existence and uniqueness of the solution $\psi_{N,t}$, from (1). For this reason, one of the most important tasks in non-equilibrium quantum statistical mechanics is the derivation of effective evolution equations approximating the solution of the Schrödinger equation (1) in physically relevant regimes.

1 - The Mean-Field Limit for Bosons

From the mathematical point of view, one of the most accessible (but still not trivial) regimes in many-body quantum mechanics is the mean-field limit for bosonic systems. In this regime, particles experience a large number of weak collisions, so that the total force on each particle can be approximated, in the spirit of the law of large numbers, by an effective average (or mean-field) potential.

A system of N bosons in the mean-field regime is described by a Hamilton operator of the form (2), with $N \gg 1$ (many collisions) and coupling constant $|\lambda| \ll 1$ (weak interactions). To make sure that the total effect of the many weak collisions is comparable with the inertia of the particles (i.e. the kinetic energy), we also require that the product $N\lambda$ is fixed, of order one. In other words, the Hamilton operator of a bosonic system in the mean-field regime is given by

$$H_{\text{mf}} = \sum_{j=1}^{N} \left[-\Delta_{x_j} + V_{\text{ext}}(x_j)\right] + \frac{1}{N}\sum_{i<j}^{N} V(x_i - x_j) \tag{3}$$

acting on $L^2_s(\mathbb{R}^{3N})$, the subspace of $L^2(\mathbb{R}^{3N})$ consisting of functions that are symmetric with respect to permutations.

It turns out that, under reasonable assumptions on V_{ext} and V, equilibrium states associated with the Hamilton operator (3) exhibit, at low temperature, complete Bose-Einstein condensation. This means that, up to a fraction vanishing as $N \to \infty$, all N particles in the system are described by the same one-particle wave function $\varphi \in L^2(\mathbb{R}^3)$.

To give a mathematically precise definition of Bose-Einstein condensation, we introduce the notion of reduced densities. For $\psi_N \in L^2_s(\mathbb{R}^{3N})$ and $k \in \{1, 2, \ldots, N\}$, we define the k-particle reduced density associated with ψ_N as the non-negative operator $\gamma_N^{(k)}$ on $L^2(\mathbb{R}^{3k})$ with the integral kernel

$$\begin{aligned}&\gamma_N^{(k)}(x_1,\dots,x_k;y_1,\dots,y_k)\\&=\int dx_{k+1}\dots dx_N\,\overline{\psi}_{N,t}(x_1,\dots,x_k,x_{k+1},\dots,x_N)\psi_{N,t}(y_1,\dots,y_k,x_{k+1},\dots,x_N).\end{aligned}$$

We choose here the normalization $\operatorname{tr}\gamma_N^{(k)}=1$, for all $N\in\mathbb{N}$ and $1\leq k\leq N$. Using $\gamma_N^{(k)}$, we can compute the expectation, in the state ψ_N, of an arbitrary k-particle observable. In fact, if A is a self-adjoint operator on $L^2(\mathbb{R}^{3k})$, a simple computation shows that

$$\left\langle\psi_{N,t},\left(A\otimes 1^{(N-k)}\right)\psi_{N,t}\right\rangle=\operatorname{tr} A\gamma_N^{(k)}\,.$$

Notice that, for exactly factorized $\psi_N=\varphi^{\otimes N}$, we easily find

$$\gamma_N^{(k)}=|\varphi\rangle\langle\varphi|^{\otimes k},\tag{4}$$

where $|\varphi\rangle\langle\varphi|$ denotes the orthogonal projection onto $\varphi\in L^2(\mathbb{R}^3)$. Bose-Einstein condensation means that (4) holds asymptotically, in the limit $N\to\infty$. More precisely, we say that a sequence $\psi_N\in L^2_s(\mathbb{R}^{3N})$ exhibits complete Bose-Einstein condensation in a one-particle state $\varphi\in L^2(\mathbb{R}^3)$ if and only if

$$\operatorname{tr}\left|\gamma_N^{(1)}-|\varphi\rangle\langle\varphi|\right|\to 0\tag{5}$$

as $N\to\infty$. Notice that (5) automatically implies that also $\gamma_N^{(k)}\to|\varphi\rangle\langle\varphi|^{\otimes k}$, for all fixed $k\in\mathbb{N}$, as $N\to\infty$ (the argument is sketched, for example, in [**32**], after Theorem 1).

With the definition (5) and with appropriate assumptions on the external potential (V_{ext} should be confining) and on V (for example, V should be bounded and positive definite), one can prove (see for example [**26**]) that the ground state ψ_N^{gs} of (3) exhibits complete Bose-Einstein condensation in the minimizer ϕ_H of the Hartree functional

$$\mathcal{E}_{\text{H}}(\varphi)=\int\left[|\nabla\varphi|^2+V_{\text{ext}}|\varphi|^2+\frac{1}{2}(V*|\varphi|^2)|\varphi|^2\right]dx\tag{6}$$

among all $\varphi\in L^2(\mathbb{R}^3)$ with $\|\varphi\|_2=1$. The physical interpretation of this result is clear: to minimize the energy, all particles, up to a fraction vanishing as $N\to\infty$, condense in the one-particle state ϕ_H, minimizing (6).

From the point of view of the dynamics, we are interested in the reaction of equilibrium states (at zero temperature, of the ground state) to perturbations.

In labs, the simplest perturbation of a many-body system is a change of the external fields. For example, we may ask what happens to a bosonic system in the ground state of (3), if we turn off the external potential V_{ext}. This leads us to the following question: what can we say about the solution of the many-body Schrödinger equation

$$i\partial_t \psi_{N,t} = \left[\sum_{j=1}^{N} -\Delta_{x_j} + \frac{1}{N} \sum_{i<j}^{N} V(x_i - x_j) \right] \psi_{N,t} \tag{7}$$

for a sequence of initial data $\psi_{N,0} = \psi_N$ exhibiting complete condensation in a one-particle state $\varphi \in L^2(\mathbb{R}^3)$? The answer is given by the next theorem, which holds true under appropriate assumptions on the interaction potential V (see discussion below).

Theorem 1.1. *Consider a sequence $\psi_N \in L^2_s(\mathbb{R}^{3N})$ exhibiting complete Bose-Einstein condensation, i.e. such that*

$$\gamma_N^{(1)} \to |\varphi\rangle\langle\varphi|$$

as $N \to \infty$, for a $\varphi \in L^2(\mathbb{R}^3)$ (for example, in the trace norm topology; since the limit is a rank-one projection, all convergence notions are actually equivalent). Let $\psi_{N,t}$ denote the solution of (7) with initial data $\psi_{N,0} = \psi_N$. Then, for every fixed $t \in \mathbb{R}$,

$$\gamma_{N,t}^{(1)} \to |\varphi_t\rangle\langle\varphi_t| \tag{8}$$

as $N \to \infty$, where φ_t is the solution of the time-dependent nonlinear Hartree equation

$$i\partial_t \varphi_t = -\Delta\varphi_t + (V * |\varphi_t|^2)\varphi_t \tag{9}$$

with initial data $\varphi_{t=0} = \varphi$.

