Effective Evolution Equations from Many-Body Quantum Mechanics

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Across the page the symbols moved in grave morrice, in the mummery of their letters, wearing quaint caps of squares and cubes. Give hands, traverse, bow to partner: so: imps of fancy of the Moors. Gone too from the world, Averroes and Moses Maimonides, dark men in mien and movement, flashing in their mocking mirrors the obscure soul of the world, a darkness shining in brightness which brightness could not comprehend. (..)
–It is very simple, Stephen said as he stood up.

(James Joyce, Ulysses)

Summary

Systems of interest in physics often consist of a very large number of interacting particles. In certain physical regimes, effective non-linear evolution equations are commonly used as an approximation for making predictions about the time-evolution of such systems. Important examples are Bose-Einstein condensates of dilute Bose gases and degenerate Fermi gases. While the effective equations are well-known in physics, a rigorous justification is very difficult. However, a rigorous derivation is essential to precisely understand the range and the limits of validity and the quality of the approximation.

In this thesis, we prove that the time evolution of Bose-Einstein condensates in the Gross-Pitaevskii regime can be approximated by the time-dependent Gross-Pitaevskii equation, a cubic non-linear Schrödinger equation. We then turn to fermionic systems and prove that the evolution of a degenerate Fermi gas can be approximated by the time-dependent Hartree-Fock equation (TDHF) under certain assumptions on the semiclassical structure of the initial data. Finally, we extend the latter result to fermions with relativistic kinetic energy. All our results provide explicit bounds on the error as the number of particles becomes large.

A crucial methodical insight on bosonic systems is that correlations can be modeled by Bogoliubov transformations. We construct initial data appropriate for the Gross-Pitaevskii regime using a Bogoliubov transformation acting on a coherent state, which amounts to studying squeezed coherent states.

As a crucial insight for fermionic systems, we point out a semiclassical structure in states close to the ground state of fermions in a trap. As a convenient language for studying the dynamics of fermionic systems, we use particle-hole transformations.

This thesis is based on the articles [BdS12, BPS13a, BPS13b].

Contents

1. Introduction

Systems of interest in physics usually consist of a very large number of particles, starting at several thousand up to numbers of order 10^{23} for samples in chemistry and even larger numbers for astronomical objects like stars. While many of these systems are believed to be described by versions of the Schrödinger equation and the laws of quantum mechanics, the derivation of their macroscopic properties from these microscopic laws presents us with challenging theoretical problems. As a matter of fact, based on heuristic arguments, in many areas of physics and chemistry effective macroscopic equations are commonly used to approximately understand the properties of such systems. However, to understand the range and the limits of validity as well as the quality of these approximations, a rigorous mathematical derivation is essential.

In this thesis, we derive two important effective theories from the microscopic laws of quantum mechanics: The Gross-Pitaevskii equation for the dynamics of Bose-Einstein condensates and the Hartree-Fock equation for the dynamics of fermionic systems. Furthermore, we extend the latter result to fermions with relativistic kinetic energy. The mathematical technique both for the fermionic and the bosonic systems is inspired by the method of coherent states introduced to study the mean-field theory of bosons [RS09, CLS11, GV79, H74]. However, coherent states are not adequate for either of the systems we consider here. To overcome this problem, we introduce Bogoliubov transformations as a tool for studying the dynamics of many-body systems. In the dilute Bose gas in the Gross-Pitaevskii regime, it is essential to find a description of the short-scale correlations in the many-body system. In the study of fermionic systems, we point out a crucial semiclassical structure in states close to the ground state.

To conclude this summary, let us give an overview for orientation in this thesis. First, we proceed to Section 1.1, where we give a short introduction to quantum mechanics and fix some conventions.

Section 1.2 is a central part of the introduction, where we introduce the idea of effective evolution equations and explain the physical background of the models considered in this thesis.

In Section 1.3 we quickly review the mathematics of second quantization to set the background for the calculations following.

Then in Section 1.4 we review the method of coherent states as used for deriving the Hartree equation for the bosonic mean-field regime. Since the method of coherent states was the main inspiration for the work in this thesis, this section conveys important ideas.

In Section 1.5 we then introduce Bogoliubov transformations, which are a crucial tool in this thesis and a main new ingredient. In Subsection 1.5.1 we explain how Bogoliubov transformations can be used to construct initial data. Bosonic Bogoliubov transformations can be used to implement correlations, and fermionic Bogoliubov transformations can be used to construct Slater determinants.

We conclude Chapter 1 with three appendices. Appendix 1.A compares different conventions for the definition of reduced density matrices and proves a useful lemma. Appendix 1.B explains in detail the global well-posedness of the effective evolution equations in this thesis. Appendix 1.C collects some notations.

In Chapters 2–4 we present the new results and their proofs obtained in [BdS12, BPS13a, BPS13b]; at the beginning of the respective chapters, we give detailed introductions to the methods and new ideas entering.

1.1. Many-body quantum mechanics

Quantum mechanics as a physical theory was invented at the beginning of the twentieth century to describe matter on the atomic scale. Nowadays the laws of quantum mechanics are believed to be fundamental to physics. In the following we will give a short introduction to the quantum mechanical description of many-body systems. As we are interested in systems at low energies, we restrict our attention to the non-relativistic theory. The pseudo-relativistic model of Chapter 4 is a special case: it is not Lorentz invariant, but it includes the effects of the relativistic dispersion relation.

We start with the description of non-relativistic N-particle systems, ignoring for the moment the question of quantum statistics (i. e. the bosonic or fermionic nature of the particles).

According to the laws of quantum mechanics the state of a system is identified with a vector ψ in a complex Hilbert space $\mathcal{H}$. For N particles in three dimensional space, we have $\mathcal{H} = L^2(\mathbb{R}^{3N})$, where we use the convention $\langle f, g\rangle = \int \overline{f}(x)g(x)\,\mathrm{d}x$ for the scalar product of $f, g \in L^2(\mathbb{R}^{3N})$. We also call $\psi \in L^2(\mathbb{R}^{3N})$ the wave function of the system and generally assume the normalization $\|\psi\|_{L^2(\mathbb{R}^{3N})} = 1$. We routinely use the identification $L^2(\mathbb{R}^{3N}) \simeq L^2(\mathbb{R}^3)^{\otimes N}$ and call $L^2(\mathbb{R}^3)$ the one-particle Hilbert space; vectors φ in $L^2(\mathbb{R}^3)$ normalized to $\|\varphi\|_{L^2(\mathbb{R}^3)} = 1$ are also called one-particle wave functions or orbitals. Quantum mechanics predicts the average of measuring an observable over a large number of repetitions of the experiment. The average is calculated from the theory as the expectation value $\langle \psi, A\psi\rangle$, where A is a selfadjoint, possibly unbounded, operator on $L^2(\mathbb{R}^{3N})$ modeling the observable. Standard examples of observables are the position operator, acting on the j-th particle as multiplication by the coordinate $x_j \in \mathbb{R}^3$, and the corresponding momentum operator $p_j = -i\nabla_{x_j}$. A special role is played by the Hamilton operator H_N, which models the total energy of the system: through the Schrödinger equation

$$i\partial_t\psi(t) = H_N\psi(t) \quad \text{with initial data } \psi(0) \in L^2(\mathbb{R}^{3N}) \tag{1.1}$$

it generates the time evolution of the state vector of the system,

$$\psi : \mathbb{R} \to L^2(\mathbb{R}^{3N}), \quad t \mapsto \psi(t).$$

We will use the notation $\psi_t = \psi(t)$ throughout. The solution of the Schrödinger equation is given through the strongly continuous unitary group $e^{-iH_N t}$ as $\psi_t = e^{-iH_N t}\psi_0$.

In this thesis, we consider Hamilton operators of the form

$$H_N = \sum_{j=1}^{N} \left(-\Delta_{x_j} + V_{\text{ext}}(x_j)\right) + \lambda \sum_{i<j}^{N} V(x_i - x_j). \tag{1.2}$$

Here, $-\Delta_{x_j}$ is the Laplace operator acting on the j-th particle ($x_j \in \mathbb{R}^3$) and the multiplication operator given by $V_{\text{ext}} : \mathbb{R}^3 \to \mathbb{R}$ describes an external potential, which we think of as modeling a trap. The term $\sum_{j=1}^{N} -\Delta_{x_j}$ corresponds to the total kinetic energy. The term $\lambda \sum_{i<j}^{N} V(x_i - x_j)$ describes pair interactions with a coupling constant $\lambda \in \mathbb{R}$ and an interaction potential $V : \mathbb{R}^3 \to \mathbb{R}$. Units were chosen such that Planck's constant is $\hbar = 1$ and particles have mass $m = 1/2$.

Next we introduce quantum statistics, the behavior of wave functions under permutation of indistinguishable particles. We define the symmetrization operator S_N by its action on $\psi \in L^2(\mathbb{R}^{3N})$ as

$$(S_N\psi)(x_1, \dots x_N) := \frac{1}{N!} \sum_{\sigma \in \mathcal{S}_N} \psi(x_{\sigma(1)}, \dots x_{\sigma(N)})$$

and the antisymmetrization operator A_N similarly by

$$(A_N\psi)(x_1, \dots x_N) := \frac{1}{N!} \sum_{\sigma \in \mathcal{S}_N} \operatorname{sgn}(\sigma) \psi(x_{\sigma(1)}, \dots x_{\sigma(N)}).$$

By $\operatorname{sgn}(\sigma)$ we denote the sign of the permutation $\sigma \in \mathcal{S}_N$. The operators S_N and A_N are orthogonal projections. As a principle of physics, bosonic indistinguishable particles are described using wave functions $\psi \in L^2_s(\mathbb{R}^{3N}) := S_N L^2(\mathbb{R}^{3N})$; fermionic indistinguishable particles by $\psi \in L^2_a(\mathbb{R}^{3N}) := A_N L^2(\mathbb{R}^{3N})$. More explicitly, $L^2_s(\mathbb{R}^{3N})$ is the subspace of $L^2(\mathbb{R}^{3N})$ consisting of all functions which are symmetric with respect to permutation of the N particles, in formula

$$L^2_s(\mathbb{R}^{3N}) = \{\psi \in L^2(\mathbb{R}^{3N}) : \psi(x_{\sigma(1)}, \dots, x_{\sigma(N)}) = \psi(x_1, \dots, x_N) \text{ for all } \sigma \in \mathcal{S}_N\}.$$

Similarly $L^2_a(\mathbb{R}^{3N})$ is the subspace of antisymmetric functions,

$$L^2_a(\mathbb{R}^{3N}) = \{\psi \in L^2(\mathbb{R}^{3N}) : \psi(x_{\sigma(1)}, \dots, x_{\sigma(N)}) = \operatorname{sgn}(\sigma)\psi(x_1, \dots, x_N) \text{ for all } \sigma \in \mathcal{S}_N\}.$$

It is a principle of physics that in three space dimensions, particles other than bosons and fermions do not exist. Since both S_N and A_N commute with $e^{-iH_N t}$, $\psi_0 \in L^2_s(\mathbb{R}^{3N})$ implies $\psi_t \in L^2_s(\mathbb{R}^{3N})$ for all times $t \in \mathbb{R}$ and analogously for the fermionic case. The well-known Pauli exclusion principle is a consequence of the antisymmetry of fermionic wave functions. It can be stated, for example, as

$$A_N(\varphi \otimes \varphi \otimes \varphi_1 \otimes \dots \otimes \varphi_{N-2}) = 0 \qquad \left(\varphi, \varphi_1, \dots \varphi_{N-2} \in L^2(\mathbb{R}^3)\right),$$

i. e. no two fermions can occupy the same one-particle orbital.

An important notion is the ground state of a system. At zero temperature the ground state ψ_0 is the minimizer of the functional $\psi \mapsto \langle \psi, H_N \psi \rangle$ among the $\psi \in L^2_s(\mathbb{R}^{3N})$ or $L^2_a(\mathbb{R}^{3N})$ (for bosonic or fermionic systems, respectively) with normalization $\|\psi\| = 1$. We study only systems at zero temperature in this thesis.

1.2. Effective evolution equations

Only in some special cases it is possible to solve the Schrödinger equation (1.1) explicitly. In fact, for large systems of interacting particles — as present in many settings of physical importance — even the numerical solution of the Schrödinger equation becomes impossible. Therefore, effective evolution equations which allow one to approximately calculate expectation values of observables are of great importance.

In systems of indistinguishable particles, the results of measurements are averages over all particles. To see how the result of such a measurement can be calculated from theory, let O be a selfadjoint operator on $L^2(\mathbb{R}^3)$, i. e. a one-particle observable. Extending it to $L^2(\mathbb{R}^{3N})$ as $O_j := \mathbb{1} \otimes \ldots \mathbb{1} \otimes O \otimes \mathbb{1} \ldots \otimes \mathbb{1}$, where the operator O acts only in the j-th factor of the tensor product, we obtain an observable on the N-particle system. For bosonic wave functions $\psi \in L^2_s(\mathbb{R}^{3N})$ (and in the same way for fermionic wave functions, since the signs cancel in the expectation value) we find

$$\langle \psi, O_1 \psi \rangle = \langle \psi, S_N O_1 S_N \psi \rangle = \frac{1}{N} \sum_{j=1}^{N} \langle \psi, O_j \psi \rangle,$$

i. e. explicitly the average over all N particles. In particular, the choice of O_1 is merely a convention and we could just as well have chosen any O_j.

We introduce the one-particle reduced density matrix $\gamma^{(1)}_\psi$ by taking the partial trace over $N-1$ particles[1] of the projection[2] $|\psi\rangle\langle\psi|$

$$\gamma^{(1)}_\psi := \operatorname{tr}_{2,\ldots N} |\psi\rangle\langle\psi|.$$

The one-particle reduced density matrix is a non-negative trace class operator on $L^2(\mathbb{R}^3)$. In terms of the one-particle reduced density matrix we can write the expectation value as

$$\langle \psi, O_1 \psi \rangle = \operatorname{tr} O \gamma^{(1)}_\psi.$$

Thus, to approximately determine the expectation value, it is sufficient to approximately determine the one-particle reduced density matrix $\gamma^{(1)}_\psi$. More precisely, for $\tilde{\gamma}$ an operator on $L^2(\mathbb{R}^3)$ to be thought of as the approximation to $\gamma^{(1)}_\psi$ we have

$$|\operatorname{tr} O \gamma^{(1)}_\psi - \operatorname{tr} O \tilde{\gamma}| \leq \|O\| \operatorname{tr} \left| \gamma^{(1)}_\psi - \tilde{\gamma} \right|$$

if O is a bounded operator, and

$$|\operatorname{tr} O \gamma^{(1)}_\psi - \operatorname{tr} O \tilde{\gamma}| \leq \|O\|_{\mathrm{HS}} \|\gamma^{(1)}_\psi - \tilde{\gamma}\|_{\mathrm{HS}}$$

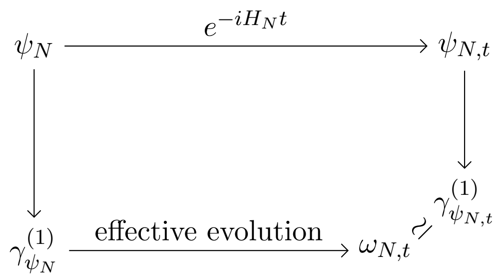
if O is a Hilbert-Schmidt operator. Our goal is thus the following: Start with an initial wave function $\psi_N \in L^2_s(\mathbb{R}^{3N})$ or $L^2_a(\mathbb{R}^{3N})$ (bosonic or fermionic, depending on the physical situation to be described). Let $\gamma^{(1)}_{\psi_N}$ be the one-particle reduced density matrix of ψ_N. Let $\psi_{N,t} = e^{-iH_N t}\psi_N$ be the solution to the Schrödinger equation with initial data ψ_N, and $\gamma^{(1)}_{\psi_{N,t}}$ its one-particle reduced density matrix. We want to find an effective evolution equation for the one-particle reduced density matrix, i. e. a differential equation for an approximating one-particle density matrix $\omega_{N,t}$ such that the solution with agreeing initial data $\omega_{N,0} = \gamma^{(1)}_{\psi_N}$ makes the difference

$$\operatorname{tr} \left| \gamma^{(1)}_{\psi_{N,t}} - \omega_{N,t} \right| \qquad \text{or} \qquad \|\gamma^{(1)}_{\psi_{N,t}} - \omega_{N,t}\|_{\mathrm{HS}}$$

[1] In general, we use the normalization that for $\|\psi\| = 1$, we have $\operatorname{tr}\gamma^{(1)}_\psi = 1$, since then "small" in the discussion here means "much smaller than one". However, in Chapters 3 and 4 it is more convenient to normalize the trace to $\operatorname{tr}\gamma^{(1)}_\psi = N$.

[2] We use the Dirac notation for projection operators, i. e. $|\psi\rangle\langle\psi|$ is the operator acting on $f \in L^2(\mathbb{R}^{3N})$ by $|\psi\rangle\langle\psi| f = \langle \psi, f \rangle \psi$.

small, for times $t > 0$ as long as possible. In other words, we want to arrive approximately at $\gamma^{(1)}_{\psi_{N,t}}$, but avoiding to calculate $\psi_{N,t}$ and instead solving an effective evolution equation starting from $\gamma^{(1)}_{\psi_N}$. Schematically in a diagram:



Surely we can not expect this to be generally possible in interacting systems, but in certain physical regimes, modeled through appropriate scaling of the parameters of the system, we prove that good approximations of this kind can be obtained. In the following, we explain the regimes considered in this thesis and introduce the respective effective equations. The scalings will be parametrized with the number of particles N, which is naturally a large number so that we are interested in the asymptotic behavior as $N \to \infty$.

The physical setting for the application of effective evolution equations can be described by the following steps which constitute a typical experiment.

Step 1 The system with a trapping external potential, e. g. $V_{\text{ext}}(x) = |x|^2$, is prepared (approximately) in the ground state ψ_N by cooling it to very low temperatures. Since the ground state is an eigenstate of the Hamilton operator the time evolution is trivial, i. e. just multiplication with a phase which does not affect any expectation values.

Step 2 The traps are switched off, $V_{\text{ext}} = 0$, so ψ_N is not an eigenstate of the Hamilton operator anymore and will thus evolve in a non-trivial way. It is this evolution that we describe with an effective evolution equation. More generally, the external potential could be changed instead of being switched off, which also leads to a non-trivial evolution.

The effective evolution equation can be studied analytically and is also numerically more accessible than the original high-dimensional Schrödinger equation.

1.2.1. The Hartree equation for the bosonic mean-field regime

Let us start with a well-known simple example of an effective evolution equation, which serves to illustrate the type of results and methods to be presented in this thesis. Consider the Hamilton operator

$$H_N = \sum_{j=1}^{N} (-\Delta_{x_j} + V_{\text{ext}}(x_j)) + \frac{1}{N} \sum_{i<j}^{N} V(x_i - x_j) \tag{1.3}$$

for N indistinguishable bosons, i. e. on $L^2_s(\mathbb{R}^{3N})$. The coupling constant has been chosen to be $1/N$, so that the interaction term is formally of order N and thus of the same order as the kinetic energy. (Considering a vector $\varphi^{\otimes N}$ as below, the kinetic energy is $\big\langle \varphi^{\otimes N}, \sum_{j=1}^{N}(-\Delta_{x_j})\varphi^{\otimes N}\big\rangle = N\big\langle \varphi, -\Delta\varphi\big\rangle = \mathcal{O}(N)$, while the double sum of the interaction term is $\mathcal{O}(N^2)$.) This means that in the limit $N \to \infty$ none of the terms becomes negligible with respect to the other, giving rise to a non-trivial limiting dynamics. Since the interaction is weak and its range of order one and thus much larger than the typical distance $N^{-1/3}$ between particles (for N particles in a volume of order one, confined by the trapping potential), in the spirit of the law of large numbers we can think of each particle as interacting with an effective potential obtained through averaging over all other particles. For this reason, we call this scaling the mean-field regime.