The first results in the direction of Theorem 1.1 have already been obtained in [**27**, **28**]. The first proof of (8) was given in [**40**], for bounded potential $V \in L^\infty(\mathbb{R}^3)$. The approach of [**40**], which will be briefly presented in the next section, has been extended to interactions with a Coulomb singularity $V(x) = \pm 1/|x|$ in [**6**, **21**]. Recently, results similar to Theorem 1.1 have been obtained, for example, in [**1**, **2**, **15**, **23**, **24**, **25**, **29**, **31**, **39**].

2 - The BBGKY Approach for Bounded Potentials

In this section, we review the main ideas in the proof of Theorem 1.1 obtained in [**40**].

First of all, we observe that, starting from the Schrödinger equation (7), we can derive a system of partial differential equations for the reduced densities $\{\gamma^{(k)}_{N,t}\}_{k=1}^N$ associated with $\psi_{N,t}$. Using the permutation symmetry of $\psi_{N,t}$, we find the so called BBGKY hierarchy

$$
\begin{aligned}
i\partial_t \gamma^{(k)}_{N,t} = & \sum_{j=1}^k \left[-\Delta_{x_j}, \gamma^{(k)}_{N,t}\right] + \frac{1}{N}\sum_{i<j}^k \left[V(x_i - x_j), \gamma^{(k)}_{N,t}\right] \\
& + \frac{N-k}{N} \sum_{j=1}^k \text{tr}_{k+1} \left[V(x_j - x_{k+1}), \gamma^{(k+1)}_{N,t}\right]
\end{aligned} \tag{10}
$$

for $k = 1, \dots, N$ (with the convention that $\gamma^{(N+1)}_{N,t} \equiv 0$). Here tr_{k+1} denotes the partial trace over the $(k+1)$-th particle (it maps operators on $L^2(\mathbb{R}^{3(k+1)})$ into operators on $L^2(\mathbb{R}^{3k})$).

What happens to the hierarchy (10), if we let $N \to \infty$? Formally, we obtain the infinite hierarchy of equations

$$
i\partial_t \gamma^{(k)}_{\infty,t} = \sum_{j=1}^k \left[-\Delta_{x_j}, \gamma^{(k)}_{\infty,t}\right] + \sum_{j=1}^k \text{tr}_{k+1} \left[V(x_j - x_{k+1}), \gamma^{(k+1)}_{\infty,t}\right] \tag{11}
$$

for $k \in \mathbb{N}$. It is then easy to check that (11) has factorized solutions. In fact, the family $\gamma^{(k)}_{\infty,t} = |\varphi_t\rangle\langle\varphi_t|^{\otimes k}$ solves the infinite hierarchy (11) if and only if φ_t solves the nonlinear Hartree equation (9).

This observation suggests a strategy to prove Theorem 1.1. The strategy consists of three steps. In the first step, one shows the compactness of the sequence $\{\gamma^{(k)}_{N,t}\}_{k=1}^N$ with respect to an appropriately chosen weak topology. In the second step, one proves that every limit point $\{\gamma^{(k)}_{\infty,t}\}_{k\geq 1}$ of the sequence $\{\gamma^{(k)}_{N,t}\}_{k=1}^N$ solves the infinite hierarchy (11). Finally, in the third step, one has to show that the factorized solution $\gamma^{(k)}_{\infty,t} = |\varphi_t\rangle\langle\varphi_t|^{\otimes k}$ is the unique solution of the infinite hierarchy (with the correct initial data). Since a compact sequence with at most one limit point always converges, these three steps immediately imply that the sequence $\{\gamma^{(k)}_{N,t}\}_{k=1}^N$ converges, as $N \to \infty$, towards the factorized limit $\gamma^{(k)}_{\infty,t} = |\varphi_t\rangle\langle\varphi_t|^{\otimes k}$, completing the proof of Theorem 1.1.

Technically, the most difficult part of this program is the proof of the uniqueness of the solution of the infinite hierarchy. Let us briefly explain how uniqueness was proven in [**40**], for bounded interaction potentials. Rewriting (11) in integral form, we find

$$\gamma^{(k)}_{\infty,t} = \mathcal{U}^{(k)}(t)\gamma^{(k)}_{\infty,0} + \int_0^t \mathcal{U}^{(k)}(t-s)B^{(k)}\gamma^{(k+1)}_{\infty,s}ds \tag{12}$$

with the free evolution

$$\mathcal{U}^{(k)}(t)\gamma^{(k)} = e^{it\sum_{j=1}^k \Delta_{x_j}}\gamma^{(k)}e^{-it\sum_{j=1}^k \Delta_{x_j}}$$

and the collision operator

$$B^{(k)}\gamma^{(k+1)} = \sum_{j=1}^k \mathrm{tr}_{k+1}\left[V(x_j - x_{k+1}), \gamma^{(k+1)}\right].$$

Iterating (12), we obtain the series expansion

$$\gamma^{(k)}_{\infty,t} = \sum_{m=0}^{n-1} \xi^{(k)}_{m,t} + \eta^{(k)}_{n,t} \tag{13}$$

with

(14)

$$\xi^{(k)}_{m,t} = \int_0^t ds_1 \dots \int_0^{s_{m-1}} ds_m \mathcal{U}^{(k)}(t-s_1)B^{(k)} \dots B^{(k+m-1)}\mathcal{U}^{(k+m)}(s_m)\gamma^{(k+m)}_{\infty,0}$$

$$\eta^{(k)}_{n,t} = \int_0^t ds_1 \dots \int_0^{s_{n-1}} ds_n \mathcal{U}^{(k)}(t-s_1)B^{(k)} \dots B^{(k+n-1)}\gamma^{(k+n)}_{\infty,s_n}.$$

To prove uniqueness, it is enough to show that the remainder term $\eta^{(k)}_{n,t}$ vanishes, in the limit $n \to \infty$ (because the other terms only depend on the initial data). To this end, we consider the trace norm of $\eta^{(k)}_{n,t}$ (defined by $\|A\|_{\mathrm{tr}} = \mathrm{tr}\,|A|$). We observe that

$$\|\mathcal{U}^{(k)}(t)\gamma^{(k)}\|_{\mathrm{tr}} = \|\gamma^{(k)}\|_{\mathrm{tr}}$$

and that, for a bounded potential $V \in L^\infty(\mathbb{R}^3)$,

$$\begin{aligned}\|B^{(k)}\gamma^{(k+1)}\|_{\mathrm{tr}} = \mathrm{tr}\left|B^{(k)}\gamma^{(k+1)}\right| &\leq \sum_{j=1}^k \mathrm{tr}\left|\left[V(x_j - x_{k+1}), \gamma^{(k+1)}\right]\right| \\ &\leq 2k\|V\|_\infty \|\gamma^{(k+1)}\|_{\mathrm{tr}}\,.\end{aligned}$$

Here we used the fact that, for a bounded operator B and a trace-class operator A, $\|AB\|_{\mathrm{tr}}, \|BA\|_{\mathrm{tr}} \leq \|A\|_{\mathrm{tr}}\|B\|$. Applying the last two bounds to the error term $\eta_{n,t}^{(k)}$, we find that

$$\left\|\eta_{n,t}^{(k)}\right\| \leq \frac{(2t\|V\|_\infty)^n}{n!}k(k+1)\dots(k+n-1) \leq 2^k(4t\|V\|_\infty)^n. \tag{15}$$

This proves the uniqueness for $|t| \leq 1/(8\|V\|_\infty)$. Iterating the same argument, we get uniqueness for all times.