For bosons, a physically important and mathematically tractable class of initial data is given by factorized wave functions

$$\psi_N = \varphi^{\otimes N} \in L^2_s(\mathbb{R}^{3N}) \tag{1.4}$$

where $\varphi \in L^2(\mathbb{R}^3)$; written more explicitly $\psi_N(x_1,\ldots,x_N) = \prod_{j=1}^N \varphi(x_j)$. In fact, for vanishing interaction $V=0$, the ground state (at zero temperature) is exactly of the form (1.4), and this form is approximately correct for non-vanishing interaction in the mean-field regime in the sense that the ground state $\psi_{N,\mathrm{g}}$ satisfies $\operatorname{tr}\left|\gamma^{(1)}_{\psi_{N,\mathrm{g}}} - \gamma^{(1)}_{\varphi^{\otimes N}}\right| = \operatorname{tr}\left|\gamma^{(1)}_{\psi_{N,\mathrm{g}}} - |\varphi\rangle\langle\varphi|\right| \to 0$ as $N\to\infty$, with φ the minimizer of the Hartree functional given below. A simple proof of this fact in the case $\hat{V}\geq 0$ can be found in [GS12, Lemma 1][3]. This phenomenon is known as Bose-Einstein condensation and was first predicted in 1924 by Bose and Einstein, who considered non-interacting bosons at positive temperature.

For a state approximately given by $\psi_N \simeq \varphi^{\otimes N}$, the energy in the mean-field regime is expected to be approximately

$$\begin{aligned}
\left\langle \varphi^{\otimes N}, H_N \varphi^{\otimes N}\right\rangle &= \left\langle \varphi^{\otimes N}, \left[\sum_{j=1}^N(-\Delta_{x_j} + V_{\mathrm{ext}}(x_j)) + \frac{1}{N}\sum_{i<j}^N V(x_i - x_j)\right]\varphi^{\otimes N}\right\rangle \\
&= N\left\langle \varphi^{\otimes N}, (-\Delta_{x_1} + V_{\mathrm{ext}}(x_1))\varphi^{\otimes N}\right\rangle + \frac{N(N-1)}{2N}\left\langle \varphi^{\otimes N}, V(x_1-x_2)\varphi^{\otimes N}\right\rangle \\
&\simeq N\int \mathrm{d}x \left(|\nabla\varphi|^2 + V_{\mathrm{ext}}|\varphi|^2\right) + \frac{N}{2}\int \mathrm{d}x\mathrm{d}y\, |\varphi(x)|^2 V(x-y)|\varphi(y)|^2 \\
&=: N\mathcal{E}_{\mathrm{Hartree}}(\varphi).
\end{aligned}$$

Here we introduced the Hartree energy functional $\mathcal{E}_{\mathrm{Hartree}}$.

Now suppose that, after having prepared the trapped ground state, the confining trap is switched off, so now $V_{\mathrm{ext}} = 0$. The former ground state $\psi_N \simeq \varphi^{\otimes N}$ is no longer stationary and evolves non-trivially. However, we may expect that since in the mean-field regime the interaction is weak, at any later time t we still have an approximately factorized wave function,

$$\psi_{N,t} = e^{-iH_N t}\psi_N \simeq \varphi_t^{\otimes N}, \tag{1.5}$$

wherein φ_t should be a one-particle orbital evolved with an appropriate, self-consistent, effective evolution equation. The evolution equation for φ_t can be obtained as the evolution equation canonically associated with the Hartree energy functional:

$$i\partial_t\varphi_t = -\Delta\varphi_t + (V * |\varphi_t|^2)\varphi_t, \quad \varphi_0 = \varphi. \tag{1.6}$$

This is a non-linear Schrödinger equation for $\varphi_t \in L^2(\mathbb{R}^3)$ instead of a linear Schrödinger equation for $\psi_{N,t} \in L^2(\mathbb{R}^{3N})$, so the dimension has been extremely reduced at the cost of a

[3] Notice that in [GS12] a different indicator of condensation (the number of particles outside the Hartree ground state) is used, but by [KP10, Lemma 2.3] it implies the convergence of the reduced density.

non-linearity which models the interaction. The energy $\mathcal{E}_{\mathrm{Hartree}}(\varphi_t)$ as well as the L^2-norm of φ_t are conserved with respect to the evolution (1.6).

To give the reader a feeling of the results that we prove in this thesis, we now make (1.5) more precise citing the following theorem. The theorem holds if the interaction potential is dominated by the Laplacian (the kinetic energy of one particle) in the sense that $V^2 \leq C(1-\Delta)$ holds as an operator inequality for some $C > 0$. This is true for example for the physically important case of the attractive and repulsive Coulomb potential.

Theorem 1.2.1 ([RS09, CLS11]). *Suppose $V^2 \leq C(1-\Delta)$ for some $C > 0$. Let $\varphi \in H^1(\mathbb{R}^3)$ with $\|\varphi\|_{L^2} = 1$ and let φ_t be the solution to the Hartree equation* (1.6) *with initial data $\varphi_0 = \varphi$. Let $\psi_{N,t} = e^{-iH_N t}\varphi^{\otimes N}$ be the solution to the Schrödinger equation $i\partial_t \psi_{N,t} = H_N \psi_{N,t}$ with mean-field Hamiltonian* (1.3) *(with $V_{ext} = 0$) and initial data $\psi_{N,0} = \varphi^{\otimes N}$. Then there exist constants $D, K > 0$ such that*

$$\operatorname{tr}\left|\gamma^{(1)}_{\psi_{N,t}} - |\varphi_t\rangle\langle\varphi_t|\right| \leq \frac{1}{N} D e^{K|t|} \quad \text{for all } t \in \mathbb{R}.$$

Notice that the projection $|\varphi_t\rangle\langle\varphi_t|$ is the one-particle reduced density matrix of $\varphi_t^{\otimes N}$.

Since the method of [RS09, CLS11] was the main inspiration for the work in this thesis, we review it in detail in Section 1.4. This method has been developed starting in [H74, GV79] for the study of the classical limit. A remarkable feature of this method is that it provides explicit strong estimates for the rate of convergence as $N \to \infty$. Furthermore it also allows us to understand the behavior of the fluctuations in the limit, and in particular was used to prove a central limit theorem [BKS11].

We conclude this subsection with a short overview of rigorous results on the dynamics of bosonic systems in the mean-field limit. The first rigorous proof of validity of the Hartree equation in the sense that $\gamma^{(1)}_{N,t} \to |\varphi_t\rangle\langle\varphi_t|$ as $N \to \infty$ was obtained in [S80], for bounded interaction potentials. The method of [S80] was extended to particles interacting through a Coulomb potential [EY01], both in the attractive and repulsive case.

A different approach to obtain control of the rate of convergence towards the Hartree evolution was developed in [KP10, P11] with the advantage that it can be extended to potentials with more severe singularities. The convergence towards the Hartree dynamics was proved as propagation of Wigner measures in [AN11] for regular interaction potentials. In [FKS09] the convergence towards the Hartree dynamics was proven as an Egorov-type theorem, for particles interacting through a Coulomb potential.

In [GMM10, GMM11, GM12] it was shown how an approximation in Fock space norm (instead of the trace norm of reduced densities) can be obtained by considering next-order corrections to the Hartree dynamics. Many-body quantum dynamics in one and two dimensions in appropriate mean-field limits have been studied in [AGT07, KSS11] and were found to give rise to Schrödinger equations with local non-linearity.

The study of the spectral properties of bosonic mean-field Hamiltonians also received a lot of attention in the last years. A first proof of the emergence of a Bogoliubov excitation spectrum has been found in [S11] for systems of bosons in a box and in [GS12] in the presence of an external potential. A more general approach to the analysis of the excitation spectrum of bosonic mean-field systems was given in [LNSS12].

A setting combining mean-field and semiclassical limit for bosonic systems has been considered in [GMP03] and [FGS07]. This setting is similar to the joint mean-field and semiclassical limit that naturally emerges in fermionic mean-field systems, as we will explain in Subsection 1.2.3.

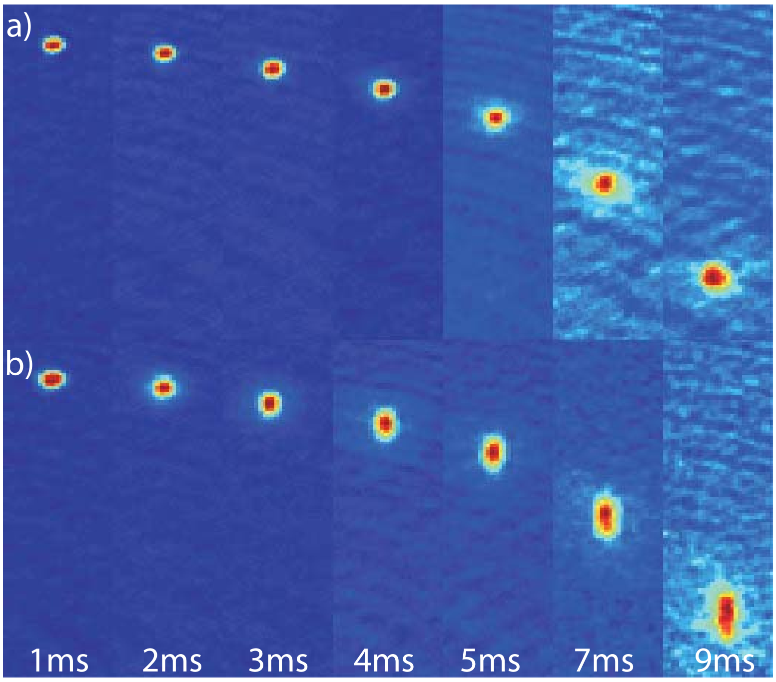


Fig. 1.: Experiment: At $t = 0$ms a Bose-Einstein condensate is released from (a) an almost isotropic and (b) an anisotropic trap and expands. Shown is (in false colors) the absorption of a beam of light by the condensate cloud. The initial condensate consists of more than 50,000 chromium atoms at a temperature of about 10^{-6}K.
From [GWH+05] with permission of the authors. Copyright 2005 by The American Physical Society.

1.2.2. The Gross-Pitaevskii equation for the dilute Bose gas

In dilute trapped Bose gases at very low temperatures Bose-Einstein condensation can be observed in experiments, in the sense that a macroscopic fraction of particles is found to occupy the same one-particle orbital. This is similar to the ground state for the bosonic mean-field system that we discussed above, despite the physical regime being very different. The first experimental evidence of this phenomenon was obtained in 1995 [AEM+95, DMA+95] and it was rewarded with a Nobel prize in 2001.

In typical experiments, the gas of bosonic particles is initially trapped using electromagnetic fields and cooled down to very low temperatures. At a critical temperature, a phase transition occurs and a condensate is formed. Afterwards the trapping fields are switched off or changed and the time evolution of the condensate is observed. We show an example of data obtained in this way in Figure 1: after releasing the condensate from the trap, the condensate cloud expands and, in Figure 1(b), also changes its shape. On the fundamental level, the dynamics are described by many-body quantum mechanics. In the work presented in this thesis we show rigorously that the dynamics of Bose-Einstein condensates can be approximated with an effective evolution equation, the time-dependent Gross-Pitaevskii equation.

We now introduce the theoretical picture for the description of a condensate by Gross-Pitaevskii theory. We start by making the notion of Bose-Einstein condensation rigorous, following the idea of using reduced density matrices as hinted at in the mean-field setting in the previous section. Considering the simplest non-trivial case, a factorized wave function in $L^2_s(\mathbb{R}^{3N})$ of the form

$$\psi_N = S_N\left(\varphi^{\otimes k_1} \otimes \varphi_\perp^{\otimes k_2}\right), \quad \langle \varphi, \varphi_\perp \rangle = 0, \quad k_1 + k_2 = N, \tag{1.7}$$

we can simply count the number of tensor factors φ and speak of macroscopic occupation of the orbital φ if k_1 is large, close to the total number of particles N. However, for systems with interaction, the ground state is not factorized. To come up with a more general notion of macroscopic occupation and Bose-Einstein condensation, let us consider the example of a sequence $(\psi_N)_{N\in\mathbb{N}}$ of the form (1.7) with $k_2 = N^\alpha$, where $\alpha \in [0,1)$. For the trace norm one finds

$$\operatorname{tr}\left|\gamma^{(1)}_{\psi_N} - |\varphi\rangle\langle\varphi|\right| = \frac{2}{N^{1-\alpha}}. \tag{1.8}$$

In ψ_N we have a fraction $k_1/N \to 1$ (as $N \to \infty$) of the particles in the condensate orbital φ. Motivated by this example, we speak of complete (or 100%) Bose-Einstein condensation if

$$\operatorname{tr}\left|\gamma^{(1)}_{\psi_N} - |\varphi\rangle\langle\varphi|\right| \to 0 \qquad (N \to \infty)$$

for some $\varphi \in L^2(\mathbb{R}^3)$. We then say that the one-particle orbital φ is macroscopically occupied. Equivalently, complete Bose-Einstein condensation occurs if the largest eigenvalue of $\gamma^{(1)}_{\psi_N}$ converges to one as $N \to \infty$. The definition given in this paragraph is meaningful also for non-factorized ψ_N, and thus also in systems with strong interaction.

Bose-Einstein condensation is difficult to prove mathematically, however there is a model of physical importance in which Bose-Einstein condensation has been rigorously proven. This model is the trapped Bose gas of N particles in the Gross-Pitaevskii regime, in which the idea of the scaling is to model diluteness by making the effective range of interaction very small. More precisely, the Hamiltonian is taken to be

$$H_N = \sum_{j=1}^N (-\Delta_{x_j} + V_{\text{ext}}(x_j)) + N^2 \sum_{i<j}^N V(N(x_i - x_j)) \tag{1.9}$$

on $L^2_s(\mathbb{R}^{3N})$. The interaction potential is repulsive, i. e. $V \geq 0$, spherically symmetric and decaying sufficiently fast at infinity. The scaling of the potential is chosen such that the range of the interaction[4] is of order N^{-1}, much smaller than the typical distance $N^{-1/3}$ of particles (for N particles trapped in a volume of order one). This means that collisions are very rare and in this sense the model (1.9) describes a dilute gas. The N^2 in front of the potential is chosen such that collisions are very strong and thus despite diluteness not negligible, the interaction term being formally[5] of order N. Since the interaction is so strong and short-ranged, the Gross-Pitaevskii regime is very different from the mean-field regime discussed before, where collisions are frequent but weak. Indeed factorized wave functions are not sufficient as an approximation in the Gross-Pitaevskii regime. Correlations play an important role in the Gross-Pitaevskii regime as we will now discuss.

[4] We will introduce below the scattering length, which measures the effective range of a potential. The scattering length of the rescaled potential $N^2V(Nx)$ appearing in the Hamiltonian (1.9) is $a = a_0/N$.

[5] To see this, use symmetry of the wave function to write the interaction term as $\frac{1}{2}\sum_{i\neq j}^N N^2 V(N(x_i - x_j)) = \frac{N}{2}\sum_{j=2}^N N^2 V(N(x_1 - x_j))$. The particle at x_1 mostly interacts with the particles in a volume of size N^{-3}. Since in volumes of order one there are N particles, the particle at x_1 can interact with N^{-2} particles, so $\sum_{j=2}^N V(N(x_1 - x_j)) = \mathcal{O}(N^{-2})$.

Let us introduce $f\colon \mathbb{R}^3 \to \mathbb{R}$ as the solution to the zero-energy scattering equation [LSSY05]

$$\left(-\Delta + \frac{1}{2}V\right) f = 0 \quad \text{with boundary condition } f(x) \to 1 \text{ as } |x| \to \infty. \tag{1.10}$$

(For a physical interpretation, notice that this is the stationary Schrödinger equation with energy eigenvalue $E = 0$ for two particles in relative coordinates.) The solution satisfies $0 \leq f \leq 1$ and has the asymptotic form

$$f(x) \simeq 1 - \frac{a_0}{|x|} \quad \text{for } |x| \gg a_0, \tag{1.11}$$

where

$$a_0 := (8\pi)^{-1} \int V f \mathrm{d}x \tag{1.12}$$

is called the scattering length of the potential V. The scattering length plays a central role in describing the effect of correlations. In fact, it was proven in [LSY00] that the quantum-mechanical ground state energy

$$E_N = \inf_{\substack{\psi \in L^2_s(\mathbb{R}^{3N}) \\ \|\psi\|=1}} \langle \psi, H_N \psi \rangle \tag{1.13}$$

is approximated by the Gross-Pitaevskii energy in the sense that

$$\lim_{N\to\infty} \frac{E_N}{N} = \min_{\substack{\varphi \in L^2(\mathbb{R}^3) \\ \|\varphi\|=1}} \mathcal{E}_{\mathrm{GP}}(\varphi),$$

where the Gross-Pitaevskii energy functional is defined as

$$\mathcal{E}_{\mathrm{GP}}(\varphi) := \int \mathrm{d}x \, \left(|\nabla\varphi|^2 + V_{\mathrm{ext}}|\varphi|^2 + 4\pi a_0 |\varphi|^4\right). \tag{1.14}$$

Here, the scattering length appears in front of the quartic term. Hence, in leading order the ground state energy per particle depends on the interaction potential V only through its scattering length. The importance of correlations in the ground state can now be seen observing that for factorized, i. e. uncorrelated, wave functions we have

$$\begin{aligned} \langle \varphi^{\otimes N}, H_N \varphi^{\otimes N} \rangle &\simeq N \int \mathrm{d}x \, \left(|\nabla\varphi|^2 + V_{\mathrm{ext}}|\varphi|^2\right) + \frac{N}{2} \int \mathrm{d}x\mathrm{d}y \, |\varphi(x)|^2 N^3 V(N(x-y)) |\varphi(y)|^2 \\ &\to N \int \mathrm{d}x \, \left(|\nabla\varphi|^2 + V_{\mathrm{ext}}|\varphi|^2 + \frac{b}{2}|\varphi|^4\right) \qquad (N \to \infty), \end{aligned}$$

where in the last step we took the limit to a delta distribution. The constant in front of the quartic term is $b = \int V \mathrm{d}x$. Since $\frac{b}{2} > 4\pi a_0$ (this follows from 1.12 and the fact that $f \leq 1$ and not constant), the energy of the factorized state differs from the ground state energy in leading order! Due to this observation we expect that the ground state has a singular structure on a short length scale. Rescaling the coordinates one finds that the solution f_N of

$$\left(-\Delta_x + \frac{1}{2}N^2 V(Nx)\right) f_N(x) = 0 \quad \text{with boundary condition } f_N(x) \to 1 \text{ as } |x| \to \infty$$

is $f_N(x) = f(Nx)$. In Chapter 2 we use the function f_N in a Bogoliubov transformation to describe the correlations in the Bose-Einstein condensate on length scale $1/N$. Notice also in this context that according to [EMS06], a short-scale structure described by f_N forms almost immediately in an initially uncorrelated state $\varphi^{\otimes N}$ under the time evolution generated by the Hamiltonian (1.9).

Nevertheless, despite the presence of correlations, the notion of complete Bose-Einstein condensation introduced before still makes sense. In fact, it was proven [LS02] that the ground state ψ_N in the Gross-Pitaevskii limit exhibits complete Bose-Einstein condensation,

$$\gamma^{(1)}_{\psi_N} \to |\varphi_{\mathrm{GP}}\rangle\langle\varphi_{\mathrm{GP}}| \qquad (N \to \infty),$$

where the macroscopically occupied orbital φ_{GP} is the normalized minimizer of the Gross-Pitaevskii energy functional $\mathcal{E}_{\mathrm{GP}}$. The results of [LSY00, LS02] show that the properties of the ground state are well approximated by Gross-Pitaevskii theory.