3 - Extension to Coulomb Singularities

For $V(x) = \pm 1/|x|$, the argument presented above to show the uniqueness of the infinite hierarchy does not apply. To control the singularity of the potential, one has to use a-priori bounds on the kinetic energy; this point has been first realized in [**21**].

Uniqueness is shown to hold in the class of (time-dependent) infinite families of reduced densities $\{\gamma_{\infty,t}^{(k)}\}_{k\geq 1}$, such that

$$\|\gamma_{\infty,t}^{(k)}\|_{H_k^1} := \mathrm{tr}\left|(1-\Delta_{x_1})^{1/2}\dots(1-\Delta_{x_k})^{1/2}\gamma_{\infty,t}^{(k)}(1-\Delta_{x_k})^{1/2}\dots(1-\Delta_{x_1})^{1/2}\right| \leq C^k \tag{16}$$

for a constant $C > 0$ and all $k \in \mathbb{N}$, $t \in \mathbb{R}$. To reach this goal, we proceed as follows. First, we expand the solution as in (13). Here, however, we control the error term $\eta_{n,t}^{(k)}$ in the $\|.\|_{H_k^1}$ norm defined in (16), rather than in the trace norm. The key observation is that, on the one hand,

$$\|\mathcal{U}^{(k)}(t)\gamma^{(k)}\|_{H_k^1} = \|\gamma^{(k)}\|_{H_k^1}$$

since the Laplace operators commute with the free evolution and, on the other hand,

$$\|B^{(k)}\gamma^{(k+1)}\|_{H_k^1} \leq C\|\gamma^{(k+1)}\|_{H_{k+1}^1} \tag{17}$$

for an appropriate constant $C > 0$. The last two estimates imply, similarly as in (15), that

$$\|\eta_{n,t}^{(k)}\|_{H_k^1} \leq C^k(C|t|)^n$$

and therefore that $\eta_{n,t}^{(k)} \to 0$ as $n \to \infty$, for $|t|$ sufficiently small. This proves uniqueness, first for short time but then, by iteration (since the a-priori bounds (16) are assumed to hold uniformly in t), for all $t \in \mathbb{R}$.

To prove (17) we observe, using the notation $S_j = (1-\Delta_{x_j})^{1/2}$ and the permutation symmetry, that

$$\begin{aligned}\|B^{(k)}\gamma^{(k+1)}\|_{H^1_k} &\leq \sum_{j=1}^{k} \mathrm{tr}\left| S_1 \dots S_k \mathrm{tr}_{k+1}\left[\frac{1}{|x_j - x_{k+1}|}, \gamma^{(k+1)}\right] S_k \dots S_1 \right| \\ &\leq k\,\mathrm{tr}\left| S_1 \dots S_k \mathrm{tr}_{k+1} \frac{1}{|x_1 - x_{k+1}|}\gamma^{(k+1)} S_k \dots S_1\right| \\ &\quad + k\,\mathrm{tr}\left| S_1 \dots S_k \mathrm{tr}_{k+1}\gamma^{(k+1)} \frac{1}{|x_1 - x_{k+1}|} S_k \dots S_1\right|.\end{aligned}$$

By the cyclicity of the partial trace, and since $\mathrm{tr}|\mathrm{tr}_{k+1}A| \leq \mathrm{tr}|A|$ for every $(k+1)$-particle operator A, we find

$$\begin{aligned}\|B^{(k)}\gamma^{(k+1)}\|_{H^1_k} \leq k\,\mathrm{tr}&\left| S_1 S_{k+1}^{-1} \frac{1}{|x_1 - x_{k+1}|} S_{k+1}^{-1} S_1^{-1} S_1 \dots S_{k+1}\gamma^{(k+1)} S_{k+1} \dots S_1\right| \\ &+ k\,\mathrm{tr}\left| S_1 \dots S_{k+1}\gamma^{(k+1)} S_{k+1}\dots S_1 S_1^{-1} S_{k+1}^{-1} \frac{1}{|x_1 - x_{k+1}|} S_{k+1}^{-1} S_1\right|.\end{aligned}$$

Since $\|AB\|_{\mathrm{tr}}, \|BA\|_{\mathrm{tr}} \leq \|A\|_{\mathrm{tr}}\|B\|$ (i.e. since the space of trace class operators is a two-sided ideal in the space of bounded operators), we conclude that

$$\|B^{(k)}\gamma^{(k+1)}\|_{H^1_k} \leq 2k \left\| S_1 S_{k+1}^{-1} \frac{1}{|x_1 - x_{k+1}|} S_{k+1}^{-1} S_1^{-1}\right\| \, \|\gamma^{(k+1)}\|_{H^1_{k+1}}.$$

Treating S_1 as a simple derivative, and using the operator inequality

$$\frac{1}{|x|^2} \leq C(1-\Delta)$$

we easily find

$$\left\| S_1 S_{k+1}^{-1} \frac{1}{|x_1 - x_{k+1}|} S_{k+1}^{-1} S_1^{-1}\right\| < \infty$$

which leads us to (17) (the precise proof requires some more care to commute the non-local operator S_1 to the right of the Coulomb interaction).

Observe that the proof of uniqueness that we just sketched provides a weaker result, compared with the one for bounded potential discussed in the previous section. Here, for a Coulomb interaction, we only get uniqueness for reduced densities satisfying the a-priori bounds (16). Of course, there is a price to pay for establishing uniqueness in a smaller class of densities. To apply this result to prove Theorem 1.1 for a Coulomb interaction, one first has to show that every limit point $\{\gamma^{(k)}_{\infty,t}\}_{k\geq 1}$ of the sequence $\{\gamma^{(k)}_{N,t}\}_{k=1}^N$ of reduced densities associated with the solution of the Schrödinger equation (7) satisfies the a-priori bounds (16). This can be done by noticing that

(18)
$$\|\gamma^{(k)}_{N,t}\|_{H^1_k} = \mathrm{tr}\,(1-\Delta_{x_1})\dots(1-\Delta_{x_k})\gamma^{(k)}_{N,t} \simeq N^{-k}\left\langle \psi_{N,t}, \left[\sum_{j=1}^N -\Delta_{x_j} + N\right]^k \psi_{N,t}\right\rangle$$

up to errors converging to zero, as $N \to \infty$, and by comparing the moments of the kinetic energy operator appearing on the r.h.s. of (18) with moments of the Hamilton operator

$$H_{\mathrm{cou}} = \sum_{j=1}^N -\Delta_{x_j} + \frac{1}{N}\sum_{i<j}^N \frac{1}{|x_i - x_j|}$$

generating the many-body time evolution (moments of H_{cou} are preserved by the evolution). The details can be found in [**21**] and, for the case of a relativistic dispersion law, in [**17**].

4 - The Gross-Pitaevskii Limit

A mathematically more subtle regime, compared with the mean-field limit discussed in Sections 1-3, is the so-called Gross-Pitaevskii regime, which is used to describe trapped Bose-Einstein condensates. Since 1995, this has become a very hot topic of research, in physics and in mathematical physics, because Bose-Einstein condensates have become accessible to experiments. In the Gross-Pitaevskii regime, a gas of N bosons is described by the Hamilton operator

$$H^{\mathrm{trap}}_{\mathrm{GP}} = \sum_{j=1}^N \left[-\Delta_{x_j} + V_{\mathrm{ext}}(x_j)\right] + \sum_{i<j}^N N^2 V(N(x_i - x_j)) \tag{19}$$

where V_{ext} is an external potential, trapping the particles in a volume of order one, and $V \geq 0$ is a smooth short-range (for simplicity, compactly supported) interaction.

The pair potential scales with the number of particles N so that its scattering length is of the order N^{-1}. Let us recall that the scattering length of an interaction V is defined through the zero-energy scattering equation

$$\left(-\Delta + \frac{1}{2}V\right) f = 0 \tag{20}$$

with the boundary condition $f(x) \to 1$, as $|x| \to \infty$. For $|x|$ large (outside the support of V), we must have

$$f(x) = 1 - \frac{a_0}{|x|}$$

for a constant a_0 which is known as the scattering length of V. Equivalently, the scattering length can be defined through the integral

$$8\pi a_0 = \int V f dx. \tag{21}$$

From the definition of the scattering length a_0 of V, it is clear that the scattering length of the rescaled potential $N^2 V(N.)$ appearing in (19) is given by a_0/N, since

$$\left(-\Delta + \frac{N^2}{2} V(Nx)\right) f(Nx) = 0\,. \tag{22}$$

It has been shown in [**32**,**33**] that the ground state of (19) exhibits complete Bose-Einstein condensation (in the sense (5)) in the minimizer of the Gross-Pitaevskii energy functional

$$\mathcal{E}_{\mathrm{GP}}(\varphi) = \int \left[|\nabla\varphi|^2 + V_{\mathrm{ext}}|\varphi|^2 + 4\pi a_0|\varphi|^4\right] dx$$

among all $\varphi \in L^2(\mathbb{R}^3)$ with $\|\varphi\|_2 = 1$.

As we did in Section 1, also here it is natural to ask: what happens to the gas at equilibrium in the ground state of (19) if, at time $t = 0$, we turn off the external fields. Obviously, the gas will start to evolve and its evolution is governed by the Schrödinger equation

$$i\partial_t \psi_{N,t} = H_{\mathrm{GP}} \psi_{N,t} \tag{23}$$

with the translation invariant Hamilton operator

$$H_{\mathrm{GP}} = \sum_{j=1}^{N} -\Delta_{x_j} + \sum_{i<j}^{N} N^2 V(N(x_i - x_j))\,. \tag{24}$$

The next theorem shows that, for any fixed $t \in \mathbb{R}$, the solution $\psi_{N,t}$ of (23) still exhibits complete Bose-Einstein condensation and that the condensate wave function evolves according to the time-dependent Gross-Pitaevskii equation.

Theorem 4.1. *Let $V \geq 0$ be regular, spherically symmetric and compactly supported. Let $\psi_N \in L^2_s(\mathbb{R}^{3N})$ be a sequence with*

i) *one-particle reduced density* $\gamma^{(1)}_{N,t}$ *such that* $\gamma^{(1)}_{N,t} \to |\varphi\rangle\langle\varphi|$ *for a* $\varphi \in L^2(\mathbb{R}^3)$ *with* $\|\varphi\|_2 = 1$.

ii) *finite energy per particle, i.e.*

$$\langle \psi_N, H_{GP} \psi_N \rangle \leq CN. \tag{25}$$

Let $\psi_{N,t}$ *denote the solution of the Schrödinger equation* (23) *with initial data* $\psi_{N,t=0} = \psi_N$. *Then the one-particle reduced density* $\gamma^{(1)}_{N,t}$ *associated with* $\psi_{N,t}$ *is such that, for every fixed* $k \in \mathbb{N}$ *and* $t \in \mathbb{R}$,

$$\gamma^{(k)}_{N,t} \to |\varphi_t\rangle\varphi_t|^{\otimes k}$$

as $N \to \infty$ (*recall that, since the limit is a rank-one projection, convergence for* $k = 1$ *is equivalent to convergence for all* $k \in \mathbb{N}$). *Here* φ_t *is the solution of the time-dependent Gross-Pitaevskii equation*

$$i\partial_t \varphi_t = -\Delta\varphi_t + 8\pi a_0 |\varphi_t|^2 \varphi_t \tag{26}$$

with initial data $\varphi_{t=0} = \varphi$.

The first proof of Theorem 4.1 has been obtained in the series of papers [**18**,**19**,**20**]. A different approach has been later proposed in [**37**]. More recently, a similar statement (with a bound on the rate of the convergence, for a certain class of initial data) has been established in [**7**].

To explain the connection with Theorem 1.1 in the mean-field regime, we can write the Hamilton operator (24) as

$$H_{\text{GP}} = \sum_{j=1}^N -\Delta_{x_j} + \frac{1}{N}\sum_{i<j}^N N^3 V(N(x_i - x_j)) .$$

At first sight, it seems that the Gross-Pitaevskii regime is just a mean-field limit with the N-dependent interaction $N^3 V(N.)$ converging, in the limit of large N, to a Dirac-δ function. However, this interpretation is quite misleading.

Formally, we have $N^3 V(Nx) \to b_0 \delta(x)$, with the constant $b_0 = \int V dx$. If we believed in the analogy with the mean-field regime, we should expect the solution of (23) to be approximated by products of the solution of the Hartree equation (9), with V replaced by $b_0\delta(x)$. This leads to a nonlinear Schrödinger equation similar to the Gross-Pitaevskii equation (26), but with a different constant in front of the nonlinearity (b_0 instead of $8\pi a_0$). The analogy with the mean-field regime leads therefore to the wrong limiting equation; this is a consequence of the fact that, in the Gross-Pitaevskii regime, the solution of the Schrödinger equation develops correlations among the particles. These correlations are responsible for the emergence of the scattering length in (26).