Coming back to the experiments discussed above, the question is whether the dynamics after switching off (or changing) the trap can also be described by Gross-Pitaevskii theory, i. e. if the evolution governed by the Schrödinger equation $i\partial_t \psi_{N,t} = H_N \psi_{N,t}$ with Hamiltonian

$$H_N = \sum_{j=1}^N -\Delta_{x_j} + \sum_{i<j}^N N^2 V(N(x_i - x_j)) \tag{1.15}$$

can be approximated by the evolution equation canonically associated with $\mathcal{E}_{\mathrm{GP}}$,

$$i\partial_t \varphi_t = -\Delta\varphi_t + 8\pi a_0 |\varphi_t|^2 \varphi_t. \tag{1.16}$$

The answer is yes; in a series of articles [ESY06a, ESY06b, ESY10, ESY07, ESYS09] (see also Subsection 2.1.1 for some details on the method) and by a different method in [P10] the following result was established: Consider a family of vectors $\psi_N \in L^2_s(\mathbb{R}^{3N})$ with bounded energy per particle,

$$\langle \psi_N, H_N \psi_N \rangle \leq CN,$$

and exhibiting complete condensation in a one-particle orbital $\varphi \in H^1(\mathbb{R}^3)$ in the sense

$$\gamma^{(1)}_{\psi_N} \to |\varphi\rangle\langle\varphi| \quad (N \to \infty).$$

Then, the solution $\psi_{N,t} = e^{-iH_N t}\psi_N$ of the Schrödinger equation still exhibits complete Bose-Einstein condensation, i. e. the reduced one-particle density $\gamma^{(1)}_{\psi_{N,t}}$ associated with $\psi_{N,t}$ satisfies

$$\gamma^{(1)}_{\psi_{N,t}} \to |\varphi_t\rangle\langle\varphi_t| \quad (N \to \infty) \tag{1.17}$$

at any fixed time $t > 0$. Here φ_t is the solution of the time-dependent Gross-Pitaevskii equation (1.16) with initial data φ. This result establishes the stability of complete Bose-Einstein condensation with respect to the time-evolution, and the fact that the condensate wave function evolves according to the Gross-Pitaevskii equation.

It is now desirable to obtain explicit bounds on the rate of convergence in (1.17), not least because in view of (1.8) an explicit bound gives an indication of the number of particles outside the condensate, but also because in experiments the number of particles is always finite and it is thus important to know how large the number of particles has to be in order to obtain a good approximation. The techniques of [ESY06a, ESY06b, ESY10, ESY07, ESYS09] however do not tell us anything about the rate of convergence, since they conclude convergence from a compactness argument. We nevertheless discuss these techniques in Subsection 2.1.1 since they provide us with a better understanding of how to take into account the effect of correlations.

For an extensive review on Bose-Einstein condensation (in the state of 2007) leading from the experimental side to the mathematics, we recommend to the reader the thesis [M07].

In Chapter 2 we present our work providing quantitative bounds for (1.17), see Theorem 2.1.1 and Theorem 2.C.1. The method, while inspired by the work [RS09, CLS11] on mean-field systems, is significantly more involved due to the need of controlling the correlations. In particular, we introduce Bogoliubov transformations (see Subsection 1.5.1) as a tool to model correlations in the many-body system. On the mathematical side, the use of Bogoliubov transformations presents a close link to our work on the Hartree-Fock theory for fermionic systems, which we introduce next.

1.2.3. The Hartree-Fock equation for the fermionic mean-field regime

Another very important example of an effective evolution equation is the Hartree-Fock equation, describing the dynamics of systems of fermionic particles (e. g. electrons, neutrons, protons, some atoms) in the mean-field regime. We consider the Schrödinger equation

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

for N indistinguishable fermions, i. e. in $L^2_a(\mathbb{R}^{3N})$. As for the bosonic mean-field regime we choose the coupling constant λ small, such that kinetic and interaction energy are of the same order as $N \to \infty$. To get a heuristic estimate of the order of the kinetic energy let us consider non-interacting fermions confined to a box of volume of order one and with periodic boundary conditions (in this example the energy can easily be calculated explicitly). Due to Pauli's principle, in fermionic systems particles can easily reach high energies: since no two fermions can occupy the same one-particle orbital, they fill the eigenstates of the Laplacian in order of increasing energy until all fermions found a place. As a consequence, already in the ground state the kinetic energy is of order $N^{5/3}$, the so-called Fermi energy. We thus choose $\lambda = N^{-1/3}$. Since as a consequence of the high energy, fermions also have a high velocity — of order $N^{1/3}$ for the energetically highest occupied orbitals — we can only expect to follow their dynamics with an effective evolution equation up to times of order $N^{-1/3}$. Introducing a new time variable τ (which will be taken to be N-independent, and which is called the semiclassical time) such that the physical time becomes

$$t = N^{-1/3}\tau,$$

we obtain the Schrödinger equation

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

We define a new parameter (we call it the semiclassical parameter)

$$\varepsilon := N^{-1/3}$$

and multiply the Schrödinger equation by ε^2, resulting in

$$i\varepsilon\partial_\tau\psi_{N,\tau} = \left[\sum_{j=1}^{N}(-\varepsilon^2\Delta_{x_j}) + \frac{1}{N}\sum_{i<j}^{N}V(x_i - x_j)\right]\psi_{N,\tau}. \tag{1.18}$$

We introduce the Hamilton operator

$$H_N = \sum_{j=1}^{N}(-\varepsilon^2\Delta_{x_j}) + \frac{1}{N}\sum_{i<j}^{N}V(x_i - x_j), \qquad \varepsilon = N^{-1/3}, \tag{1.19}$$

so the Schrödinger equation is $i\varepsilon\partial_\tau\psi_{N,\tau} = H_N\psi_{N,\tau}$. With the factor $1/N$ explicitly written now, the interaction term is of the same form as in the bosonic mean-field system, but in contrast to the bosonic case we also have to deal with the semiclassical regime, the parameter ε taking the role of Planck's constant converging to zero. The factor ε in front of the time derivative makes the analysis much more involved than for the bosonic mean-field regime.

For now, let us heuristically derive the Hartree-Fock equation as the effective equation associated with the evolution (1.18). Typical initial data is prepared in an external trapping potential just like for bosons. We expect the ground state of the weakly interacting fermions in the trap to be close to the ground state of non-interacting fermions in the trap (or in a box, as above), which has the form of a Slater determinant

$$\psi_N = A_N(f_1 \otimes \ldots \otimes f_N).$$

Here $f_1, \ldots f_N \in L^2(\mathbb{R}^3)$ are orthonormal one-particle orbitals[6]. Now suppose the trap is switched off. The idea of the Hartree-Fock approximation is to approximate the evolved wave function $\psi_{N,\tau} = e^{-iH_N\tau/\varepsilon}\psi_N$ with a Slater determinant

$$A_N(f_{1,\tau} \otimes \ldots \otimes f_{N,\tau}), \tag{1.20}$$

where the orbitals evolve with an effective evolution equation. Calculating the energy of a Slater determinant we find

$$\begin{aligned}\langle\psi_N, H_N\psi_N\rangle = \int \mathrm{d}x \sum_{j=1}^{N}\varepsilon^2|\nabla f_j|^2 &+ \frac{1}{2N}\int \mathrm{d}x\mathrm{d}y \sum_{i,j=1}^{N} V(x-y)|f_j(x)|^2|f_i(y)|^2 \\ &- \frac{1}{2N}\int \mathrm{d}x\mathrm{d}y \sum_{i,j=1}^{N} V(x-y)\overline{f_j(x)}f_j(y)\, f_i(x)\overline{f_i(y)} \\ =: \mathcal{E}_{\mathrm{HF}}(f_1, \ldots, f_N),&\end{aligned} \tag{1.21}$$

where in the last step we defined the Hartree-Fock energy functional $\mathcal{E}_{\mathrm{HF}}$. The first summand containing the interaction potential V is called the direct term, the second term containing the interaction potential is called the exchange term. The self-consistent effective evolution equation (to be precise, N coupled equations, one for each orbital) is obtained as the evolution equation canonically associated with the Hartree-Fock energy functional $\mathcal{E}_{\mathrm{HF}}$:

$$i\varepsilon\partial_\tau f_{i,\tau} = -\varepsilon^2\Delta f_{i,\tau} + \frac{1}{N}\sum_{j=1}^{N}\left(V * |f_{j,\tau}|^2\right)f_{i,\tau} - \frac{1}{N}\sum_{j=1}^{N}\left(V * (f_{i,\tau}\overline{f_{j,\tau}})\right)f_{j,\tau}. \tag{1.22}$$

[6] The non-interacting Hamilton operator can be written as $H_N = \sum_{j=1}^{N} h_j$, where h is a one-particle Hamiltonian $-\Delta + V_{\mathrm{ext}}$ on $L^2(\mathbb{R}^3)$ (the subscript j meaning that it acts on the j-th particle). In this notation, the f_i would be the eigenvectors of h in order of increasing eigenvalues.

The evolution defined by (1.22) conserves the energy $\mathcal{E}_{\mathrm{HF}}$ and the orthonormality of the orbitals. The Hartree-Fock equations can be rewritten in a convenient form by introducing the one-particle reduced density matrix

$$\omega_{N,\tau} = \frac{1}{N}\sum_{j=1}^{N} |f_{j,\tau}\rangle\langle f_{j,\tau}| \tag{1.23}$$

associated with the Slater determinant (1.20). The Hartree-Fock equation (1.22) then becomes

$$i\varepsilon\partial_\tau \omega_{N,\tau} = [-\varepsilon^2\Delta + V * \rho_\tau - X_\tau, \omega_{N,\tau}]. \tag{1.24}$$

Here we have introduced the commutator $[A,B] = AB - BA$ of operators A and B. Furthermore, we introduced the configuration space density of particles $\rho_\tau(x) = \omega_{N,\tau}(x,x)$, the multiplication operator $(V * \rho_\tau)$, and the exchange operator X_τ, which is defined through its integral kernel $X_\tau(x,y) = V(x-y)\omega_{N,\tau}(x,y)$.

Conversely, if the initial data $\omega_{N,0}$ is a projection of rank N, so is $\omega_{N,\tau}$ for all τ (see Section 1.B), and thus we can decompose it in the form (1.23) to obtain the equations in the orbital form (1.22) again.

In Chapter 3 we present our work providing quantitative bounds on the difference of the one-particle reduced density matrix of the Schrödinger evolution and the Hartree-Fock evolution, for initial data satisfying certain semiclassical commutator bounds, see Theorem 3.3.1 and Theorem 3.3.2. As an important ingredient, we prove that the Hartree-Fock equation preserves the semiclassical properties of the initial data. In Chapter 4, we present similar results (Theorem 4.2.1) for the fermionic setting with relativistic dispersion relation, known to physicists as relativistic degenerate matter.

The method is again inspired by the use of coherent states as initial data in [RS09, CLS11], but in contrast to the bosonic case there are no coherent states in fermionic Fock space[7]. As a replacement for the Weyl operators creating coherent states in the bosonic Fock space, on fermionic Fock space we find degenerate Bogoliubov transformations that create Slater determinants. Since correlations are not important in the mean-field case, the Bogoliubov transformations to be used for fermions are very different from those used to implement correlations in the Gross-Pitaevskii setting. In fact, the fermionic Bogoliubov transformations to be used are particle-hole transformations. We would like to stress that the fermionic Bogoliubov transformations are better compared with the Weyl operator in Chapter 2 and [RS09, CLS11] (see Section 1.4 for a review) than with the correlation-implementing Bogoliubov transformations in Chapter 2.

The Hartree-Fock equation (1.24) still depends on N, through the semiclassical parameter $\varepsilon = N^{-1/3}$ and through the initial data. This poses the question whether the Hartree-Fock equation has a well-defined limit for $\varepsilon \to 0$. The answer is yes: the semi-classical limit of the Hartree-Fock equation is given by the non-linear Vlasov equation

$$\frac{\partial f_t}{\partial t} + 2v \cdot \nabla_x f_t + F(f_t) \cdot \nabla_v f_t = 0, \tag{1.25}$$

where $f_t(x,v) \geq 0$ is a time-dependent density in the classical phase space $\Gamma := \mathbb{R}^3 \times \mathbb{R}^3$, with x position and v momentum[8]. The force F is given self-consistenly as the mean-field

[7] It is possible to define fermionic coherent states by extending Fock space with Grassmann variables (see e. g. [CR12, FKT02, FK11]), but we found Bogoliubov transformations more convenient for us.

[8] The factor of 2 appears because we prefer to think of phase space over momentum instead of velocity, the conversion factor being the mass $m = 1/2$.

force $F(f_t) = -\nabla(V * \rho_t^f)$ with $\rho_t^f(x) = \int f_t(x,v)\mathrm{d}v$ the configuration space density of particles. For V the Coulomb potential, (1.25) is called the Vlasov-Poisson equation. The non-linear Vlasov equation describes the mean-field theory of classical particles [BH77]; it is of great importance for example in plasma physics [V68, Eq. II] and gives rise to intriguing phenomena like Landau damping [MV11].

We now present a heuristic argument that the semiclassical limit of the Hartree-Fock equation is given by the Vlasov equation. A standard tool for analyzing the semiclassical limit is the Wigner function: For γ a one-particle density matrix, it is defined as a function on phase space $\Gamma = \mathbb{R}^3 \times \mathbb{R}^3$ through

$$W_N(x,v) := \frac{1}{(2\pi)^3} \int e^{-iv\cdot\eta}\, \gamma\left(x + \varepsilon\frac{\eta}{2}, x - \varepsilon\frac{\eta}{2}\right) \mathrm{d}\eta \qquad \text{for } (x,v) \in \Gamma. \tag{1.26}$$

Even though the Wigner function in general is not a probability density on the classical phase space (Gaussians are the only pure states with non-negative Wigner function [SC83]), it is nevertheless useful for comparing quantum mechanical theories to classical theories (c. f. [B98, Chapter 15]).

In Appendix 3.A in Chapter 3 we prove that the exchange term can be neglected, so we can consider the Hartree equation

$$i\varepsilon\partial_\tau \omega_{N,\tau} = [-\varepsilon^2\Delta + V * \rho_\tau, \omega_{N,\tau}] \tag{1.27}$$

instead of the Hartree-Fock equation (1.24). To obtain the Vlasov equation, let us look at the time-derivative of the Wigner function associated with the solution $\omega_{N,\tau}$ to the Hartree equation. We find

$$\begin{aligned} &i\varepsilon\partial_\tau W_{N,\tau}(x,v)\,(2\pi)^3 \\ &= \int \mathrm{d}\eta\, e^{-iv\cdot\eta} \left(-\varepsilon^2\Delta_1 + \varepsilon^2\Delta_2\right) \omega_{N,\tau}\left(x + \varepsilon\frac{\eta}{2}, x - \varepsilon\frac{\eta}{2}\right) &(1.28) \\ &\quad + \int \mathrm{d}\eta\, e^{-iv\cdot\eta} \left((V * \rho_\tau)\left(x + \varepsilon\frac{\eta}{2}\right) - (V * \rho_\tau)\left(x - \varepsilon\frac{\eta}{2}\right)\right) \omega_{N,\tau}\left(x + \varepsilon\frac{\eta}{2}, x - \varepsilon\frac{\eta}{2}\right), &(1.29) \end{aligned}$$

wherein Δ_1 and Δ_2 denote the Laplacian acting on the first and the second argument, respectively, of the integral kernel $\omega_{N,\tau}(x_1,x_2)$. We approximate the difference in (1.29) by expanding it to linear order in ε:

$$\left((V * \rho_\tau)\left(x + \varepsilon\frac{\eta}{2}\right) - (V * \rho_\tau)\left(x - \varepsilon\frac{\eta}{2}\right)\right) = \varepsilon\eta \cdot \nabla(V * \rho_\tau)(x) + \mathcal{O}(\varepsilon^2).$$

We plug this into line (1.29) and use integration by parts to convert the factor of η into a gradient with respect to v; we obtain

$$(1.29) = \varepsilon i \nabla(V * \rho_\tau)(x) \cdot \nabla_v W_{N,\tau}(x,v) + \mathcal{O}(\varepsilon^2).$$

Furthermore it is easy to see that

$$(\Delta_1 - \Delta_2)\omega_{N,\tau}\left(x + \varepsilon\frac{\eta}{2}, x - \varepsilon\frac{\eta}{2}\right) = \frac{2}{\varepsilon}\nabla_\eta \nabla_x \omega_{N,\tau}\left(x + \varepsilon\frac{\eta}{2}, x - \varepsilon\frac{\eta}{2}\right).$$

Plugging this into (1.28), using integration by parts with respect to η and dividing the whole equation by $i\varepsilon$, we finally arrive at

$$\partial_\tau W_{N,\tau}(x,v) + 2v \cdot \nabla_x W_{N,\tau}(x,v) = \nabla_x(V * \rho_\tau)(x) \cdot \nabla_v W_{N,\tau}(x,v) + \mathcal{O}(\varepsilon). \tag{1.30}$$

To conclude, we notice that the configuration space density ρ_τ^W of the Wigner function is

$$\rho_\tau^W(x) := \int W_{N,\tau}(x,v)\mathrm{d}v = \omega_{N,\tau}(x,x) = \rho_\tau(x).$$

Thus (1.30) is indeed the Vlasov equation, up to an error term formally of order ε. The Vlasov equation has been rigorously derived starting directly from the quantum-mechanical fermionic system (1.18) in [NS81] for real-analytic potentials and in [S81] for more general potentials. It has also been derived as a semiclassical limit starting from the Hartree-Fock equation (1.24) in [GIMS98]. (The latter work is interesting as it shows that the step from the Hartree-Fock equation to the Vlasov equation also holds for particles interacting via the Coulomb potential, while the step from many-body quantum mechanics to the Hartree-Fock equation has not yet been rigorously proven in the Coulomb case.)

We conclude with a review of the literature on the mean-field dynamics of fermionic systems, which is much more limited than for bosonic systems. As far as we know, the first rigorous results concerning the evolution of fermionic system in the regime we are interested in were proven by [NS81] and [S81]. Neither [NS81] nor [S81] give a bound on the rate of convergence. More recently, in [EESY04] the many-body evolution is compared to the N-dependent Hartree dynamics described by (1.27): Under the assumption of a real-analytic potential, it is shown that, for short semiclassical times, the difference between $\gamma_{N,t}^{(1)}$ and $\omega_{N,t}$ is of order N^{-1} (when tested against appropriate observables). The results that we present in Chapter 3 are comparable with those of [EESY04]. In contrast to [EESY04] we obtain convergence for arbitrary times (i. e. for arbitrary, N-independent τ as appearing in (1.18)) and under much weaker assumptions on the regularity of the interaction potential.

A different mean-field regime of fermionic systems, characterized by $\varepsilon = 1$ in (1.18), has been considered in [BGGM03, FK11], for regular interactions and for potentials with Coulomb singularity, respectively. This alternative scaling describes physically interesting situations if the particles occupy a large volume (so that the kinetic energy per particle is of order one) and if the interaction has a long range (to make sure that also the potential energy per particle is of order one). In this thesis we are interested in the evolution of initial data describing N fermions in a volume of order one; correspondingly, we only consider the scaling with $\varepsilon = N^{-1/3}$ appearing in (1.18).

To conclude our discussion of the Hartree-Fock theory, we would like to point out that the time-dependent Hartree-Fock equation was adapted to a wide range of applications, e. g. in nuclear physics [MRSU13, BKN76]. As an example, in Figure 2 and Figure 3 we show numerical results, obtained by time-dependent Hartree-Fock methods, describing the collision of two atomic nuclei.