To understand this important point, let us consider the first equation in the BBGKY hierarchy governing the evolution of the reduced densities associated with the solution of (23):

$$i\partial_t \gamma^{(1)}_{N,t} = \left[-\Delta, \gamma^{(1)}_{N,t}\right] + (N-1)\text{tr}_2 \left[N^2 V(N(x_1-x_2)), \gamma^{(2)}_{N,t}\right].$$

Let us consider, in particular, one of the two contributions arising from the second term on the r.h.s. of the last equation. Approximating $(N-1) \simeq N$, its integral kernel is given by

$$\left[N\text{tr}_2 N^2 V(N(x_1-x_2))\gamma^{(2)}_{N,t}\right](x_1;y_1) = \int dx_2 N^3 V(N(x_1-x_2))\gamma^{(2)}_{N,t}(x_1,x_2;y_1,x_2).$$

The ansatz

$$\gamma^{(2)}_{N,t}(x_1,x_2;y_1,y_2) = \varphi_t(x_1)\varphi_t(x_2)\overline{\varphi}_t(y_1)\overline{\varphi}_t(y_2)$$

leads (in the limit of large N) to

$$\left[N\text{tr}_2 N^2 V(N(x_1-x_2))\gamma^{(2)}_{N,t}\right](x_1;y_1) \simeq b_0|\varphi_t(x_1)|^2\varphi_t(x_1)\overline{\varphi}_t(y_1)$$

and thus to the wrong limiting equation (with coupling constant b_0). If instead we use the solution of the zero energy scattering equation (22) to take into account correlations, we find the improved ansatz

$$\gamma^{(2)}_{N,t}(x_1,x_2;y_1,y_2) = f(N(x_1-x_2))f(N(y_1-y_2))\varphi_t(x_1)\varphi_t(x_2)\overline{\varphi}_t(y_1)\overline{\varphi}_t(y_2) \tag{27}$$

and we obtain, using (21) and letting $N \to \infty$,

$$\begin{aligned}\left[N\text{tr}_2 N^2 V(N(x_1-x_2))\gamma^{(2)}_{N,t}\right](x_1;y_1) \\ \simeq \int dx_2 N^3 V(N(x_1-x_2))f(N(x_1-x_2))|\varphi_t(x_2)|^2\varphi_t(x_1)\overline{\varphi}_t(y_1) \\ \simeq 8\pi a_0|\varphi_t(x_1)|^2\varphi_t(x_1)\overline{\varphi}_t(y_1)\end{aligned} \tag{28}$$

which leads us to (26), this time with the correct coupling constant. Notice that the correlation factors $f(N(x_1-x_2))$ and $f(N(y_1-y_2))$ that we introduced in the ansatz (27) to model correlations converge to one, in the limit $N \to \infty$. They are substantially different from one only when $|x_1-x_2| \lesssim N^{-1}$ or $|y_1-y_2| \lesssim N^{-1}$. Hence, they only play an important role when multiplied with the singular potential $N^3V(N.)$, otherwise they can be neglected. This is the reason why in (28) we retain only the correlation factor $f(N(x_1-x_2))$

while we neglect $f(N(y_1 - y_2))$. This is also the reason why the ansatz (27) is not in contradiction with the fact that $\psi_{N,t}$ exhibits complete Bose-Einstein condensation, which implies that $\gamma^{(k)}_{N,t} \to |\varphi_t\rangle\langle\varphi_t|^{\otimes k}$, as $N \to \infty$, for every fixed $k \in \mathbb{N}$.

This heuristic discussion explains that a very important step to obtain a proof of Theorem 4.1 consists in showing that the solution of the many-body Schrödinger equation (23) does indeed develop a short scale correlation structure which can be described, in good approximation, by the solution of the zero-energy scattering equation (22). For small interaction potential V, this goal can be reached by means of the energy estimate in the next proposition, whose proof can be found in [**19**] (a similar bound can also be obtained with no assumption on the size of V, making use of the wave operators associated with the Schrödinger operator $-\Delta + V/2$; the details can be found in [**20**]).

Proposition 4.2. *Let $V \geq 0$ be regular, spherically symmetric and with short range (for simplicity, compactly supported). Assume additionally that*

$$\alpha = \sup_{r \geq 0} x^2 V(x) + \int V(x)|x|^{-1} dx \tag{29}$$

is small enough. Then there exists $c > 0$ such that

$$\langle \psi_N, H^2_{GP} \psi_N \rangle \geq cN^2 \int dx_1 \dots dx_N \left| \nabla_{x_1} \nabla_{x_2} \frac{\psi_N(x_1, \dots, x_N)}{f(N(x_1 - x_2))} \right|^2 \tag{30}$$

for all $\psi_N \in L^2_s(\mathbb{R}^{3N})$.

Let $\psi_{N,t}$ be the solution of the Schrödinger equation (23), with initial data $\psi_N \in L^2_s(\mathbb{R}^{3N})$ satisfying the bound

$$\langle \psi_N, H^2_{\mathrm{GP}} \psi_N \rangle \leq CN^2$$

for a constant $C > 0$ independent of N (at the end, this assumption can be relaxed with a simple approximation argument and one only needs the condition (25) on the expectation of H_{GP} for Theorem 4.1 to hold true). Then (30) implies that

$$\begin{aligned} \int dx_1 \dots dx_N \left| \nabla_{x_1} \nabla_{x_2} \frac{\psi_{N,t}(x_1, \dots, x_N)}{f(N(x_1 - x_2))} \right|^2 &\leq CN^{-2} \langle \psi_{N,t}, H^2_{\mathrm{GP}} \psi_{N,t} \rangle \\ &= CN^{-2} \langle \psi_N, H^2_{\mathrm{GP}} \psi_N \rangle \leq C \end{aligned} \tag{31}$$

for an appropriate constant $C > 0$ (changing from line to line).

The bound (31) shows exactly that $\psi_{N,t}$ has a short scale correlation structure that can be described by the solution of the zero-energy scattering equation

(22). It is crucial to observe that, in (31), we first divide $\psi_{N,t}$ by $f(N(x_1 - x_2))$ removing the correlations between particles one and two. Only afterwards we take derivatives in the variables x_1 and x_2. Without dividing by $f(N(x_1 - x_2))$, the integral in (31) would be of order N.

Observe that, in (30), we use an estimate for the second moment of H_{GP} to identify correlations. It is natural to ask whether an estimate for the first moment would also suffice. The presence of the correlations clearly lowers the energy; however, even in a completely uncorrelated product state $\varphi^{\otimes N}$, the expectation of H_{GP} is of the order N, the same order as for the ground state of H_{GP}. So, it is difficult to distinguish between correlated and uncorrelated states by looking only at the expectation of H_{GP} (to do so, one would need to compare the expectation $\langle \psi_N, H_{\text{GP}} \psi_N \rangle$ with the Gross-Pitaevskii energy $\mathcal{E}_{\text{GP}}(\varphi)$ of the orbital $\varphi \in L^2(\mathbb{R}^3)$ into which ψ_N exhibits condensation; this approach has been followed in [**37**]). It is simpler to distinguish between correlated and uncorrelated states by looking at the expectation of H_{GP}^2. It follows from (30) (or from a simple direct computation) that $\langle \varphi^{\otimes N}, H_{\text{GP}}^2 \varphi^{\otimes N} \rangle$ is of the order N^3 and hence by a factor of N larger than for states with the correct correlations.