1.3. Second quantization

In this section we quickly review second quantization; see e. g. [RS80, Sections II.4 and VIII.10] and [RS75, Section X.7] for details. As long as we work with states of exactly N particles, the formalism of second quantization is just a convenient language for calculations. In our derivation of the Gross-Pitaevskii equation in Chapter 2 however, second quantization is indispensable since we consider states that do not have an exact number of particles. We introduce the fermionic and bosonic setting both at once, pointing out differences only where necessary.

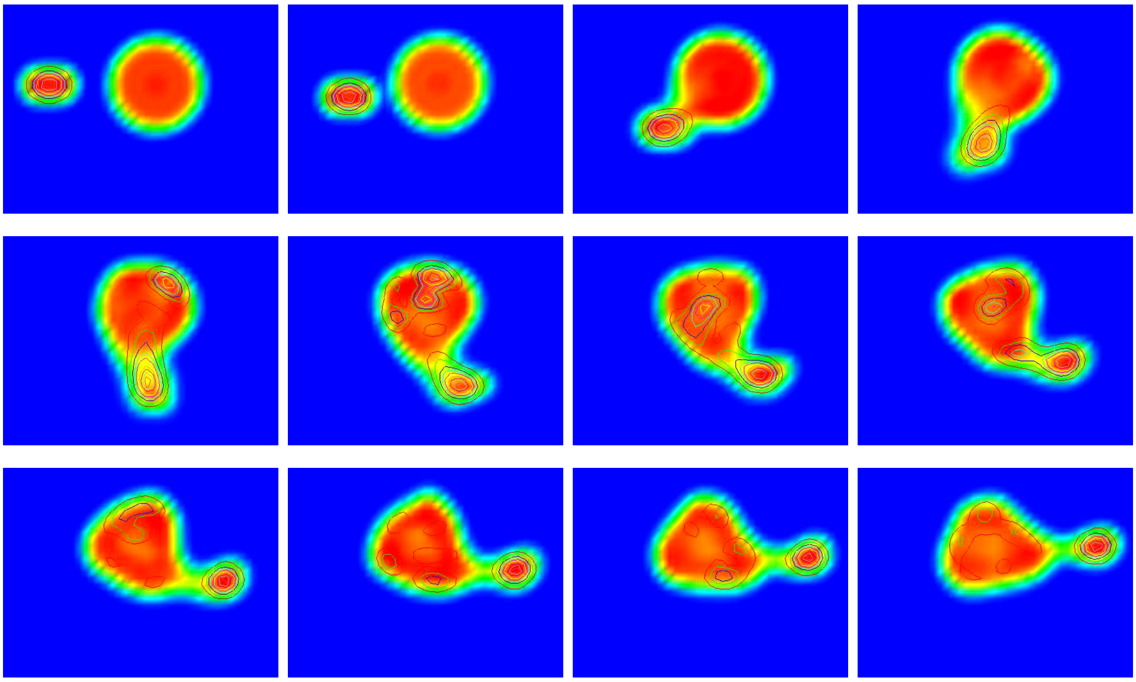


Fig. 2.: TDHF numerics: Excentric collision of a nucleus of Magnesium-24 with a nucleus of Lead-208. Time from left to right and up to down. Colors correspond to the total density, contour lines to the density of energetically lowest one-particle wave functions in Magnesium-24. The Lead-208 nucleus has a radius of about 6fm. From [M14].

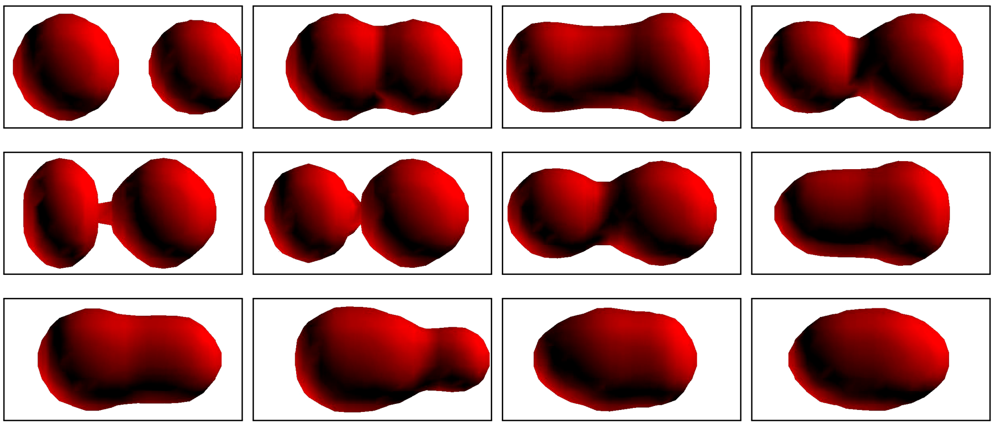


Fig. 3.: TDHF numerics: A nucleus of Carbon-12 collides with a nucleus of Oxygen-16, with initial relative energy 100MeV. Time from left to right and up to down. From [M14].

Fock space is defined as the Hilbert space direct sum

$$\mathcal{F} := \bigoplus_{n\geq 0} S_n L^2(\mathbb{R}^{3n}) \qquad \text{(bosons)},$$
$$\mathcal{F} := \bigoplus_{n\geq 0} A_n L^2(\mathbb{R}^{3n}) \qquad \text{(fermions)},$$

where A_n is the antisymmetrization operator and S_n the symmetrization operator, both as introduced in Section 1.1. By convention $L^2(\mathbb{R}^0) = L^2(\mathbb{R}^3)^{\otimes 0} = \mathbb{C}$. A vector $\psi \in \mathcal{F}$ can be written as a sequence $\psi = (\psi^{(0)}, \psi^{(1)}, \ldots)$, where $\psi^{(n)} \in A_n L^2(\mathbb{R}^{3n})$ for the fermionic and $\psi^{(n)} \in S_n L^2(\mathbb{R}^{3n})$ for the bosonic case. The vector (both in the fermionic and the bosonic Fock space)

$$\Omega := (1, 0, 0, \ldots)$$

is called vacuum vector and describes a state not containing any particle. The scalar product on Fock space (with respect to which Fock space is a Hilbert space) is

$$\langle \psi, \varphi \rangle = \sum_{n\geq 0} \langle \psi^{(n)}, \varphi^{(n)} \rangle_{L^2(\mathbb{R}^{3n})}, \qquad \psi, \varphi \in \mathcal{F}.$$

In fact, any sequence $\psi = (\psi^{(0)}, \psi^{(1)}, \ldots)$ with $\psi^{(n)} \in S_n L^2(\mathbb{R}^{3n})$ satisfying

$$\sum_{n\geq 0}^{\infty} \|\psi^{(n)}\|^2 < \infty$$

is an element of the bosonic Fock space, and analogously for $\psi^{(n)} \in A_n L^2(\mathbb{R}^{3n})$ an element of fermionic Fock space.

In Fock space we can describe states where the number of particles is not exactly determined. The vector $\psi = (\psi^{(0)}, \psi^{(1)}, \ldots) \in \mathcal{F}$ describes a coherent superposition of states with different numbers of particles; the n-particle component is described by $\psi^{(n)}$. The probability to find n particles in a measurement is given by $\|\psi^{(n)}\|^2$. We will generally identify states of exactly N particles, $\psi_N \in L^2_s(\mathbb{R}^{3N})$ or $\psi_N \in L^2_a(\mathbb{R}^{3N})$, with

$$(0, \ldots, 0, \psi_N, 0, \ldots) \in \mathcal{F},$$

i. e. $\psi^{(n)} = 0$ for all $n \neq N$ and $\psi^{(N)} = \psi_N$.

For calculations it is convenient to use creation and annihilation operators. In the bosonic case, they are defined for every one-particle orbital $f \in L^2(\mathbb{R}^3)$ by their action on the individual elements of the sequence $\psi \in \mathcal{F}$ as

$$\left(a(f)\psi\right)^{(n)}(x_1, \ldots x_n) := \sqrt{n+1} \int \overline{f}(x) \psi^{(n+1)}(x, x_1, \ldots x_n) \mathrm{d}x \qquad \text{(annihilation operator)},$$
$$\left(a^*(f)\psi\right)^{(n)}(x_1, \ldots x_n) := \frac{1}{\sqrt{n}} \sum_{k=1}^{n} f(x_k) \psi^{(n-1)}(x_1, \ldots \hat{x}_k \ldots x_n) \qquad \text{(creation operator)}.$$

The notation $\hat{x}_k$ means that the argument x_k is left out. The sum in the definition of the creation operator is required to make the result of applying $a^*(f)$ symmetric with respect to permutation of particles, so that we stay in the bosonic Fock space. The domain of the bosonic creation and annihilation operators is equal to the domain of $\mathcal{N}^{1/2}$, with $\mathcal{N}$ being the number operator

$$(\mathcal{N}\psi)^{(n)} := n\psi^{(n)}, \qquad D(\mathcal{N}) := \Big\{\psi \in \mathcal{F} : \sum_{n\geq 0} n^2 \|\psi^{(n)}\|^2 < \infty\Big\} \tag{1.31}$$

on bosonic Fock space. The physical interpretation is that $\mathcal{N}$ counts the number of particles of the Fock space vector ψ. The bosonic creation and annihilation operators are densely defined and closed, but unbounded. The creation operator $a^*(f)$ is the adjoint of the annihilation operator $a(f)$. Notice that $a(f)$ is antilinear in f while $a^*(f)$ is linear in f. The bosonic operators satisfy the canonical commutation relations (CCR)

$$[a(f), a^*(g)] = \big\langle f, g\big\rangle,\ [a(f), a(g)] = [a^*(f), a^*(g)] = 0 \qquad \text{for all } f, g \in L^2(\mathbb{R}^3). \tag{1.32}$$

For fermions the definition is similar but taking into account the antisymmetry,

$$\left(a(f)\psi\right)^{(n)}(x_1, \dots x_n) := \sqrt{n+1}\int \overline{f}(x)\psi^{(n+1)}(x, x_1, \dots x_n)\mathrm{d}x \qquad \text{(annihilation operator)},$$

$$\left(a^*(f)\psi\right)^{(n)}(x_1, \dots x_n) := \frac{1}{\sqrt{n}}\sum_{k=1}^{n}(-1)^{k-1} f(x_k)\psi^{(n-1)}(x_1, \dots \hat{x}_k \dots x_n) \quad \text{(creation operator)}.$$

The fermionic operators satisfy the canonical anticommutation relations (CAR)

$$\{a(f), a^*(g)\} = \big\langle f, g\big\rangle,\ \{a(f), a(g)\} = \{a^*(f), a^*(g)\} = 0 \qquad \text{for all } f, g \in L^2(\mathbb{R}^3), \tag{1.33}$$

where we have introduced the anticommutator $\{A, B\} = AB + BA$. In particular, this means that for fermions $a^*(f)^2 = 0$, implementing Pauli's exclusion principle. Unlike the bosonic operators, the fermionic creation and annihilation operators are bounded operators, a property that we will heavily use in the derivation of the Hartree Fock equation in Chapter 3. Indeed we have, using the CAR (1.33),

$$\|a(f)\psi\|^2 = \langle a(f)\psi, a(f)\psi\rangle = \langle \psi, a^*(f)a(f)\psi\rangle = \|f\|_2^2\|\psi\|^2 - \langle \psi, a(f)a^*(f)\psi\rangle \leq \|f\|_2^2\|\psi\|^2\,,$$

which implies that the fermionic operators satisfy

$$\|a(f)\| \leq \|f\|_2 \quad \text{and} \quad \|a^*(f)\| \leq \|f\|_2. \tag{1.34}$$

The fermionic number operator is defined by the same expressions as the bosonic number operator (1.31), just on the fermionic Fock space.

Both for fermions and bosons, for any annihilation operator $a(f)$, we have

$$a(f)\Omega = 0.$$

The (anti)commutation relations make it possible to do many calculations in a systematic way. Both in the fermionic and bosonic case, it is useful to introduce the operator-valued distributions a_x^* and a_x. Actually

$$\left(a_x\psi\right)^{(n)}(x_1, \dots x_n) := \sqrt{n+1}\psi^{(n+1)}(x, x_1, \dots, x_n) \tag{1.35}$$

defines a densely defined operator (the expression makes sense on continuous wave functions), which we think of as destroying a particle at $x \in \mathbb{R}^3$. It is easy to see that

$$a(f) = \int \overline{f}(x)a_x\mathrm{d}x.$$

On the other hand, a_x^* can not be defined in a useful way as an operator, since its domain would only contain the zero-vector (for a lucid discussion, see [W96]). Nevertheless we can make sense of it as a quadratic form through

$$\langle \varphi, a_x^* \psi \rangle := \langle a_x \varphi, \psi \rangle, \tag{1.36}$$

or by considering it as a distribution, since by formally integrating against a test function $f \in L^2(\mathbb{R}^3)$ we can take a_x^* back to the well-defined operator

$$\int f(x) a_x^* \mathrm{d}x = a^*(f).$$

In terms of the operator-valued distributions, the canonical commutation relations on bosonic Fock space read

$$[a_x, a_y^*] = \delta(x-y) \qquad \text{and} \qquad [a_x, a_y] = [a_x^*, a_y^*] = 0,$$

where δ is the Dirac delta distribution. The canonical anticommutation relations on fermionic Fock space read

$$\{a_x, a_y^*\} = \delta(x-y) \qquad \text{and} \qquad \{a_x, a_y\} = \{a_x^*, a_y^*\} = 0.$$

A product of creation and annihilation operators is called normal-ordered if all creation operators are to the left of all annihilation operators. From (1.36) and the CCR/CAR in the distributional sense it is clear that non-normal-ordered products of operator-valued distributions are often singular, and thus require a more careful treatment than normal-ordered products.

As an example for the use of operator-valued distributions, let us derive a useful representation of the number operator $\mathcal{N}$: Interpreting the integral in a weak sense, we have

$$\langle \psi, \int a_x^* a_x \, \mathrm{d}x \, \varphi \rangle = \int \langle \psi, a_x^* a_x \varphi \rangle \mathrm{d}x = \int \langle a_x \psi, a_x \varphi \rangle \mathrm{d}x = \langle \psi, \mathcal{N} \varphi \rangle,$$

or shorter $\mathcal{N} = \int \mathrm{d}x \, a_x^* a_x$.

For a one-particle operator O on $L^2(\mathbb{R}^3)$ with dense domain $D(O)$, let $O^{(n)}$ be the closure of the operator (restriction to the symmetric/antisymmetric subspace is simple)

$$\sum_{j=1}^{n} \mathbb{1} \otimes \cdots \mathbb{1} \otimes \underset{j\text{-th factor}}{O} \otimes \mathbb{1} \otimes \cdots \mathbb{1} : \; D(O)^{\otimes n} \to L^2(\mathbb{R}^{3N}).$$

We then introduce the second quantization $\mathrm{d}\Gamma(O)$ of the one-particle operator O by

$$(\mathrm{d}\Gamma(O)\psi)^{(n)} := O^{(n)} \psi^{(n)},$$

which naturally has the domain

$$D(\mathrm{d}\Gamma(O)) := \Big\{ \psi \in \mathcal{F} : \psi^{(n)} \in D(O^{(n)}) \text{ for all } n \in \mathbb{N}, \text{ and } \sum_{n \geq 0} \lVert O^{(n)} \psi^{(n)} \rVert^2_{L^2(\mathbb{R}^{3n})} < \infty \Big\}.$$

If O is essentially selfadjoint on some $D \subset L^2(\mathbb{R}^3)$, then $\mathrm{d}\Gamma(O)$ restricted to the subspace $\big\{ \psi \in \mathcal{F} : \text{ only finitely many } \psi^{(n)} \neq 0, \text{ and } \psi^{(n)} \in D^{\otimes n} \text{ for all } n \in \mathbb{N} \big\}$ is essentially selfadjoint, too (using [RS80, Theorems VIII.33 and VIII.3]).

If the operator O on $L^2(\mathbb{R}^3)$ has an integral kernel $O(x,y)$ we have

$$\mathrm{d}\Gamma(O) = \int \mathrm{d}x\mathrm{d}y\, O(x,y) a_x^* a_y. \tag{1.37}$$

Expressions like the last one should again be interpreted as quadratic forms. As an example, we have already discussed the number operator $\mathcal{N} = \mathrm{d}\Gamma(\mathbb{1})$. A more complicated example for the use of the operator-valued distributions is given by the second quantized Hamilton operator. On the one hand we have the Hamilton operator $\mathcal{H}$ defined as an operator on fermionic or bosonic Fock space by

$$(\mathcal{H}\psi)^{(n)} = \mathcal{H}^{(n)}\psi^{(n)}, \quad \text{where } \mathcal{H}^{(n)} = \sum_{j=1}^{n} -\Delta_{x_j} + \sum_{i<j}^{n} V(x_i - x_j).$$

On the other hand, we have

$$\tilde{\mathcal{H}} = \int \mathrm{d}x \nabla_x a_x^* \nabla_x a_x + \frac{1}{2}\int \mathrm{d}x\mathrm{d}y\, V(x-y) a_x^* a_y^* a_y a_x$$

defined as a quadratic form on e. g.

$$\mathcal{F}_0^{\mathcal{S}} := \left\{ \psi \in \mathcal{F} : \text{ only finitely many } \psi^{(n)} \neq 0, \text{ and } \psi^{(n)} \in \mathcal{S}(\mathbb{R}^{3n}) \text{ for all } n \in \mathbb{N} \right\},$$

with $\mathcal{S}(\mathbb{R}^{3n})$ denoting Schwartz space. As discussed in Section 1.B, under general assumptions on the potential, $\mathcal{H}^{(n)}$ is essentially selfadjoint on $\mathcal{S}(\mathbb{R}^{3n})$ (and on the symmetric/antisymmetric subspace), and consequently, $\mathcal{H}$ is essentially selfadjoint on $\mathcal{F}_0^{\mathcal{S}}$ by the dense-range criterion [RS80, Theorem VIII.3][9]. Now for $\varphi, \psi \in \mathcal{F}_0^{\mathcal{S}}$, one can use (1.35) to check that $\langle \varphi, \mathcal{H}\psi \rangle = \langle \varphi, \tilde{\mathcal{H}}\psi \rangle$, so $\mathcal{H}$ and $\tilde{\mathcal{H}}$ coincide as quadratic forms on $\mathcal{F}_0^{\mathcal{S}}$.

Even for bounded operators O, the operator $d\Gamma(O)$ does not have to be bounded. However, on fermionic Fock space, if O is trace class then $d\Gamma(O)$ is a bounded operator. This fact and other important bounds are shown in Lemma 3.4.1 in Section 3.4. We caution the reader that this does not hold in the bosonic case.

Finally, let us remark that occasionally we use the notation $a^\sharp(f)$ for an equation that holds both for an annihilation operator $a(f)$ and a creation operator $a^*(f)$ in this place.

1.4. Derivation of the Hartree equation using coherent states

Since it inspired the strategies followed in Chapters 2–4, we give a review on the method of coherent states [RS09, CLS11] for proving Theorem 1.2.1. Our review is based on the presentation [S08]. *The main message we would like to convey in this section is that after introducing appropriate fluctuation dynamics, the problem is reduced to proving a bound of the type* (1.45)*. The central object is* $\langle U_N(t,0)\Omega, \mathcal{N} U_N(t,0)\Omega \rangle$*, which we call the number of fluctuations, and the central task is to bound the number of fluctuations uniformly in* N*, for example using Grönwall's lemma. This idea was the main inspiration for the work in this thesis.*

[9] Furthermore, since $\mathcal{H}^{(n)}$ is selfadjoint on (the symmetric/antisymmetric subspace of) $H^2(\mathbb{R}^{3n})$, $\mathcal{H}$ is selfadjoint on $\{\psi \in \mathcal{F} : \psi^{(n)} \in H^2(\mathbb{R}^{3n}), \sum_{n\geq 0} \|\mathcal{H}^{(n)}\psi^{(n)}\|^2_{L^2(\mathbb{R}^{3n})} < \infty\}$.