Starting from the estimate (31), we conclude that the solution $\psi_{N,t}$ of the Schrödinger equation (23) and therefore also the corresponding reduced densities $\{\gamma_{N,t}^{(k)}\}_{k=1}^N$ have a correlation structure that can be described, in good approximation, by $f(N.)$. Hence, if $\gamma_{N,t}^{(k)}$ converges, in the limit of large N, towards a limit point $\gamma_{\infty,t}^{(k)}$ then, in good approximation,

$$\gamma_{N,t}^{(k)}(x_1, \dots, x_k; y_1, \dots, y_k) \simeq \prod_{i<j}^{k} f(N(x_i - x_j)) f(N(y_i - y_j))\, \gamma_{\infty,t}^{(k)}(x_1, \dots, x_k; y_1, \dots, y_k).$$

Inserting this expression in the BBGKY governing the evolution of the reduced densities $\{\gamma_{N,t}^{(k)}\}_{k=1}^N$ and letting $N \to \infty$, we end up, similarly as in (28), with the infinite hierarchy

$$\text{(32)} \qquad i\partial_t \gamma_{\infty,t}^{(k)} = \sum_{j=1}^{k} \left[-\Delta_{x_j}, \gamma_{\infty,t}^{(k)} \right] + 8\pi a_0 \sum_{j=1}^{k} \text{tr}_{k+1} \left[\delta(x_j - x_{k+1}), \gamma_{\infty,t}^{(k+1)} \right].$$

with the correct coupling constant proportional to the scattering length in front of the interaction. Like in the mean-field regime, also here it is easy to verify that the factorized densities $\gamma_{\infty,t}^{(k)} = |\varphi_t\rangle\langle\varphi_t|^{\otimes k}$ are a solution of the infinite hierarchy (32) if and only if φ_t solves the Gross-Pitaevskii equation (26). Hence, to conclude the proof of Theorem 4.1, what is left is a proof of the uniqueness of the solution of (32). Here, one has to face two new challenges, compared with the mean-field case.

First of all, it is now more difficult to prove that limit points $\{\gamma^{(k)}_{\infty,t}\}_{k\geq 1}$ of the sequence $\{\gamma^{(k)}_{N,t}\}_{k=1}^N$ satisfy a-priori estimates of the form

$$\|\gamma^{(k)}_{\infty,t}\|_{H^1_k} = \operatorname{tr}\left|(1-\Delta_{x_1})^{1/2}\dots(1-\Delta_{x_k})^{1/2}\gamma^{(k)}_{\infty,t}(1-\Delta_{x_k})^{1/2}\dots(1-\Delta_{x_1})^{1/2}\right| \leq C^k \tag{33}$$

uniformly in t. Because of the short scale correlation structure, for finite N the reduced densities $\gamma^{(k)}_{N,t}$ do not satisfy these bounds, at least not uniformly in N. While the solution $f(N.)$ of the zero energy scattering equation is always bounded between 0 and 1, it varies on the scale N^{-1}, and therefore its derivatives are large, in the limit $N \to \infty$. Only after letting $N \to \infty$, correlations disappear and (33) can hold true.

So, to prove (33), we first have to introduce a cutoff function, setting $\Theta^{(k)}_N = \prod_{j=1}^k \theta_j$, with

$$\theta_j(x_1,\dots,x_N) \simeq \begin{cases} 0 & \text{if there exists } i \neq j \text{ with } |x_j - x_i| \leq \ell, \\ 1 & \text{it } |x_j - x_i| \gg \ell \text{ for all } i \neq j. \end{cases}$$

On the support of $\Theta^{(k)}_N$, there is no particle in a ball of radius ℓ around $x_1,\dots,x_k$. If ℓ is not too small (it turns out, if $\ell \gg N^{-1/2}$), derivatives in the variables $x_1,\dots,x_k$ are not affected by the short scale correlations structure, and one can prove that

$$\operatorname{tr}\Theta^{(k)}_N(x_1,\dots,x_N)(1-\Delta_{x_1})^{1/2}\dots(1-\Delta_{x_k})^{1/2}\gamma^{(k)}_{N,t}(1-\Delta_{x_k})^{1/2}\dots(1-\Delta_{x_1})^{1/2} \leq C^k \tag{34}$$

uniformly in N. On the other hand, if ℓ is not too large (it turns out, if $\ell \ll N^{-1/3}$), one can show that the cutoff function $\Theta^{(k)}_N$, which is only effective in a small part of the configuration space, with a volume that vanishes as $N \to \infty$, becomes negligible in the limit of large N. Hence, with the right choice of $N^{-1/2} \ll \ell \ll N^{-1/3}$, one can first prove (34) and then show that (34) implies (33) for the limit points $\{\gamma^{(k)}_{\infty,t}\}_{k\geq 1}$ of the sequence $\{\gamma^{(k)}_{N,t}\}_{k=1}^N$; the details can be found in [**20**].

The second challenge one has to face to show the uniqueness of the solution of the infinite hierarchy (32) is the fact that, in contrast with the Coulomb potential considered in Section 3, the δ-interaction appearing on the r.h.s of

(32) cannot be controlled by the kinetic energy (because in three dimensions, the L^∞ norm is not bounded by the H^1-norm). So, the a-priori estimates (33) are not enough, here, to control the error term in the expansion (13). Instead, to show that $\eta_{n,t}^{(k)}$ tends to zero, as $n \to \infty$, one has to make use of the smoothing effect of the free evolution operators; in [**18**] this goal was reached through an expansion of $\eta_{n,t}^{(k)}$ in a sum of terms associated with certain Feynman graphs. More recently, a simpler proof of the uniqueness of the infinite hierarchy (32) has been obtained in [**14**] (combining ideas from [**30**] with the quantum de Finetti Theorem).

5 - Fermions in the Mean-Field Regime

In this section, we switch to fermions. We consider a system of N particles, described by a wave function $\psi_N \in L^2_a(\mathbb{R}^{3N})$, the subspace of $L^2(\mathbb{R}^{3N})$ consisting of functions that are antisymmetric with respect to permutations.

As in the previous sections, we focus on Hamilton operators with two-body interactions, having the form

$$H_N = \sum_{j=1}^N -\Delta_{x_j} + \lambda \sum_{i<j}^N V(x_i - x_j). \tag{35}$$

Physically, we are interested in the mean-field regime, in which the N particles are initially trapped in a volume of order one. Because of the fermionic statistics, the kinetic energy of N particles in a volume of order one is of order $N^{5/3}$, much larger than for bosons. To make sure that kinetic and potential energy are of the same order, here we have to choose the coupling constant $\lambda = N^{-1/3}$. Furthermore, the fact that the kinetic energy is of order $N^{5/3}$ means that the kinetic energy per particle is, in average, of order $N^{2/3}$; this implies that particles move very fast, with an average speed of the order $N^{1/3}$. For this reason, we can only follow the evolution of the system for short times, of the order $N^{-1/3}$. After rescaling time, we end up with the N-particle Schrödinger equation

$$iN^{1/3}\partial_t \psi_{N,t} = \left[\sum_{j=1}^N -\Delta_{x_j} + \frac{1}{N^{1/3}} \sum_{i<j}^N V(x_i - x_J)\right] \psi_{N,t}. \tag{36}$$

Here, t denotes the rescaled time variable; we are interested in t of order one. It is convenient to rewrite (36) in a more familiar form. We set $\varepsilon = N^{-1/3}$ and we multiply (36) on the left and on the right with ε^2. We obtain

$$i\varepsilon\partial_t \psi_{N,t} = \left[\sum_{j=1}^N -\varepsilon^2\Delta_{x_j} + \frac{1}{N} \sum_{i<j}^N V(x_i - x_J)\right] \psi_{N,t}. \tag{37}$$

Notice that we recover the same N^{-1} factor in front of the potential energy which characterized the mean field limit for bosons. The difference is that now, in the fermionic case, the mean-field limit is coupled with a semiclassical limit with $\varepsilon = N^{-1/3}$ playing the role of Planck's constant and converging to zero, as $N \to \infty$.