We consider the bosonic mean-field regime introduced in Section 1.2.1, i. e. N bosons in three-dimensional space, described by the Hamilton operator

$$H_N = \sum_{j=1}^{N} -\Delta_{x_j} + \frac{1}{N}\sum_{i<j}^{N} V(x_i - x_j). \tag{1.38}$$

We consider the time evolution given by the Schrödinger equation $i\partial_t \psi_{N,t} = H_N \psi_{N,t}$ with initial data $\psi_{N,0} = \varphi^{\otimes N} \in L^2_s(\mathbb{R}^{3N})$, where the one-particle orbital is $\varphi \in L^2(\mathbb{R}^3)$ with $\|\varphi\|_2 = 1$. We would like to prove that for the solution $\psi_{N,t} = e^{-iH_N t}\varphi^{\otimes N}$ to the Schrödinger equation the one-particle reduced density matrix $\gamma^{(1)}_{N,t} = \operatorname{tr}_{2,\dots N}|\psi_{N,t}\rangle\langle\psi_{N,t}|$ satisfies

$$\gamma^{(1)}_{N,t} \to |\varphi_t\rangle\langle\varphi_t| \quad (N \to \infty \text{ at any fixed } t)$$

in trace norm topology. Here φ_t is the solution to the Hartree equation

$$i\partial_t\varphi_t = -\Delta\varphi_t + (V * |\varphi_t|^2)\varphi_t \quad \text{with initial data } \varphi_0 = \varphi. \tag{1.39}$$

Furthermore, we would like to obtain quantitative estimates on the rate of convergence.

Here we present the method of Rodnianski and Schlein [RS09], giving

$$\operatorname{tr}\left|\gamma^{(1)}_{N,t} - |\varphi_t\rangle\langle\varphi_t|\right| \leq \frac{C}{\sqrt{N}} e^{Kt},$$

which was later refined by [CLS11] to provide the optimal rate of convergence N^{-1}. This approach was originally proposed by [H74] for studying the classical limit of quantum mechanics; it was later extended by [GV79] to a larger class of potentials. In this approach, the N-body system is embedded in bosonic Fock space $\mathcal{F}$ and coherent states are considered as initial data. Since coherent states do not have an exact number of particles, in the end one has to project back from $\mathcal{F}$ to the N-particle space $L^2_s(\mathbb{R}^{3N})$. Actually, for the one-particle density matrix $\gamma^{(1)}_{\text{coh},t}$ of a coherent state with expected number of particles N, Rodnianski and Schlein prove that the rate of convergence is $\operatorname{tr}\left|\gamma^{(1)}_{\text{coh},t} - |\varphi_t\rangle\langle\varphi_t|\right| = \mathcal{O}(N^{-1})$, but in projecting to the N-particle space they loose a factor $N^{-1/2}$.

For N-particle vectors $\psi_N \in L^2(\mathbb{R}^{3N})$, the one-particle reduced density matrix can be expressed as

$$\gamma^{(1)}_{\psi_N}(x,y) = \frac{1}{N}\langle\psi_N, a^*_y a_x \psi_N\rangle.$$

For vectors in Fock space, $\psi \in \mathcal{F}$, this is generalized to

$$\gamma^{(1)}_{\psi}(x,y) = \frac{1}{\langle\psi, \mathcal{N}\psi\rangle}\langle\psi, a^*_y a_x \psi\rangle.$$

Using the operator-valued distributions the Hamiltonian can be lifted to Fock space by

$$\mathcal{H}_N = \int \mathrm{d}x\, \nabla_x a^*_x \nabla_x a_x + \frac{1}{2N}\int \mathrm{d}x\mathrm{d}y\, V(x-y) a^*_x a^*_y a_y a_x.$$

The operator $\mathcal{H}_N$ restricted to the subspace $L^2_s(\mathbb{R}^{3N})$ of Fock space coincides with H_N given in (1.38). Furthermore, $\mathcal{H}_N$ conserves the number of particles, i. e. it commutes with $\mathcal{N}$, so that the n-particle subspaces evolve independently,

$$\left(e^{-i\mathcal{H}_N t}\psi\right)^{(n)} = e^{-i\mathcal{H}^{(n)}_N t}\psi^{(n)}.$$

Here $\mathcal{H}_N^{(n)}$ is the restriction of $\mathcal{H}_N$ to $L^2(\mathbb{R}^{3n})$. In particular, starting with initial data in the N-particle subspace, the evolution stays in the N-particle subspace for all times.

For $f \in L^2(\mathbb{R}^3)$ one defines the Weyl operator

$$W(f) = \exp(a^*(f) - a(f)).$$

One then introduces the coherent state with one-particle orbital $f \in L^2(\mathbb{R}^3)$ as

$$W(f)\Omega = e^{-\|f\|_2^2/2} e^{a^*(f)}\Omega = e^{-\|f\|_2^2/2} \sum_{n\geq 0} \frac{(a^*(f))^n}{n!}\Omega = e^{-\|f\|_2^2/2} \sum_{n\geq 0} \frac{1}{\sqrt{n!}} f^{\otimes n} \in \mathcal{F}.$$

(Here we used the Baker-Campbell-Hausdorff formula $e^{A+B} = e^{-\frac{1}{2}[A,B]}e^A e^B$ (for A, B operators that commute with their commutator $[A,B]$) with the canonical commutation relations (1.32) and then expanded the exponential.) Since $W(f)$ is unitary, coherent states are always normalized, $\|W(f)\Omega\| = 1$. Apparently coherent states are linear combinations of states with all possible particle numbers. Coherent states have an extremely wide use in quantum mechanics. For us, their usefulness is due to the algebraic properties listed in the following standard lemma:

Lemma 1.4.1 (Bosonic Weyl operators)**.** *Let $f, g \in L^2(\mathbb{R}^3)$.*

(i) *Weyl operators satisfy the Weyl relations*

$$W(f)W(g) = W(g)W(f)e^{-2i\,\mathrm{Im}\langle f,g\rangle_{L^2}} = W(f+g)e^{-i\,\mathrm{Im}\langle f,g\rangle_{L^2}}.$$

(ii) *$W(f)$ is a unitary operator on $\mathcal{F}$ and $W(f)^{-1} = W^*(f) = W(-f)$. (By a common abuse of notation $W^*(f) = W(f)^*$.)*

(iii) *We have*

$$W^*(f)a(g)W(f) = a(g) + \langle g, f\rangle \qquad \text{and} \qquad W^*(f)a^*(g)W(f) = a^*(g) + \langle f, g\rangle. \quad (1.40)$$

In terms of the operator-valued distributions

$$W^*(f)a_x W(f) = a_x + f(x), \qquad W^*(f)a_x^* W(f) = a_x^* + \overline{f(x)}.$$

(iv) *Coherent states are eigenvectors of all annihilation operators,*

$$a(g)W(f)\Omega = \langle g, f\rangle W(f)\Omega.$$

(v) *The expected number of particles in a coherent state $W(f)\Omega$ is*

$$\big\langle W(f)\Omega, \mathcal{N} W(f)\Omega\big\rangle = \|f\|_2^2.$$

Proof of the lemma. The Weyl relations follow from the canonical commutation relations and the Baker-Campbell-Hausdorff formula. Unitarity is clear since the exponent is anti-selfadjoint. The identity $W^*(f) = W(-f)$ follows by taking the hermitian conjugation into the exponent. The properties (iii) are proved by writing $W^*(f)a(g)W(f) - a(g)$ as an integral over the derivative with respect to a dummy variable. Property (iv) follows from (iii). Finally, (v) is obtained by writing $\mathcal{N} = \int \mathrm{d}x\, a_x^* a_x$ and using (iii). □

Rodnianski and Schlein study the dynamics of coherent states with expected number of particles equal to N. Let $\varphi \in L^2(\mathbb{R}^3)$ with $\|\varphi\|_2 = 1$. Consider the Schrödinger equation in bosonic Fock space, $i\partial_t \psi_{N,t} = \mathcal{H}_N \psi_{N,t}$, with initial data chosen to be a coherent state

$$\psi_{N,0} = W(\sqrt{N}\varphi)\Omega.$$

The solution is given by $\psi_{N,t} = e^{-i\mathcal{H}_N t} W(\sqrt{N}\varphi)\Omega$. One expects $\psi_{N,t}$ to be approximately coherent again, i. e. of the form $W(\sqrt{N}\varphi_t)\Omega$, where φ_t should be the solution of the Hartree equation (1.39) with initial data $\varphi_0 = \varphi$. This holds in terms of the reduced densities, and as the first step of the proof, one expresses the difference between $\gamma^{(1)}_{N,t}$, the one-particle reduced density matrix associated with $\psi_{N,t}$, and $|\varphi_t\rangle\langle\varphi_t|$, the one-particle reduced density matrix associated with $\varphi_t^{\otimes N}$, in terms of a unitary fluctuation dynamics. Consider

$$\gamma^{(1)}_{N,t}(x,y) = \frac{1}{N}\langle \Omega, W^*(\sqrt{N}\varphi) e^{i\mathcal{H}_N t} a_y^* a_x e^{-i\mathcal{H}_N t} W(\sqrt{N}\varphi)\Omega\rangle.$$

One then inserts $\mathbb{1} = W(\sqrt{N}\varphi_t)W^*(\sqrt{N}\varphi_t)$ on the left and the right of $a_y^* a_x$. Using Lemma 1.4.1 (iii) and defining the unitary fluctuation dynamics

$$U_N(t,s) = W^*(\sqrt{N}\varphi_t) e^{-i\mathcal{H}_N(t-s)} W(\sqrt{N}\varphi_s) \tag{1.41}$$

one obtains

$$\begin{aligned} \gamma^{(1)}_{N,t}(x,y) - \varphi_t(x)\overline{\varphi}_t(y) &= \frac{1}{N}\big\langle U_N(t,0)\Omega, a_y^* a_x U_N(t,0)\Omega\big\rangle && (1.42)\\ &+ \frac{\varphi_t(x)}{\sqrt{N}}\big\langle U_N(t,0)\Omega, a_y^* U_N(t,0)\Omega\big\rangle && (1.43)\\ &+ \frac{\overline{\varphi}_t(y)}{\sqrt{N}}\big\langle U_N(t,0)\Omega, a_x U_N(t,0)\Omega\big\rangle. && (1.44) \end{aligned}$$

The N-dependence of the first term on the r. h. s. is already optimal; we can estimate it in Hilbert-Schmidt norm by

$$\left\| \frac{1}{N}\big\langle U_N(t,0)\Omega, a^*_{(.)} a_{(.)} U_N(t,0)\Omega\big\rangle \right\|_{\mathrm{HS}} \leq \frac{1}{N}\big\langle U_N(t,0)\Omega, \mathcal{N} U_N(t,0)\Omega\big\rangle.$$

It is now sufficient to prove the key bound

$$\big\langle U_N(t,0)\Omega, \mathcal{N} U_N(t,0)\Omega\big\rangle \leq C e^{K|t|}, \tag{1.45}$$

which can be done using Grönwall's lemma. We will prove the same bound for a simpler evolution $\tilde{U}_N(t,0)$ in some detail below. The bound for $U_N(t,0)$ is more central (in fact, it is a key point), but its proof is much more involved (although based on similar ideas), so we refer the reader to [RS09, S08] for the details.

We could also control (1.43) and (1.44) in this way to obtain a bound of order $N^{-1/2}$, but here we will explain the technical argument allowing us to improve the rate (this inspired the argument used to improve the trace norm estimate in Theorem 3.3.1 from $N^{1/2}$ to $N^{1/6}$). The starting point is to notice that $U_N(t,s)$ is a unitary evolution determined by the equation

$$i\partial_t U_N(t,s) = \mathcal{L}_N(t) U_N(t,s), \quad U_N(s,s) = \mathbb{1}$$

with generator

$$\begin{aligned}\mathcal{L}_N(t) &= \left(i\partial_t W^*(\sqrt{N}\varphi_t)\right) W(\sqrt{N}\varphi_t) + W^*(\sqrt{N}\varphi_t)\mathcal{H}_N W(\sqrt{N}\varphi_t) \\ &= \mathcal{H}_N + \int \mathrm{d}x\,(V * |\varphi_t|^2)(x) a_x^* a_x + \int \mathrm{d}x\mathrm{d}y\, V(x-y)\overline{\varphi}_t(x)\varphi_t(y) a_y^* a_x \\ &\quad + \frac{1}{2}\int \mathrm{d}x\mathrm{d}y\, V(x-y)\left(\varphi_t(x)\varphi_t(y) a_x^* a_y^* + \overline{\varphi}_t(x)\overline{\varphi}_t(y) a_x a_y\right) \\ &\quad + \frac{1}{\sqrt{N}}\int \mathrm{d}x\mathrm{d}y\, V(x-y) a_x^*\left(\varphi_t(y) a_y^* + \overline{\varphi}_t(y) a_y\right) a_x.\end{aligned} \tag{1.46}$$

The Hartree equation (1.39) is needed for cancelling the terms linear in a_x^* or a_x between the two summands in (1.46). This cancellation is crucial since individually, the linear terms are of order $N^{1/2}$, and we must not get anything larger than order one (w. r. t. N) here in the generator to be able to apply Grönwall's lemma.

Now, if $U_N(t,0)$ conserved the parity $(-1)^{\mathcal{N}}$, we would immediately know that the expectation values $\langle U_N(t,0)\Omega, a_y^* U_N(t,0)\Omega\rangle$ and $\langle U_N(t,0)\Omega, a_x U_N(t,0)\Omega\rangle$ vanish completely. However, the summand in the last line of the generator violates parity, but we notice that it is formally of order $N^{-1/2}$. Therefore one introduces a new dynamics $\tilde{U}_N$, generated by

$$\begin{aligned}\tilde{\mathcal{L}}_N(t) = \mathcal{H}_N &+ \int \mathrm{d}x\,(V * |\varphi_t|^2)(x) a_x^* a_x + \int \mathrm{d}x\mathrm{d}y\, V(x-y)\overline{\varphi}_t(x)\varphi_t(y) a_y^* a_x \\ &+ \frac{1}{2}\int \mathrm{d}x\mathrm{d}y\, V(x-y)\left(\varphi_t(x)\varphi_t(y) a_x^* a_y^* + \overline{\varphi}_t(x)\overline{\varphi}_t(y) a_x a_y\right),\end{aligned}$$

i. e. the parity-violating term has been dropped. In fact, using the Duhamel formula

$$\begin{aligned}U_N(t,0) - \tilde{U}_N(t,0) &= U_N(t,0)\left(1 - U_N(t,0)^*\tilde{U}_N(t,0)\right) \\ &= -i\int_0^t \mathrm{d}s\, U_N(t,s)\left(\mathcal{L}_N(s) - \tilde{\mathcal{L}}_N(s)\right)\tilde{U}_N(s,0)\end{aligned}$$

and (1.47) below (and an analogous bound for the expectation of $\mathcal{N}^4$), one can prove that

$$\|(U_N(t,0) - \tilde{U}_N(t,0))\Omega\| \leq \frac{C}{\sqrt{N}} e^{K|t|}.$$

Since $\tilde{U}_N$ conserves the parity it can be inserted in (1.43) and (1.44), and eventually one obtains the estimate

$$\begin{aligned}\|\gamma_{N,t}^{(1)} - |\varphi_t\rangle\langle\varphi_t|\|_{\mathrm{HS}} &\leq \frac{1}{N}\langle U_N(t,0)\Omega, \mathcal{N} U_N(t,0)\Omega\rangle \\ &\quad + \frac{2}{\sqrt{N}}\|(U_N(t,0) - \tilde{U}_N(t,0))\Omega\| \|(\mathcal{N}+1)^{1/2} U_N(t,0)\Omega\| \\ &\quad + \frac{2}{\sqrt{N}}\|(U_N(t,0) - \tilde{U}_N(t,0))\Omega\| \|(\mathcal{N}+1)^{1/2} \tilde{U}_N(t,0)\Omega\| \\ &\leq \frac{1}{N}\langle U_N(t,0)\Omega, \mathcal{N} U_N(t,0)\Omega\rangle \\ &\quad + \frac{C}{N} e^{K|t|}\|(\mathcal{N}+1)^{1/2} U_N(t,0)\Omega\| + \frac{C}{N} e^{K|t|}\|(\mathcal{N}+1)^{1/2}\tilde{U}_N(t,0)\Omega\|.\end{aligned}$$

The next step is to prove that

$$\big\langle \tilde{U}_N(t,0)\Omega, (\mathcal{N}+1)\tilde{U}_N(t,0)\Omega\big\rangle \leq Ce^{K|t|}. \tag{1.47}$$

Notice that the generator of $\tilde{U}_N(t,s)$ contains terms not conserving the number of particles, so it is non-trivial to bound this expectation value. (From a physical point of view, this is because $U_N(t,s)$ describes fluctuations around the Hartree evolution and the fluctuations are expected to grow in time. For us the important point is that they must not grow with N.) To obtain a bound, one computes the time derivative using the generator $\tilde{\mathcal{L}}_N$ of $\tilde{U}_N$,

$$\begin{aligned}
&\frac{\mathrm{d}}{\mathrm{d}t}\big\langle \tilde{U}_N(t,0)\Omega, (\mathcal{N}+1)\tilde{U}_N(t,0)\Omega\big\rangle \\
&\quad = \big\langle \tilde{U}_N(t,0)\Omega, [\tilde{\mathcal{L}}_N(t), \mathcal{N}]\tilde{U}_N(t,0)\Omega\big\rangle \\
&\quad = 4\,\mathrm{Im}\int \mathrm{d}x\mathrm{d}y\, V(x-y)\varphi_t(x)\varphi_t(y)\big\langle \tilde{U}_N(t,0)\Omega, a_x^* a_y^* \tilde{U}_N(t,0)\Omega\big\rangle,
\end{aligned}$$

and estimates the last line using the well-known lemma that creation and annihilation operators are bounded with respect to the number operator:

Lemma 1.4.2. *Let $f \in L^2(\mathbb{R}^3)$. Then, for any $\psi \in \mathcal{F}$, we have the following bounds for the bosonic creation and annihilation operators:*

$$\begin{aligned}
\|a(f)\psi\| &\leq \|f\|_2 \|\mathcal{N}^{1/2}\psi\|, \\
\|a^*(f)\psi\| &\leq \|f\|_2 \|(\mathcal{N}+1)^{1/2}\psi\|, \\
\|\phi(f)\psi\| &\leq 2\|f\|_2 \|(\mathcal{N}+1)^{1/2}\psi\|.
\end{aligned} \tag{1.48}$$

Here we introduced the selfadjoint field operator $\phi(f) := a^*(f) + a(f)$.

Proof. The first inequality follows by writing out the definition of the annihilation operator and using the Cauchy-Schwarz inequality on the integrals. The second inequality follows from the first and the CCR. □

Assuming the potential to satisfy $V^2 \leq C(1-\Delta)$ for some $C > 0$, one obtains

$$\left|\frac{\mathrm{d}}{\mathrm{d}t}\big\langle \tilde{U}_N(t,0)\Omega, (\mathcal{N}+1)\tilde{U}_N(t,0)\Omega\big\rangle\right| \leq C\big\langle \tilde{U}_N(t,0)\Omega, (\mathcal{N}+1)\tilde{U}_N(t,0)\Omega\big\rangle.$$

Applying Grönwall's lemma, this implies (1.47).

As mentioned before, the proof of (1.45) is similar, but requires extra work to control terms which are cubic in creation/annihilation operators.

Finally, one obtains

$$\|\gamma_{N,t}^{(1)} - |\varphi_t\rangle\langle\varphi_t|\|_{\mathrm{HS}} \leq \frac{C}{N}e^{K|t|} \tag{1.49}$$

and according to Lemma 1.A.1, Hilbert-Schmidt norm and trace norm here only differ by at most a factor of 2. The estimate (1.49) here is for the one-particle reduced density matrix of a solution to the Schrödinger equation with coherent state as initial data, but one can project onto the N-particle component to obtain the result for initial data $\varphi^{\otimes N}$, see [CLS11] for the optimal way.

After this review, we summarize the general strategy: For initial data obtained by applying a unitary operator to the vacuum, one introduces fluctuation dynamics U_N in the spirit of (1.41). For a well-chosen unitary (i. e. well-chosen initial data and well-chosen effective evolution) one can then bound the difference between $\gamma_{N,t}^{(1)}$ and its approximation by the number of fluctuations $\langle U_N(t,0)\Omega, \mathcal{N} U_N(t,0)\Omega \rangle$. The main task is to control this quantity, which is typically done invoking Grönwall's lemma.

This general strategy is the basis for the results in Chapter 2 (Derivation of the Gross-Pitaevskii equation) and Chapter 3 and 4 (Derivation of the Hartree-Fock equation). However, for the Gross-Pitaevskii setting as well as for the Hartree-Fock setting, coherent states are not well-adapted initial data. In fact, we use Bogoliubov transformations to define pertinent initial data. We then obtain bounds in terms of the number of fluctuations. To control the number of fluctuations we have to develop new ideas beyond the bosonic mean-field setting which we will explain in the respective chapters.

1.5. Bogoliubov transformations

In this chapter, we introduce the theory of Bogoliubov transformations. In particular, we comment on the similarities and highlight the differences between the bosonic and fermionic Bogoliubov transformations employed in this work.

Let us start with the abstract theory following [S07]. In the most general setting, with an abstract one-particle Hilbert space $\mathfrak{h}$, it is necessary to introduce the conjugate linear map $J : \mathfrak{h} \to \mathfrak{h}^*$ such that $(Jg)(f) = \langle g, f \rangle_{\mathfrak{h}}$ $(f, g \in \mathfrak{h})$. In this thesis we only consider quantum mechanical systems which have one-particle space $\mathfrak{h} = L^2(\mathbb{R}^3)$, so we choose to formulate the theory using explicit complex conjugation.

The appropriate language for studying Bogoliubov transformations is generalized creation and annihilation operators. We give the bosonic and fermionic definitions at the same time; unless we point out differences everything holds for bosons as well as for fermions. For $f, g \in L^2(\mathbb{R}^3)$ the generalized operators are defined as

$$A(f,g) := a(f) + a^*(\overline{g}), \quad A^*(f,g) := a^*(f) + a(\overline{g}) = (A(f,g))^* . \tag{1.50}$$

Let us define

$$\mathcal{J} = \begin{pmatrix} 0 & J \\ J & 0 \end{pmatrix},$$

where $J : L^2(\mathbb{R}^3) \to L^2(\mathbb{R}^3)$ is complex conjugation, i. e. $Jf = \overline{f}$ for $f \in L^2(\mathbb{R}^3)$. We observe that

$$A^*(f,g) = A(\mathcal{J}(f,g)). \tag{1.51}$$

Notice that A^* is linear in its arguments whereas A is antilinear in its arguments. The canonical commutation relations (i. e. for the bosonic operators) take the form

$$\begin{gathered} [A(f_1,g_1), A^*(f_2,g_2)] = \big\langle (f_1,g_1), \mathcal{S}(f_2,g_2) \big\rangle_{L^2(\mathbb{R}^3)\oplus L^2(\mathbb{R}^3)}, \\ \text{where } \mathcal{S} = \begin{pmatrix} \mathbb{1} & 0 \\ 0 & -\mathbb{1} \end{pmatrix} : L^2(\mathbb{R}^3) \oplus L^2(\mathbb{R}^3) \to L^2(\mathbb{R}^3) \oplus L^2(\mathbb{R}^3). \end{gathered} \tag{1.52}$$

The canonical anticommutation relations (i. e. for the fermionic operators) take the form

$$\{A(f_1,g_1), A^*(f_2,g_2)\} = \big\langle (f_1,g_1), (f_2,g_2) \big\rangle_{L^2(\mathbb{R}^3)\oplus L^2(\mathbb{R}^3)}. \tag{1.53}$$

We caution the reader that in general $\{A(f_1,g_1), A(f_2,g_2)\} \neq 0$ and $[A(f_1,g_1), A(f_2,g_2)] \neq 0$.

A Bogoliubov transformation is an isomorphism $\nu : L^2(\mathbb{R}^3) \oplus L^2(\mathbb{R}^3) \to L^2(\mathbb{R}^3) \oplus L^2(\mathbb{R}^3)$ such that

$$A^*(\nu(f,g)) = A(\nu\mathcal{J}(f,g)) \tag{1.54}$$

and for bosons

$$[A(\nu(f_1,g_1)), A^*(\nu(f_2,g_2))] = \big\langle (f_1,g_1), \mathcal{S}(f_2,g_2)\big\rangle, \tag{1.55}$$

while for fermions

$$\{A(\nu(f_1,g_1)), A^*(\nu(f_2,g_2))\} = \big\langle (f_1,g_1), (f_2,g_2)\big\rangle. \tag{1.56}$$

The bosonic property (1.55) is equivalent to

$$\nu^*\mathcal{S}\nu = \mathcal{S}; \tag{1.57}$$

the fermionic property (1.56) is equivalent to

$$\nu^*\nu = \mathbb{1}. \tag{1.58}$$

In short, a Bogoliubov transformation linearly combines creation and annihilation operators in such a way that the new operators $B(f,g) := A(\nu(f,g))$ satisfy the CCR or CAR again and also the property $B^*(f,g) = B(\mathcal{J}(f,g))$. (Physically, one can think of the new operators as describing quasiparticles.)

The property (1.54) implies that (both for bosons and fermions)

$$\nu\mathcal{J} = \mathcal{J}\nu, \tag{1.59}$$

which implies that ν can be decomposed into blocks as

$$\nu = \begin{pmatrix} u & \overline{v} \\ v & \overline{u} \end{pmatrix}, \tag{1.60}$$

where $u, v : L^2(\mathbb{R}^3) \to L^2(\mathbb{R}^3)$ are bounded operators. Here we wrote $\overline{u}$ for JuJ, which is again a linear operator. If u has an integral kernel $u(x,y)$, then $\overline{u(x,y)}$ is the integral kernel of $\overline{u}$. As a consequence of (1.57), in the bosonic case the blocks have to satisfy

$$u^*u = 1 + v^*v \text{ and } \overline{v}^*u = \overline{u}^*v, \tag{1.61}$$

and for fermions as a consequence of (1.58)

$$u^*u = 1 - v^*v \text{ and } \overline{v}^*u = -\overline{u}^*v. \tag{1.62}$$

Conversely, if u and v satisfy the appropriate (bosonic or fermionic) condition then a matrix of the form (1.60) defines a Bogoliubov transformation.

A bosonic or fermionic Bogoliubov transformations ν is called implementable on the bosonic or fermionic Fock space $\mathcal{F}$, respectively, if there exists a unitary operator $R_\nu : \mathcal{F} \to \mathcal{F}$ such that

$$R_\nu^* A(f,g) R_\nu = A(\nu(f,g)). \tag{1.63}$$

According to the Shale-Stinespring condition (see e. g. [S07, Theorem 9.5] or [R78]), a Bogoliubov transformation is implementable if and only if the block v is a Hilbert-Schmidt operator.

The quantum-mechanical time-evolution generated by a quadratic Hamiltonian is an example of a Bogoliubov transformation [BD06], explaining why it can be expressed in terms of the classical evolution. However, the Bogoliubov transformations that we use in this thesis play a different role, which is to construct initial data for the many-body dynamics. To elaborate on the role of Bogoliubov transformations, recall that for $\psi \in \mathcal{F}$ the one-particle reduced density matrix is the operator on $L^2(\mathbb{R}^3)$ with integral kernel

$$\gamma_\psi^{(1)}(x,y) = \frac{1}{\langle \psi, \mathcal{N}\psi \rangle} \langle \psi, a_y^* a_x \rangle.$$

We define the pairing density[10] α_ψ as the operator with integral kernel

$$\alpha_\psi(x,y) = \frac{1}{\langle \psi, \mathcal{N}\psi \rangle} \langle \psi, a_y a_x \psi \rangle.$$

For $\psi \in L^2(\mathbb{R}^{3N})$ the pairing density vanishes; only for Fock space vectors that do not have an exact number of particles the pairing density can be non-zero.

A vector $\psi \in \mathcal{F}$ is called a quasifree pure state if it is of the form $\psi = R_\nu \Omega$ for some implementable Bogoliubov transformation ν. (In the language of quasiparticles, $R_\nu \Omega$ is the quasiparticle vacuum.) Quasifree states are particularly useful due to the fact that all higher-order correlation functions (which includes all k-particle reduced density matrices)

$$\langle \psi, a_{x_1}^\sharp \cdots a_{x_k}^\sharp \psi \rangle$$

can be expressed using only the one-particle reduced density matrix and the pairing density by Wick's theorem [S07, Theorem 10.2]:

$$\begin{aligned} \langle \psi, A(f_1,g_1) \cdots A(f_{2m},g_{2m})\psi \rangle = \sum_{\sigma \in P_{2m}} (\pm 1)^\sigma \, &\langle \psi, A(f_{\sigma(1)}, g_{\sigma(1)}) A(f_{\sigma(2)}, g_{\sigma(2)})\psi \rangle \\ &\times \cdots \langle \psi, A(f_{\sigma(2m-1)}, g_{\sigma(2m-1)}) A(f_{\sigma(2m)}, g_{\sigma(2m)})\psi \rangle. \end{aligned}$$

The expectation values on the r. h. s. are straightforwardly expanded in $\gamma_\psi^{(1)}$ and α_ψ. (Expectation values with an odd number of creation/annihilation operators vanish. The set of pairings P_{2m} is defined in (3.77). In the fermionic case $(\pm 1)^\sigma = \operatorname{sgn}(\sigma)$, in the bosonic case $(\pm 1)^\sigma = 1$.)

Furthermore, it is an easy calculation to see that for a quasifree pure state $\psi = R_\nu \Omega$ with Bogoliubov transformation ν of the form (1.60), the one-particle reduced density matrix is

$$\gamma_\psi^{(1)} = \frac{1}{\langle \psi, \mathcal{N}\psi \rangle} v^* v$$

and the pairing density

$$\alpha_\psi = \frac{1}{\langle \psi, \mathcal{N}\psi \rangle} v^* \overline{u}.$$

We have $\langle \psi, \mathcal{N}\psi \rangle = \|v\|_{\mathrm{HS}}^2$, so the Shale-Stinespring condition ensures that the number of particles in quasifree states (in the quasiparticle vacuum) is finite. As a consequence of (1.61)

[10] Since in this chapter we adapted the normalization $\operatorname{tr} \gamma_\psi^{(1)} = 1$, compared to Chapters 3 and 4 extra factors appear in the following equations.

or (1.62) the one-particle reduced density matrix $\gamma = \gamma_\psi^{(1)}$ and the pairing density $\alpha = \alpha_\psi$ of a quasifree pure state ψ satisfy

$$\gamma\alpha = \alpha\overline{\gamma} \quad \text{and} \quad \gamma^2 - \alpha\overline{\alpha} = -\gamma\frac{1}{\langle \psi, \mathcal{N}\psi \rangle} \quad \text{(bosons)} \tag{1.64}$$

or

$$\gamma\alpha = \alpha\overline{\gamma} \quad \text{and} \quad \gamma^2 - \alpha\overline{\alpha} = \gamma\frac{1}{\langle \psi, \mathcal{N}\psi \rangle} \quad \text{(fermions)}, \tag{1.65}$$

respectively.

1.5.1. Problem-specific constructions

Having introduced the abstract theory, let us now give concrete constructions for the fermionic and the bosonic Bogoliubov transformations used in this thesis. Afterwards we will also discuss the differences.

In the fermionic case, we are interested in the mean-field regime, i. e. correlations can be neglected and the initial data we are interested in is approximately a Slater determinant. We are therefore interested in finding a unitary operator R on Fock space such that $R\Omega$ coincides with a given Slater determinant. This is indeed possible by choosing R as the unitary implementor of an appropriate Bogoliubov transformation. We will now give an explicit construction of R as a particle-hole transformation. Assume $(f_i)_{i=1}^\infty$ to be an orthonormal basis in $L^2(\mathbb{R}^3)$. Define

$$R_\nu\Omega := a^*(f_1)\cdots a^*(f_N)\Omega$$

(this is exactly the Slater determinant $A_N(f_1 \otimes \ldots \otimes f_N)$) and define transformed creation operators by

$$R_\nu a^*(f_i)R_\nu^* := \begin{cases} a(f_i) & \text{for } i \leq N \\ a^*(f_i) & \text{for } i > N. \end{cases}$$

An intuitive way of thinking of this transformation is that the Slater determinant $R_\nu\Omega$ constitutes a Fermi sea, while $R_\nu a^*(f_i)R_\nu^*$ for $i \leq N$ creates holes in the Fermi sea. Clearly the transformed operators satisfy the canonical anticommutation relations and $R_\nu\Omega$ is a vacuum for them. It is easy to see that R_ν is isometric and thinking of the occupation number representation of Fock space, it is clear that R_ν is surjective. This implies that R_ν is unitary. Furthermore its action on creation/annihilation operators coincides with the Bogoliubov transformation given by

$$\nu = \begin{pmatrix} u & \overline{v} \\ v & \overline{u} \end{pmatrix} = \begin{pmatrix} 1 - \sum_{j=1}^N |f_j\rangle\langle f_j| & \sum_{j=1}^N |f_j\rangle\langle \overline{f}_j| \\ \sum_{j=1}^N |\overline{f}_j\rangle\langle f_j| & 1 - \sum_{j=1}^N |\overline{f}_j\rangle\langle \overline{f}_j| \end{pmatrix}. \tag{1.66}$$

It is an amusing exercise to derive identities for particle-hole transformations. For example, using the representation $\mathcal{N} = \sum_{i=1}^\infty a^*(f_i)a(f_i)$, we find

$$R_\nu\mathcal{N}R_\nu^* = \left(N - \sum_{i=1}^N a^*(f_i)a(f_i)\right) + \sum_{i=N+1}^\infty a^*(f_i)a(f_i).$$

In physical terms, this can be interpreted as the number of holes plus the number of particles, or in total as the number of excitations w. r. t. the Fermi sea. Restricting to the N-particle subspace, we obtain $R_\nu \mathcal{N} R_\nu^* = 2\big(N - \sum_{i=1}^N a^*(f_i)a(f_i)\big)$, so in this case the number of excitations is two times the number of holes.

We now turn to the bosonic case. It is a natural question whether it is also possible for bosons to find a Bogoliubov transformation R such that $R\Omega = \psi_N$ for a given N-particle wave function ψ_N, e. g. $\psi_N = \varphi^{\otimes N}$. However, for states with an exact number of particles we have $\alpha = 0$, so if ψ_N was a quasifree state, by (1.64), its one-particle reduced density matrix would have to satisfy

$$\gamma^2 = -\gamma N^{-1}.$$

But γ^2 is clearly a positive operator and so is γ, leading to a contradiction. So bosonic states with exact number of particles are never quasifree. This is the reason why in the bosonic case we use Weyl operators and coherent states and go through the extra complications of leaving the N-particle subspace.

In view of Section 1.4 it is natural to ask if coherent states are quasifree, and if the coherent states method can be reformulated in the framework of Bogoliubov transformations. For the definition of quasifree states used in this thesis, one finds that coherent states are not quasifree: Using Lemma 1.4.1 (iv), one finds that the second formula in (1.64) is not satisfied.

After these negative results, let us now explain the pertinent choice of initial data in bosonic Fock space for the Gross-Pitaevskii regime. As pointed out in Section 1.2.2 correlations play an important role in the Gross-Pitaevskii regime. On the other hand, we know from the discussion of the mean-field regime in Section 1.4 that coherent states are useful to describe condensates. In Chapter 2, we therefore use a Bogoliubov transformation to implement appropriate correlations on a given coherent state. Concretely, we use the Bogoliubov transformation implemented by the unitary operator

$$T(k) := \exp\left(\frac{1}{2}\int \mathrm{d}x\mathrm{d}y\,\big(k(x,y)a_x^*a_y^* - \overline{k}(x,y)a_xa_y\big)\right). \tag{1.67}$$

The integral kernel $k(x,y)$ is defined as

$$k(x,y) := -Nw(N(x-y))\varphi(x)\varphi(y),$$

where $w(x) := 1 - f(x)$ with f the solution of the zero-energy scattering equation (1.10). The initial data to be used is of the form

$$W(\sqrt{N}\varphi)T(k)\psi,$$

for ψ a vector in bosonic Fock space with bounded number of particles and bounded energy. For $\psi = \Omega$, this vector is a Bogoliubov transformed coherent state. (However, by moving $T(k)$ to the left of the Weyl operator, the argument of the Weyl operator, i. e. the condensate wave function, is also transformed.) In quantum optics such states are known as squeezed coherent states and $T(k)$ is called a squeezing operator.

As shown in Lemma 2.2.1 the operator $T(k)$ acts on creation and annihilation operators as a Bogoliubov transformation

$$T^*(k)a(f)T(k) = a(\mathrm{ch}(k)(f)) + a^*(\mathrm{sh}(k)(\overline{f})),$$
$$T^*(k)a^*(f)T(k) = a^*(\mathrm{ch}(k)(f)) + a(\mathrm{sh}(k)(\overline{f})),$$

where $\mathrm{ch}(k)$ and $\mathrm{sh}(k)$ are the bounded operators on $L^2(\mathbb{R}^3)$ defined by the absolutely convergent series

$$\mathrm{ch}(k) := \sum_{n\geq 0}\frac{1}{(2n)!}(k\overline{k})^n \qquad \text{and} \qquad \mathrm{sh}(k) := \sum_{n\geq 0}\frac{1}{(2n+1)!}(k\overline{k})^n k.$$

Products of k and $\overline{k}$ here have to be understood in the sense of operators.

In Lemma 2.4.3 we show that the bosonic Bogoliubov transformation $T(k)$ only changes the expected number of particles by order one (small compared to the number N of particles in the bulk) while it is easy to see that it affects expectation values of the kinetic energy on order N. The last effect is important to ensure that states of the form $W(\sqrt{N}\varphi)T(k)\psi$ approximate the ground state energy correctly, see Remark (ii) after Theorem 3.3.1. In this sense the bosonic Bogoliubov transformations $T(k)$ only introduce correlations and do not create the bulk of the particles.

In our proofs, for the initial data introduced above, we compare the Fock space vectors evolved by the Schrödinger equation with Fock space vectors of the same form as the initial data, but with parameters $f_{i,t}$, $i = 1, \dots N$ or $\varphi_t^{(N)}$ (and $k_t(x,y) = -Nw(N(x-y))\varphi_t^{(N)}(x)\varphi_t^{(N)}(y)$) that are evolved with the Hartree-Fock equation or modified Gross-Pitaevskii equation[11], respectively. More precisely we introduce fluctuation dynamics following this idea, see (2.33) and (3.36).