As in the bosonic case, the choice of the initial data is dictated by physics. Interesting data are equilibrium states for N-particle systems described by Hamilton operators of the form

$$H_N^{\text{trap}} = \sum_{j=1}^N \left[-\varepsilon^2 \Delta_{x_j} + V_{\text{ext}}(x_j) \right] + \frac{1}{N} \sum_{i<j}^N V(x_i - x_j) \tag{38}$$

with a trapping potential V_{ext}. In particular, at or close to zero temperature, we are interested in the solution of (37) for initial data close to the ground state of a Hamilton operator of the form (38). The ground state of (38) is expected (and in certain cases, also known) to be well approximated by a Slater determinant, which is an N-particle wave function of the form

$$\psi_{\text{slater}}(x_1, \dots, x_N) = \frac{1}{\sqrt{N!}} \det \left(f_i(x_j) \right)_{1 \le i,j \le N} . \tag{39}$$

Here $\{f_j\}_{j=1}^N$ is an orthonormal system in $L^2(\mathbb{R}^3)$. It is useful to compute the one-particle reduced density associated with the Slater determinant (39); its integral kernel is given by

$$\begin{aligned} \omega_N(x;y) &= N \int dx_2 \dots dx_N \, \overline{\psi}_{\text{slater}}(x, x_2, \dots, x_N) \psi_{\text{slater}}(y, x_2, \dots, x_N) \\ &= \sum_{j=1}^N \overline{f}_j(x) f_j(y). \end{aligned} \tag{40}$$

In other words, ω_N is the orthogonal projection onto the N-dimensional subspace of $L^2(\mathbb{R}^3)$ spanned by the N orbitals $f_1, \dots, f_N$ defining (39). Notice that, here and in the rest of this section, we will normalize one-particle reduced density differently than for bosons, requiring their trace to be N (rather than one). It is interesting to remark that Slater determinant are quasi-free states; the expectation $\langle \psi_{\text{slater}}, A \psi_{\text{slater}} \rangle$ of an arbitrary observable A can be expressed in terms of the reduced one-particle density ω_N (higher order correlation functions can be expressed in terms of ω_N by means of Wick's theorem). For example, a simple computation shows that the expectation of the Hamilton operator (38) in a Slater determinant with reduced one particle density ω_N is given by the Hartree-Fock energy functional

$$\mathcal{E}_{\mathrm{HF}}(\omega_N) = \mathrm{tr}\ \left[-\varepsilon^2\Delta + V_{\mathrm{ext}}(x)\right]\omega_N + \frac{1}{2N}\int dxdy\, V(x-y)\ \left[\omega_N(x;x)\omega_N(y;y) - |\omega_N(x;y)|^2\right]. \tag{41}$$

It seems natural, at this point, to study the solution of (37) for initial data close to a Slater determinant. Similarly as in the bosonic case, we may expect that the evolution of an approximate Slater determinant remains close to an evolved Slater determinant, and that the evolution of the Slater determinant can be described by the time-dependent Hartree-Fock equation associated with the energy functional (41), having the form

$$i\varepsilon\partial_t\omega_N = \left[-\varepsilon^2\Delta + V * \rho_t - X_t;\omega_N\right] \tag{42}$$

with $\rho_t(x) = N^{-1}\omega_{N,t}(x;x)$ and $X_t(x;y) = N^{-1}V(x-y)\omega_{N,t}(x;y)$. It turns out, however, that, in contrast with the bosonic case, not every initial Slater determinant will remain close, during its many-body evolution, to an evolved Slater determinant. Instead, Slater determinants minimizing the energy (41) (approximating therefore the ground state of (38)) inherit a semiclassical structure which plays a crucial role in the study of their time-evolution.

To understand this point, let us consider the simple example of N free fermions described by the Hamilton operator $H_{\mathrm{free}} = \sum_{j=1}^N -\Delta_{x_j}$ acting on $L^2(\Lambda^N)$, with $\Lambda = [0;1]^3$ and periodic boundary conditions. The eigenstates of the one-particle Hamiltonian $-\Delta$ are plane waves $f_p(x) = e^{-ip\cdot x}$, for $p \in 2\pi\mathbb{Z}^3$; the corresponding eigenvalue is p^2. The ground state for the many-body Hamiltonian H_{free} is therefore a Slater determinant, constructed with the N eigenmodes $f_p \in L^2(\Lambda)$ having the smallest possible energies (because of the required antisymmetry, we cannot have two particles in the same mode). The one-particle reduced density of the ground state is therefore given by

$$\begin{aligned}\omega_N(x;y) &= \sum_{p\in 2\pi\mathbb{Z}^3:|p|\leq cN^{1/3}} e^{ip\cdot(x-y)} \\ &= \sum_{p\in 2\pi N^{-1/3}\mathbb{Z}^3:|p|\leq c} e^{ip\cdot\frac{x-y}{\varepsilon}} \\ &\simeq N\int_{|p|\leq c} e^{ip\cdot(x-y)/\varepsilon} = Ng((x-y)/\varepsilon)\end{aligned}$$

for an appropriate function g with $g(z)\to 0$ as $|z|\to\infty$ (the precise form of g will not be needed for the next discussion). We conclude that the ground state of this system of free fermions is a Slater determinant, with reduced one-particle density having an integral kernel $\omega_N(x;y)$ localized close to the diagonal (such that $\omega_N(x;y) \simeq 0$, for $|x-y| \gg \varepsilon$).

More generally, if instead of free fermions in a box we considered a system of free fermions in a trapping potential, we would expect the integral kernel of the one-particle reduced density ω_N of the ground state Slater determinant to oscillate on the short length-scale ε in the $(x-y)$-direction and at the same time to exhibit a smooth profile in the $(x+y)$-direction. In other words, we expect the integral kernel of ω_N to have the form

$$\omega_N(x;y) \simeq N\rho((x+y)/2)g((x-y)/\varepsilon) \tag{43}$$

with regular functions ρ, g or, more generally, to be a linear combination of contributions of this form. If we turn on an interaction among the particles, the ground state will no longer be a Slater determinant. If the interaction is of mean-field type, however, we may still expect that Slater determinants provide a good approximation. Also in this case, we expect the relevant Slater determinants, namely those minimizing the Hartree-Fock energy (41), to have reduced densities exhibiting the semiclassical structure (43).