For comparison, we mention that bosonic Bogoliubov transformations have also been used in [BKS11] (to describe the limit of the fluctuation dynamics and prove a central limit theorem) and in [GMM10, GMM11, GM12] (to obtain an approximation for the mean-field system which holds in Fock space norm, not only for reduced densities). However, in these works, not only is the goal different, but also the choice of the Bogoliubov transformations: In [BKS11], it is used that the fluctuation dynamics $U_N(t,0)$ (1.41) in the limit $N \to \infty$ converges to a dynamics $U_\infty(t,0)$ with generator

$$\begin{aligned}\mathcal{L}_\infty(t) = &\int \mathrm{d}x\, \nabla_x a_x^* \nabla_x a_x + \int \mathrm{d}x\, (V * |\varphi_t|^2)(x) a_x^* a_x + \int \mathrm{d}x\mathrm{d}y\, V(x-y)\overline{\varphi}_t(x)\varphi_t(y) a_y^* a_x \\ &+ \frac{1}{2}\int \mathrm{d}x\mathrm{d}y\, V(x-y)\left(\varphi_t(x)\varphi_t(y) a_x^* a_y^* + \overline{\varphi}_t(x)\overline{\varphi}_t(y) a_x a_y\right),\end{aligned}$$

which is quadratic in creation/annihilation operators and thus implements a Bogoliubov transformation. In [GMM10, GMM11], a Bogoliubov transformation of the form (1.67) with time-dependent kernel k_t is used in defining a fluctuation dynamics, and the kernel is chosen to satisfy a complicated non-linear equation such that terms of the form a^*a^* in the generator are cancelled. The idea of [GM12] is similar, but the interaction potential is scaled as $N^{3\beta}V(N^\beta .)$ with $\beta < 1/3$, which is reminiscent of the Gross-Pitaevskii scaling ($\beta = 1$) but less singular (in fact giving rise to a Gross-Pitaevskii equation with $b = \int V \mathrm{d}x$ replacing $8\pi a_0$ [ESY10]).

1.A. Reduced density matrices and normalization conventions

In this section, we give an overview of the definitions of reduced densities, pointing out the differences in normalization between Chapters 1 and 2 and Chapters 3 and 4. We also state a useful lemma concerning bosonic one-particle reduced density matrices.

Chapters 1 and 2, bosonic convention.

In the bosonic case, by the convention usually followed, the reduced density matrices are all normalized such that their trace is one (for consistency, we also use this convention for

[11] The modified Gross-Pitaevskii equation is introduced in (2.4). For $N \to \infty$, its solutions converge to the solution of the Gross-Pitaevskii equation with the same initial data.

fermions in Chapter 1). The k-particle reduced density matrix associated with $\psi_N \in L^2(\mathbb{R}^{3N})$ is then defined as the non-negative trace class operator $\gamma_N^{(k)}$ on $L^2(\mathbb{R}^{3k})$ with integral kernel

$$\gamma_N^{(k)}(\mathbf{x},\mathbf{x}') := \int \mathrm{d}x_{k+1}\dots \mathrm{d}x_N\, \psi_N(\mathbf{x},x_{k+1},\dots,x_N)\overline{\psi}_N(\mathbf{x}',x_{k+1},\dots,x_N), \tag{1.68}$$

where $\mathbf{x} = (x_1,\dots,x_k)$. Since we always assume that wave functions are normalized to $\|\psi_N\| = 1$, we have $\mathrm{tr}\ \gamma_N^{(k)} = 1$. In more compact notation

$$\gamma_N^{(k)} = \mathrm{tr}_{k+1,\dots,N}|\psi_N\rangle\langle\psi_N|,$$

where $|\psi\rangle\langle\psi|$ is the projection on $\psi_N \in L^2(\mathbb{R}^{3N})$, and $\mathrm{tr}_{k+1,\dots,N}$ the partial trace over all but k particles. For Fock space vectors $\psi \in \mathcal{F}$, the k-particle reduced density matrix is defined as the non-negative trace class operators on $L^2(\mathbb{R}^{3k})$ with integral kernel

$$\gamma_\psi^{(k)}(x_1,\dots,x_k,y_1,\dots,y_k) := \frac{\langle\psi, a_{y_1}^*\dots a_{y_k}^* a_{x_k}\dots a_{x_1}\psi\rangle}{\langle\psi,\mathcal{N}(\mathcal{N}-1)\dots(\mathcal{N}-k+1)\psi\rangle},$$

where $\mathcal{N}$ is the number operator. Using the definition (1.35) of the annihilation operator a_x it is easy to check that for $\psi \in L^2(\mathbb{R}^{3N})$ both definitions of $\gamma_\psi^{(k)}$ coincide.

As the standard example of a one-particle reduced density matrix for bosonic systems, we mention the case of a wave function given as an N-fold tensor product, $\psi_N = \varphi^{\otimes N}$ with one-particle orbital $\varphi \in L^2(\mathbb{R}^3)$, for which we have $\gamma_N^{(k)} = |\varphi\rangle\langle\varphi|^{\otimes k}$.

Chapters 3 and 4, fermionic convention.
In the fermionic case, by the convention usually followed, the one-particle reduced density matrix is normalized such that it is a projection. This normalization is very convenient when using Bogoliubov transformations.

The k-particle reduced density matrix associated with $\psi_N \in L^2(\mathbb{R}^{3N})$ is then defined as the non-negative trace class operator $\gamma_N^{(k)}$ on $L^2(\mathbb{R}^{3k})$ with integral kernel

$$\gamma_N^{(k)}(\mathbf{x},\mathbf{x}') := \frac{N!}{(N-k)!}\int \mathrm{d}x_{k+1}\dots \mathrm{d}x_N\, \psi_N(\mathbf{x},x_{k+1},\dots,x_N)\overline{\psi}_N(\mathbf{x}',x_{k+1},\dots,x_N). \tag{1.69}$$

Since we assume that $\|\psi_N\| = 1$, we have $\mathrm{tr}\ \gamma_N^{(k)} = \frac{N!}{(N-k)!}$. For Fock space vectors $\psi \in \mathcal{F}$, the k-particle reduced density matrix is defined as the non-negative trace class operator on $L^2(\mathbb{R}^{3k})$ with integral kernel

$$\gamma_\psi^{(k)}(x_1,\dots,x_k,y_1,\dots,y_k) := \langle\psi, a_{y_1}^*\dots a_{y_k}^* a_{x_k}\dots a_{x_1}\psi\rangle.$$

As the standard example of a one-particle reduced density matrix for fermionic systems, we mention the case of a wave function given as a Slater determinant of N orthonormal orbitals, $\psi_N = A_N\,(f_1\otimes\dots\otimes f_N)$, for which we have $\gamma_N^{(1)} = \sum_{j=1}^N |f_j\rangle\langle f_j|$. A useful property of fermionic one-particle density matrices is that, while $\mathrm{tr}\left|\gamma_N^{(1)}\right| = N$, in operator norm $\|\gamma_N^{(1)}\| \leq 1$.

Trace norm and Hilbert-Schmidt norm
We close with a Lemma telling us that for the difference of exact one-particle reduced density matrix and Hartree one-particle density matrix in the bosonic case, the trace norm is at most twice the Hilbert-Schmidt norm. For comparison, notice that for a general operator A, one only has the inequality $\|A\|_{\mathrm{HS}} \leq \mathrm{tr}|A|$.

Lemma 1.A.1 ([RS09], attributed to R. Seiringer)**.** *Let $\gamma \geq 0$ be a trace class operator on a separable Hilbert space $\mathfrak{h}$ with $\operatorname{tr}\gamma = 1$, and let $\varphi \in \mathfrak{h}$. Then*

$$\operatorname{tr}\big|\gamma - |\varphi\rangle\langle\varphi|\big| \leq 2\|\gamma - |\varphi\rangle\langle\varphi|\|_{HS}.$$

Proof. We set $A := \gamma - |\varphi\rangle\langle\varphi|$, which is trace class and selfadjoint. We claim that A has at most one negative eigenvalue and this eigenvalue has maximal multiplicity one. Assume there are two negative eigenvalues $\mu_1 < 0$ and $\mu_2 < 0$ (possibly $\mu_1 = \mu_2$),

$$A\psi_1 = \mu_1\psi_1, \quad A\psi_2 = \mu_2\psi_2.$$

We can assume the eigenvectors to be orthogonal, $\big\langle\psi_1, \psi_2\big\rangle = 0$. Now consider an arbitrary vector $\omega \in \operatorname{span}\{\psi_1, \psi_2\}$, $\omega = a\psi_1 + b\psi_2$. Then

$$\big\langle\omega, A\omega\big\rangle = \mu_1|a|^2\|\psi_1\|^2 + \mu_2|b|^2\|\psi_2\|^2 < 0.$$

By definition of A, this implies

$$0 \leq \big\langle\omega, \gamma\omega\big\rangle < \big\langle\omega, |\varphi\rangle\langle\varphi|\omega\big\rangle = |\big\langle\omega, \varphi\big\rangle|^2.$$

But given an arbitrary vector, in any two-dimensional subspace one can find a vector which is orthogonal to it. In particular there exists $\omega \in \operatorname{span}\{\psi_1, \psi_2\}$ such that

$$|\big\langle\omega, \varphi\big\rangle|^2 = 0.$$

This contradiction concludes the proof of the claim.

Let us denote the eigenvalues of A by λ_j, indexed by $j \geq 0$, counting the multiplicity. Since $\operatorname{tr} A = 0$ by linearity of the trace, there exists exactly one negative eigenvalue $\lambda_0 < 0$ (unless $A = 0$, for which the lemma is trivial). Thus, again from $\operatorname{tr} A = 0$, we conclude that $|\lambda_0|$ equals the sum of all other eigenvalues, $\sum_{j\geq 1}\lambda_j$. Thus

$$\operatorname{tr}|A| = \sum_{j\geq 0}|\lambda_j| = 2|\lambda_0| = 2\|A\| \leq 2\|A\|_{\mathrm{HS}}.$$

For the last equality in the line we used that $\|A\| = \sup_{\lambda\in\sigma(A)}|\lambda|$ and $\lambda_j \leq |\lambda_0|$. □

1.B. Well-posedness of evolution equations

In this section we comment on the well-posedness both of the linear many-body Schrödinger equation and the non-linear effective evolution equations that we derive. Generally, no difficulties appear under the assumptions used in this thesis. In the later chapters we just assume the equations to be well-posed and do not comment on the background anymore. We do not strive for the strongest results here.

Hamilton operators and the Schrödinger equation

It is well established that Hamilton operators H_N of the form (1.2) are selfadjoint on $L^2_s(\mathbb{R}^{3N})$ and $L^2_a(\mathbb{R}^{3N})$. Indeed, if the potentials V_{ext} and V are real-valued and in $L^2(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$, then by the Kato-Rellich theorem [RS75, Theorem X.12 and X.15], H_N is selfadjoint on the domain $H^2(\mathbb{R}^{3N})$ and essentially selfadjoint on any core of the Laplacian, e. g. on Schwartz space $\mathcal{S}(\mathbb{R}^{3N})$ or on the smooth functions with compact support $C_0^\infty(\mathbb{R}^{3N})$. Furthermore, by the Kato-Rellich theorem the Hamiltonian is bounded from below, so the ground state energy $E_N = \inf_{\|\psi\|=1} \langle \psi, H_N\psi \rangle$ is finite. In particular, the Kato-Rellich theorem allows for the Coulomb potential. Since the Hamiltonian commutes with the projections S_N and A_N, it is simple to establish selfadjointness also on the symmetric and antisymmetric subspace.

For the preparation of initial data, one typically considers the Hamiltonian with added external potential that models a trap with $V_{\text{ext}}(x) \to \infty$ as $|x| \to \infty$. If $V_{\text{ext}} \geq 0$, such a potential can be added under very general assumptions, and the Hamilton operator is essentially selfadjoint on $C_0^\infty(\mathbb{R}^{3N})$ [RS75, Theorem X.29]. For our results however, Hamilton operators with trapping potentials are not necessary since we consider the initial data to be given by assumption.

Since the Hamiltonian is selfadjoint, it generates a strongly continuous unitary group, denoted $e^{-iH_N t}$, which provides us with the unique solution $\psi_t = e^{-iH_N t}\psi$ to the time-dependent Schrödinger equation

$$i\partial_t \psi_t = H_N \psi_t \quad \text{with initial data } \psi \in H^2(\mathbb{R}^{3N}).$$

In particular, the Schrödinger equation is globally well-posed.

For the pseudo-relativistic Hamiltonian in Chapter 4, that is (with $m > 0$)

$$H_N = \sum_{j=1}^{N} \sqrt{-\Delta_{x_j} + m^2} + \lambda \sum_{i<j}^{N} V(x_i - x_j),$$

similar statements hold with the domain $H^2(\mathbb{R}^{3N})$ replaced by $H^1(\mathbb{R}^{3N})$. In fact, the kinetic energy operator $\sum_{j=1}^N \sqrt{-\Delta_{x_j} + m^2}$ is selfadjoint on $H^1(\mathbb{R}^{3N})$, and for bounded potentials as we require in Chapter 4, the interaction is trivial to add.

Generally, for second quantized Hamilton operators corresponding to an (essentially) selfadjoint Hamilton operator given in first quantization, we also have (essential) selfadjointness; see Section 1.3.

Hartree- and Gross-Pitaevskii equations

The following results on non-linear Schrödinger equations in $\mathbb{R}^n$ are taken from [C96]. We consider only the case of $n \geq 3$ space dimensions.

Consider the wave function $u_t : \mathbb{R}^n \to \mathbb{C}$ where $t \in I$, I being an (possibly infinite) interval. We are interested in global well-posedness for the Cauchy problem of the non-linear Schrödinger equation,

$$\begin{cases} i\partial_t u_t &= -\Delta u_t - g(u_t) \text{ for almost all } t \in \mathbb{R}; \\ u_0 &= \varphi. \end{cases} \tag{1.70}$$

Here[12] $g \in C(H^1(\mathbb{R}^n), H^{-1}(\mathbb{R}^n))$ (or more generally $g = g_1 + \ldots + g_k$, where each g_i individually satisfies the conditions given here for g). Assume that there exists the antiderivative G, $G' = g$, where $G \in C^1(H^1(\mathbb{R}^n), \mathbb{R})$. Assume furthermore that there exist exponents $r, \rho \in \big[2, 2n/(n-2)\big)$ such that

[12] By $H^{-m}(\mathbb{R}^n)$ we denote the dual of $H^m(\mathbb{R}^n)$, a space of distributions. The test function space $\mathcal{D}(\mathbb{R}^n)$ is dense in $H^{-m}(\mathbb{R}^n)$. Despite $H^m(\mathbb{R}^n)$ being a Hilbert space, one does not identify $H^{-m}(\mathbb{R}^n)$ with $H^m(\mathbb{R}^n)$, but rather $L^2(\mathbb{R}^n)$ with its dual. We have $L^2(\mathbb{R}^n) \subset H^{-m}(\mathbb{R}^n) \subset \mathcal{D}'(\mathbb{R}^n)$. As an example, the Laplacian takes the energy space $H^1(\mathbb{R}^n)$ to $H^{-1}(\mathbb{R}^n)$. For more details, see [C96, Remark 2.3.8].

- g can be written as a mapping[13] $H^1(\mathbb{R}^n) \to L^{\rho'}(\mathbb{R}^n)$ followed by continuous injection $L^{\rho'}(\mathbb{R}^n) \to H^{-1}(\mathbb{R}^n)$;
- (local Lipschitz condition) for every $M > 0$ there exists a constant $C_M < \infty$ such that

$$\|g(v) - g(u)\|_{\rho'} \leq C_M \|v - u\|_r$$

for all $u, v \in H^1(\mathbb{R}^n)$ with $\|u\|_{H^1} + \|v\|_{H^1} \leq M$.

Moreover, assume that for all $u \in H^1(\mathbb{R}^n)$ we have $\operatorname{Im}(g(u)\overline{u}) = 0$ almost everywhere in $\mathbb{R}^n$.

For $u \in H^1(\mathbb{R}^n)$, one can define an energy functional

$$E(u) = \frac{1}{2}\int_{\mathbb{R}^n} |\nabla u(x)|^2 \mathrm{d}x - G(u).$$

We then have the following result on local well-posedness for the Cauchy problem of the non-linear Schrödinger equation (1.70):

Theorem 1.B.1 ([C96, Theorem 4.3.1])**.** *For g as above, the following holds:*

(i) *For every $\varphi \in H^1(\mathbb{R}^n)$ there exist $T_1, T_2 > 0$ and a unique maximal solution $u_{(.)}$ on the interval $(-T_1, T_2)$ such that*

$$u_{(.)} \in C\left((-T_1, T_2), H^1(\mathbb{R}^n)\right) \quad \text{and} \quad u_{(.)} \in C^1\left((-T_1, T_2), H^{-1}(\mathbb{R}^n)\right).$$

Here, u is maximal in the sense that we have the blow-up alternative: if $T_2 < \infty$, then $\|u_t\|_{H^1} \to \infty$ as $t \to T_2-$, and analogously for $-T_1$.

(ii) *There is conservation of mass and energy, that is*

$$\|u_t\|_2 = \|\varphi\|_2 \quad \text{and} \quad E(u_t) = E(\varphi)$$

for all $t \in (-T_1, T_2)$.

(iii) *The solution depends on the initial data in a continuous way, in the sense that T_1 and T_2 are lower semicontinuous as functions of φ, and that, if we have a sequence of initial data*

$$\varphi_m \to \varphi \text{ in } H^1(\mathbb{R}^n)$$

and $[-T_3, T_4] \subset (-T_1, T_2)$, then

$$u_{m,(.)} \to u_{(.)} \quad \text{in } C\left([-T_3, T_4], H^1(\mathbb{R}^n)\right).$$

(Here $u_{m,(.)}$ is the maximal solution with initial datum φ_m.)

Here $u_{(.)}$ is a solution in the sense that the differential equation (1.70) is satisfied in the space of distributions $H^{-1}(\mathbb{R}^n)$.

The assumptions of the theorem are in particular satisfied for (see [C96, Remark 4.3.2]):

- The Hartree equation: $g(u) = V_{\text{ext}} u + \left(V * |u|^2\right) u$, if we take a real-valued external potential $V_{\text{ext}} \in L^p(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$ for some $p > 3/2$, and an even, real-valued interaction potential $V \in L^q(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$ for some $q > 3/4$.

[13] We use the notation ρ' for the conjugate exponent defined through $1/\rho + 1/\rho' = 1$.

- The modified Gross-Pitaevskii equation (2.25) in Chapter 2: This is a special case of the Hartree equation, where $g(u) = \left(N f_N V_N * |u|^2\right) u$, with $f_N V_N(x) = N^2 f(Nx) V(Nx)$. Here f is the solution to the zero-energy scattering equation, and by the assumptions of Theorem 2.1.1 we have $N f_N V_N \in L^1 \cap L^3(\mathbb{R}^3, (1+|x|^6)\mathrm{d}x)$, which implies $N f_N V_N \in L^q(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$ with $q = 3 > 3/4$.
- The Gross-Pitaevskii equation: $g(u) = V_{\text{ext}} u + \lambda |u|^2 u$, with V_{ext} as in the Hartree equation and $\lambda \in \mathbb{R}$ a coupling constant.

A similar result holds if the external potential has up to quadratic growth at infinity [C96, Section 9.2]. Since the physically most interesting situation is a vanishing external potential, we do not give the precise statement here.

A discussion of propagation of regularity and smoothing effects can be found in [C96, Chapter 5]. However, we are particularly interested in the modified Gross-Pitaevskii equation (2.25) where the non-linearity depends on N, and, to be able to apply Grönwall's lemma to control the expectation of $\mathcal{N}$ in Chapter 2, we need estimates on Sobolev norms that are independent of N. For this reason, in Proposition 2.3.1 in Chapter 2 we reprove some regularity properties of the Gross-Pitaevskii equation and the modified Gross-Pitaevskii equation. In particular, we prove that for initial data in $H^n(\mathbb{R}^3)$ also the solution lives in $H^n(\mathbb{R}^3)$; our derivation of the Gross-Pitaevskii equation uses $H^4(\mathbb{R}^3)$. Under the assumptions of Theorem 2.1.1 on the potential, it is easy to see that for $u \in H^2(\mathbb{R}^3)$ we have $g(u_t) = \left(N f_N V_N * |u_t|^2\right) u_t \in L^2(\mathbb{R}^3)$, so our calculations in Chapter 2 are well-defined (of particular importance the cancellations in the linear terms of the generator).