To characterize the semiclassical structure (43), it is useful to consider certain commutators. The kernel of $[x, \omega_N]$ is given by

$$[x, \omega_N](x;y) = (x-y)\omega_N(x;y) \tag{44}$$

For ω_N with the semiclassical structure (43), we have $\omega_N(x;y) \simeq 0$ if $|x-y| \gg \varepsilon$. Hence the factor $(x-y)$ on the r.h.s. of (44) is small, giving a contribution proportional to ε. Similarly, consider the commutator

$$[\varepsilon\nabla, \omega_N](x;y) = \varepsilon(\nabla_x + \nabla_y)\,\omega_N(x;y) \tag{45}$$

For ω_N of the form (43), both derivatives ∇_x and ∇_y may hit the factor $g((x-y)/\varepsilon)$, generating large contributions. The sum $(\nabla_x + \nabla_y)$, however, can only hit the smooth profile function $\rho((x+y)/2)$, generating contributions of order one. Hence the operator $\varepsilon(\nabla_x + \nabla_y)$ on the r.h.s. of (45) is small, of order ε, if ω_N has the form (43). Summarizing, for ω_N carrying the semiclassical structure described above, we expect the commutator bounds

$$\begin{aligned} \text{tr}\ |[x, \omega_N]| &\leq CN\varepsilon \\ \text{tr}\ |[\varepsilon\nabla, \omega_N]| &\leq CN\varepsilon \end{aligned} \tag{46}$$

to hold true (recall the normalization $\text{tr}\omega_N = N$).

From this discussion, we conclude that physically interesting initial data are approximate Slater determinants with reduced one-particle density ω_N satisfying the commutator bounds (46). The next theorem describes the evolution of such initial states.

Theorem 5.1. *Let* $V \in L^1(\mathbb{R}^3)$ *with*

$$\int dp\, |\widehat{V}(p)|(1+p^2) < \infty. \tag{47}$$

Let ω_N *be a sequence of orthogonal projections onto* $L^2(\mathbb{R}^3)$ *with* $\operatorname{tr}\omega_N = N$ *and such that the commutator bounds in* (46) *hold true. Furthermore, let* $\psi_N \in L^2_a(\mathbb{R}^{3N})$ *be a sequence of many-body wave functions with one-particle reduced density* $\gamma_N^{(1)}$ *satisfying*

$$\operatorname{tr}\left|\gamma_N^{(1)} - \omega_N\right| \leq C.$$

Let $\psi_{N,t}$ *be the solution of the many-body Schrödinger equation* (37) *with initial data* $\psi_{N,0} = \psi_N$*, and let* $\gamma_{N,t}^{(1)}$ *be the one-particle reduced density associated with* $\psi_{N,t}$*. Then there exist constants* $C, c > 0$ *such that*

$$\left\|\gamma_{N,t}^{(1)} - \omega_{N,t}\right\|_{HS} \leq C \exp(c \exp(c|t|)) \tag{48}$$

where $\omega_{N,t}$ *is the solution of the time-depenent non-linear Hartree-Fock equation* (42) *with initial data* $\omega_{N,0} = \omega_N$ *(here* $\|A\|_{HS}^2 = \operatorname{tr}(A^*A)$ *is the Hilbert-Schmidt norm of the operator* A*).*

The proof of Theorem 5.1 can be found in [**10**] and, for fermions with relativistic dispersion, in [**11**]. We conclude this section with some observations concerning Theorem 5.1.

Remarks:

1) Recall that, in this section, we normalize one-particle reduced densities so that their trace is N. As a consequence, their Hilbert-Schmidt norm is typically of the order $N^{1/2}$ (we consider reduced density close to orthogonal projections). The fact that the r.h.s. of (48) is of order one, uniformly in N, means that the solution of the Hartree-Fock equation $\omega_{N,t}$ is a good approximation for the reduced density $\gamma_{N,t}^{(1)}$ associated with the solution of the many-body Schrödinger equation (37).

2) With some minor additional assumptions, it is also possible to derive bounds on the distance between $\gamma_{N,t}^{(1)}$ and $\omega_{N,t}$ in the trace-norm topology.

3) It is also possible to prove convergence for higher order reduced densities; the relative rate of convergence, in the Hilbert-Schmidt norm, is always of the order $N^{-1/2}$.

4) It is simple to check that the contribution of the exchange term in the Hartree-Fock equation (42) is negligible, under the assumption (47). Hence, (48) remains valid if we replace $\omega_{N,t}$ with the solution $\widetilde{\omega}_{N,t}$ of the fermionic Hartree equation

$$i\varepsilon\partial_t\widetilde{\omega}_{N,t} = \left[-\varepsilon^2\Delta + (V * \widetilde{\rho}_t), \widetilde{\omega}_{N,t}\right] \tag{49}$$

with $\widetilde{\rho}_t(x) = N^{-1}\widetilde{\omega}_{N,t}(x;x)$ and with initial data $\widetilde{\omega}_{N,0} = \omega_N$.

5) In contrast with the bosonic case, here the limiting equation (either the Hartree-Fock equation (42) or the Hartree equation (49)) still depends on N (through the parameter $\varepsilon = N^{-1/3}$). It is therefore natural to ask what happens to the solution $\omega_{N,t}$ of the Hartree-Fock equation or to the solution $\widetilde{\omega}_{N,t}$ of the Hartree equation (49), as $N \to \infty$. It turns out that, in this limit, the Hartree-Fock and the Hartree dynamics can be approximated by the classical Vlasov equation. More precisely, the Wigner transform associated with $\omega_{N,t}$ (or with $\widetilde{\omega}_{N,t}$), which is defined through

$$W_{N,t}(x,v) = \frac{1}{(2\pi)^{3/2}N}\int \omega_{N,t}\left(x + \frac{\varepsilon y}{2}, x - \frac{\varepsilon y}{2}\right) e^{iy\cdot v}dy$$

is expected to converge, in the limit of large N, towards the solution of the Vlasov equation

$$\partial_t W_{\infty,t}(x,v) + v\cdot\nabla_x W_{\infty,t}(x,v) + \nabla(V * \rho_{\infty,t})\cdot\nabla_v W_{\infty,t}(x,v) = 0$$

assuming that this is the case for the initial data. Rigorous mathematical results on the convergence from Hartree to Vlasov can be found for example in [**3**, **34**] and, more recently, in [**9**] (this last work is the only one which can be applied to approximate Slater determinants).

6) The first mathematically rigorous results concerning the dynamics of fermions in the mean-field limit discussed in this section go back to [**35**, **41**], where the many-body evolution was directly compared with the Vlasov dynamics. In [**16**], the solution of the Schrödinger equation (37) was compared, like in Theorem 5.1, with the solution of the Hartree-Fock (or Hartree) equation, but only under the assumption of analytic interaction and short time. Different scalings have been considered in [**4**, **5**, **22**, **36**].

7) At positive temperature, physically interesting initial data are not Slater determinants, but instead quasi-free mixed states, which are believed to

provide a good approximation for thermal Gibbs states associated with the Hamilton operator (38). In [**8**], it is shown that the evolution of approximately quasi-free mixed states with one-particle reduced density satisfying commutator bounds similar to (46) remains close to a quasi-free mixed state and that the evolution of the quasi-free mixed state is determined by the time-dependent Hartree-Fock equation (42) (or by the Hartree equation (49)).

8) The main restriction of Theorem 5.1 is the assumption on the regularity of the potential. It would be very interesting to extend Theorem 5.1 to Coulomb intearction $V(x) = \pm 1/|x|$; some partial results in this direction have been recently obtained in [**38**].

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