Since in Chapter 2 we only study the case of repulsive interaction $V \geq 0$ and $V_{\text{ext}} = 0$, conservation of energy implies that $\|u_t\|_{H^1}$ is bounded uniformly in time. This decides the blow-up alternative for global existence.

Non-relativistic Hartree-Fock equations

Notice that for the following discussion of the well-posedness of the Hartree-Fock equation, we use the normalization of the one-particle densities that $\operatorname{tr} \omega_N = N$ — like in Chapter 3 and Chapter 4, and differing from the convention elsewhere in Chapter 1.

We now discuss well-posedness for the Hartree-Fock Cauchy problem

$$\begin{cases} i\partial_t \omega_{N,t} &= [-\Delta + V * \rho_t - X_t \,,\, \omega_{N,t}], \\ \omega_{N,0} &= \omega_N. \end{cases} \tag{1.71}$$

In the normalization here, the configuration space density of particles is $\rho_t(x) = \frac{1}{N}\omega_{N,t}(x,x)$, $(V * \rho_t)$ is a multiplication operator, and the exchange operator X_t is defined through its integral kernel $X_t(x,y) = \frac{1}{N} V(x-y)\omega_{N,t}(x,y)$. For the discussion in this section, N is a fixed parameter, and thus we also set the semiclassical parameter $\varepsilon = 1$ in this section.

The solution $\omega_{N,t}$ to the Hartree-Fock equation should for all times t be a fermionic one-particle density matrix, i. e. a selfadjoint trace class operator on $L^2(\mathbb{R}^3)$ with $0 \leq \omega_{N,t} \leq 1$. Typical initial data is given as a rank-N projection, $\omega_N = \sum_{i=1}^N |f_i\rangle\langle f_i|$, which is the one-particle reduced density matrix of the Slater determinant $A_N(f_1 \otimes \cdots \otimes f_N) \in L^2_a(\mathbb{R}^{3N})$. Here $(f_j)_{j=1}^N$ is an orthonormal system in $L^2(\mathbb{R}^3)$.

Let us now define the appropriate Banach spaces to rigorously solve the Cauchy problem, following [BdF76] and [BdF74]. Denoting by $\mathcal{S}_1(L^2(\mathbb{R}^3))$ the trace class operators on $L^2(\mathbb{R}^3)$, we define

$$H_1^{-\Delta} := \left\{ T \in \mathcal{S}_1(L^2(\mathbb{R}^3)) : T \text{ is selfadjoint and } (-\Delta+1)^{1/2} T (-\Delta+1)^{1/2} \in \mathcal{S}_1(L^2(\mathbb{R}^3)) \right\}.$$

This is analogous to Sobolev spaces for functions, and should be understood as the space of one-particle density matrices T with finite kinetic energy (formally the kinetic energy can be rewritten as $\mathrm{tr}(-\Delta)T = \mathrm{tr}(-\Delta)^{1/2}T(-\Delta)^{1/2}$ by cyclicity of the trace). Equipped with the norm $\|T\|_{1,-\Delta} := \mathrm{tr}|(-\Delta+1)^{1/2}T(-\Delta+1)^{1/2})|$, $H_1^{-\Delta}$ is a Banach space. We can consider the commutator with the Laplacian as an operator a, (formally) acting on $T \in H_1^{-\Delta}$ by $aT := i[-\Delta, T]$. We denote by $D(a) \subset H_1^{-\Delta}$ the domain of the operator a, as defined in [BdF76, Equation (4.2)], and equip $D(a)$ with the graph norm of a to make it a Banach space. One can easily check that e. g. for $T = \sum_{i=1}^N |f_i\rangle\langle f_i|$ with all $f_i \in H^3(\mathbb{R}^3)$ we have $T \in D(a)$.

We have the following result for global well-posedness.

Theorem 1.B.2 ([BdF76, Proposition 5.5 and Section 6])**.** *Assume $V : \mathbb{R}^3 \to \mathbb{R}$ is almost everywhere differentiable and satisfies $V^2 \leq C(-\Delta+1)$, for some $C > 0$.*

If $0 \leq \omega_N \leq \mathbb{1}$ and $\omega_N \in H_1^{-\Delta}$, then there exists a unique mild solution[14] $\omega_{N,(.)}$ to the Cauchy problem (1.71) *defined on all the positive real axis.*

Furthermore, if $\omega_N \in D(a)$, then the solution is the unique global classical solution, in the sense that

- *we have $\omega_{N,(.)} \in C^1\big([0,\infty), H_1^{-\Delta}\big)$ and $\omega_{N,(.)} \in C\big([0,\infty), D(a)\big)$;*
- *the Hartree-Fock equation* (1.71) *is explicitly satisfied.*

The assumption $V^2 \leq C(-\Delta+1)$ is easily checked to be satisfied with our assumptions of Theorem 3.3.1 on the potential. Consequently, for initial data $\omega_N \in D(a)$, all our calculations in Chapter 3 are valid. We notice that the earlier result of [BdF74], while it requires the potential V to be bounded (which is satisfied in Chapter 3), requires less regularity from the initial data. The result for Coulomb interaction given here is nevertheless of interest to us, since it shows that Hartree-Fock theory also in this case is well-defined, while we can not yet provide a proof of its validity.

The Hartree-Fock energy functional (1.21) can be generalized to

$$\begin{aligned}\mathcal{E}_{\mathrm{HF}}(\omega_N) = \mathrm{tr}(-\Delta)\omega_N &+ \frac{1}{2N}\int \mathrm{d}x\mathrm{d}y\, V(x-y)\omega_N(x,x)\omega_N(y,y)\\ &- \frac{1}{2N}\int \mathrm{d}x\mathrm{d}y\, V(x-y)|\omega_N(x,y)|^2.\end{aligned}$$

For $\omega_N = \sum_{i=1}^N |f_i\rangle\langle f_i|$ this coincides with $\mathcal{E}_{\mathrm{HF}}(f_1, \dots, f_N)$ given in (1.21). One has the well-known conservation laws of energy and number of particles,

$$\mathcal{E}_{\mathrm{HF}}(\omega_{N,t}) = \mathcal{E}_{\mathrm{HF}}(\omega_{N,0}), \quad \text{and} \quad \mathrm{tr}\,\omega_{N,t} = \mathrm{tr}\,\omega_{N,0}.$$

Furthermore, for initial data being a projection, also $\omega_{N,t}$ is a projection. This can be proven noticing that

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

[14] Mild solution means a solution to the variation-of-constant integral equation

$$\omega_{N,t}x = e^{it\Delta}\omega_N e^{-it\Delta}x + i\int_0^t e^{i(t-s)\Delta}[\omega_{N,s}, V*\rho_s - X_s]e^{-i(t-s)\Delta}x\,\mathrm{d}s \quad \text{for all } x \in L^2(\mathbb{R}^3).$$

and $(\omega_{N,0})^2 = \omega_{N,0}$; i. e. $(\omega_{N,t})^2$ solves the same Cauchy problem as $\omega_{N,t}$. Consequently, by uniqueness of the solution, we have $(\omega_{N,t})^2 = \omega_{N,t}$ for all times t. In particular, we obtain the useful fact that $0 \leq \omega_{N,t} \leq \mathbb{1}$ for all times t.

Pseudo-relativistic Hartree-Fock equations

In Chapter 4 we consider the pseudo-relativistic Hartree-Fock equation of the form

$$\begin{cases} i\partial_t \omega_{N,t} &= [\sqrt{-\Delta+1} + V * \rho_t - X_t, \omega_{N,t}], \\ \omega_{N,0} &= \omega_N, \end{cases} \tag{1.72}$$

As explained when we introduced the non-relativistic Hartree-Fock equation (1.24), for initial data given as a finite-rank projection (i. e. $\omega_N = \sum_{i=1}^N |\phi_i\rangle\langle\phi_i|$, which is the class of initial data relevant in this thesis), the density matrix formulation of the Hartree-Fock equation is equivalent to the Hartree-Fock equation for the orbitals,

$$\begin{cases} i\partial_t f_{i,t} &= \sqrt{-\Delta+1} f_{i,t} + \dfrac{1}{N}\displaystyle\sum_{j=1}^N \left(V * |f_{j,t}|^2\right) f_{i,t} - \dfrac{1}{N}\displaystyle\sum_{j=1}^N \left(V * (f_{i,t}\overline{f_{j,t}})\right) f_{j,t}, \\ f_{i,0} &= \phi_i \quad \text{for all } i = 1, \dots, N \end{cases} \tag{1.73}$$

The properties of the Hartree-Fock equation in orbital form (with Coulomb potential) are established in the literature [FL07, L07] and the methods can easily be applied to the equation with regular potential.

We first establish local well-posedness. Global well-posedness will be obtained from the conservation laws. Local well-posedness for the semi-relativistic Hartree-Fock equations with Coulomb interaction was proven as a side-result in [FL07], essentially reducing it to proving a local Lipschitz condition on the non-linearity, which in turn follows along the lines of [L07]. We assume

$$V \in L^1(\mathbb{R}^3) \quad \text{and} \quad \int |\widehat{V}(p)|(1+|p|)^2 \mathrm{d}p < \infty, \tag{1.74}$$

which makes the problem less delicate than it is for the Coulomb potential. The case $s = 1$ of the following theorem is needed in Chapter 4.

Theorem 1.B.3. *Suppose $s \geq 1/2$ and that (1.74) holds. Let $\boldsymbol{\phi} = (\phi_k)_{k=1}^N$ be a collection of initial data with $\phi_k \in H^s(\mathbb{R}^3)$ for all $k = 1, \dots, N$.*

Then there exists a unique solution $\boldsymbol{f}_{(.)} = \left(f_{k,(.)}\right)_{k=1}^N$ to the orbital Hartree-Fock equations (1.73) with $f_{k,0} = \phi_k$ such that

$$f_{k,(.)} \in C^0\left([0,T), H^s(\mathbb{R}^3)\right) \cap C^1\left([0,T), H^{s-1}(\mathbb{R}^3)\right) \quad \text{for all } k = 1, \dots, N.$$

Here $T \in (0,\infty]$ is the maximal time of existence, and we have the blow-up alternative: If $T < \infty$, then $\lim_{t\to T-} \sum_{k=1}^N \|f_{k,t}\|_{H^{1/2}} = \infty$.

Additionally, $\boldsymbol{f}_{(.)}$ depends continuously on the initial data $\boldsymbol{\phi}$ and we have the conservation laws that for all $0 \leq t < T$

- *$\mathcal{E}_{HF}(\boldsymbol{f}_t) = \mathcal{E}_{HF}(\boldsymbol{\phi})$ (where $\mathcal{E}_{HF}$ was defined in (1.21)),*
- *$\langle f_{k,t}, f_{l,t}\rangle = \langle \phi_k, \phi_l\rangle$ for all $k, l \in \{1, \dots, N\}$.*

Here $\boldsymbol{f}_{(.)}$ is a solution in the sense that (1.73) is satisfied in the space of distributions $H^{s-1}(\mathbb{R}^3)$, the relevant case for us being $s = 1$.

The proof of Theorem 1.B.3 follows the strategy of [FL07] and reduces the problem to proving the following local Lipschitz condition:

Lemma 1.B.4. *Suppose that* (1.74) *holds. Let* $\boldsymbol{F} := (F_1, \dots, F_N)$ *be a Hartree-Fock-like non-linearity, i. e. for* $\boldsymbol{f} = (f_k)_{k=1}^N$

$$F_k(\boldsymbol{f}) := \sum_{j=1}^N \left(V * |f_j|^2\right) f_k - \sum_{j=1}^N \left(V * \left(f_k \overline{f_j}\right)\right) f_j.$$

Let $s \geq 1/2$. *Then for all* $\boldsymbol{f}, \boldsymbol{g} \in H^{s,N}$ *and* $r = \max(s-1, 1/2)$ *we have*

$$\begin{aligned} \|\boldsymbol{F}(\boldsymbol{f}) - \boldsymbol{F}(\boldsymbol{g})\|_{H^{s,N}} &\leq C \left(\|\boldsymbol{f}\|_{H^{s,N}}^2 + \|\boldsymbol{g}\|_{H^{s,N}}^2\right) \|\boldsymbol{f} - \boldsymbol{g}\|_{H^{s,N}}, \\ \|\boldsymbol{F}(\boldsymbol{f})\|_{H^{s,N}} &\leq C \|\boldsymbol{f}\|_{H^{r,N}}^2 \|\boldsymbol{f}\|_{H^{s,N}}. \end{aligned} \tag{1.75}$$

Here $H^{s,N}$ *is the* N*-fold cartesian product of* $H^s(\mathbb{R}^3)$ *equipped with the norm* $\|\boldsymbol{f}\|_{H^{s,N}} := \left(\sum_{k=1}^N \|f_k\|_{H^s}^2\right)^{1/2}$.

The proof of this lemma follows the strategy of [L07, Lemma 1] but is slightly simpler since we have $\|(1-\Delta)^\alpha V\|_\infty < \infty$ for all $0 \leq \alpha \leq 1$.

For the regular potentials we consider, the pseudo-relativistic Hartree-Fock equation is always globally well-posed. In fact, direct and exchange term in the Hartree-Fock energy functional both are bounded below since $\|V\|_\infty < \infty$. This provides a bound on the $H^{1/2}$-norm in terms of the conserved total energy and thus global well-posedness. (In the repulsive case, even with a singular potential, global well-posedness follows from local well-posedness due to the fact that the sum of direct and exchange term in the energy is non-negative if $V \geq 0$, so that the conserved energy (4.4) provides a bound on the $H^{1/2}$-norm.)

Notice however that there has been interest in the pseudo-relativistic Hartree-Fock equation with attractive Coulomb potential, in which case the equation has blow-up solutions. These solutions describe stars collapsing under gravitational attraction [HS09]; see also [FL07]. Under our assumptions on the potential there is no blow-up.

1.C. Remarks on notation

Generally we use a plain $\|x\|$ when we use the norm of the space in which x lives. In this thesis, these are typically L^2 spaces of wave functions, $L^2(\mathbb{R}^3)$ or $L^2(\mathbb{R}^{3N})$, or fermionic or bosonic Fock space. Norms of L^p spaces are denoted by $\|\cdot\|_p$, where $1 \leq p \leq \infty$.

We denote by $H^s(\mathbb{R}^n)$ the Sobolev space of functions that have s derivatives in $L^2(\mathbb{R}^n)$, and $s \geq 0$ is allowed to have non-integer values. The Sobolev norms are denoted by $\|\cdot\|_{H^s}$.

The operator norm is also denoted by $\|\cdot\|$. Important other norms on operators are the Hilbert-Schmidt norm, denoted by $\|\cdot\|_{\mathrm{HS}}$, or by $\|\cdot\|_2$ when we think about the integral kernel of the operator. The trace norm is denoted by $\operatorname{tr}|\cdot|$. In general $\|A\| \leq \|A\|_{\mathrm{HS}} \leq \operatorname{tr}|A|$. We also have the useful estimates $\operatorname{tr}|AB| \leq \|A\| \operatorname{tr}|B|$, $\|AB\|_{\mathrm{HS}} \leq \|A\| \|B\|_{\mathrm{HS}}$. We caution the reader that in general, even if A has a sufficiently regular integral kernel $a(x,x)$ to define the integral, nevertheless $\operatorname{tr}|A| \neq \int \mathrm{d}x |a(x,x)|$.

We use the Dirac notation for projection operators, i. e. for ψ a vector in a Hilbert space $\mathfrak{h}$, $|\psi\rangle\langle\psi|$ is the operator acting on $f \in \mathfrak{h}$ by $|\psi\rangle\langle\psi| f = \langle\psi, f\rangle \psi$. For multiplication operators, we use the same letter to denote the operator as for the corresponding function.

The time-dependence is generally denoted with a subscript, i. e. u_t instead of $u(t)$. Derivatives are explicitly written as ∂_t or $\mathrm{d}/\mathrm{d}t$. We sometimes write $u_{(.)}$ and similar expressions when we want to highlight that we consider u as a function of the argument in the place indicated by (.).

We use the symbol C (and sometimes K and D) for constants that can change from step to step. Dependencies on other quantities are mentioned when relevant. If it is necessary to fix a specific constant, we introduce the constant explicitly and denote it by e. g. C_1, C_2, ...

For tensor products we use the shorthand $\varphi^{\otimes N}$ to mean $\bigotimes_{i=1}^N \varphi$, and similarly $L^2(\mathbb{R}^3)^{\otimes N}$ for $\bigotimes_{i=1}^N L^2(\mathbb{R}^3)$ and $|\varphi\rangle\langle\varphi|^{\otimes k}$ for $|\varphi\rangle\langle\varphi| \otimes |\varphi\rangle\langle\varphi| \otimes \cdots \otimes |\varphi\rangle\langle\varphi|$.

We use $[A, B] = AB - BA$ for the commutator of two operators A and B (domain questions should be clear from the context) and $\{A, B\} AB + BA$ for the anticommutator.

2. Quantitative Derivation of the Gross-Pitaevskii Equation

In this chapter we prove that the evolution of the condensate of a dilute Bose gas can be described with the time-dependent Gross-Pitaevskii equation. This chapter closely follows the article [BdS12].

We use the bosonic convention tr $\gamma_N^{(k)} = 1$ for the normalization of density matrices, see Section 1.A.

2.1. Introduction

To give the reader a heuristic understanding of the difficulties of the problem, we start by reviewing the BBGKY hierarchy method, on which the first derivations of the Gross-Pitaevskii equation were based. As a key idea, this discussion suggests to not directly compare to the Gross-Pitaevskii equation but to use the modified Gross-Pitaevskii equation (2.4) in a first step and obtain cancellations from the zero-energy scattering equation.

Afterwards, in Subsection 2.1.2, we explain our new approach, based on modeling the correlation structure with Bogoliubov transformations, and then give the statement of our main results.

2.1.1. The BBGKY hierarchy

The use of the BBGKY hierarchy for deriving effective evolution equations from many-body quantum mechanics goes back to the derivation of the Hartree equation for the mean-field limit. The first rigorous derivation of the Hartree equation (1.39) was obtained by this method in [S80] for bounded interaction potentials. The basic idea is to study directly the time-evolution of the family of reduced densities $\gamma_{N,t}^{(k)}$, $k = 1, 2, \ldots, N$.

Rewriting the Schrödinger equation (with mean-field Hamiltonian (1.3), with $V_{\text{ext}} = 0$) in terms of the density matrix $\gamma_{N,t}^{(N)} = |\psi_{N,t}\rangle\langle\psi_{N,t}|$ as

$$i\partial_t \gamma_{N,t}^{(N)} = [H_N, \gamma_{N,t}^{(N)}]$$

and taking the partial trace, one derives a hierarchy[1] of N coupled equations, known as the Bogoliubov–Born–Green–Kirkwood–Yvon hierarchy:

$$i\partial_t \gamma_{N,t}^{(k)} = \sum_{j=1}^{k} \left[-\Delta_j, \gamma_{N,t}^{(k)}\right] + \frac{1}{N}\sum_{i<j}^{k} \left[V(x_i - x_j), \gamma_{N,t}^{(k)}\right] + \frac{N-k}{N}\sum_{j=1}^{k} \operatorname{tr}_{k+1}\left[V(x_j - x_{k+1}), \gamma_{N,t}^{(k+1)}\right],$$

[1]The system is called a hierarchy because the equation for $\gamma_{N,t}^{(k)}$ depends on $\gamma_{N,t}^{(k+1)}$.

for $k = 1, \dots N$, with the convention that $\gamma_{N,t}^{(k)} = 0$ for $k > N$, and with tr_{k+1} the partial trace over the $(k+1)$-th factor of the tensor product.

As $N \to \infty$, the BBGKY hierarchy converges, at least formally, towards an infinite hierarchy of coupled equations. The limiting hierarchy is solved by tensor products $|\varphi_t\rangle\langle\varphi_t|^{\otimes k}$ of the projection on the solution φ_t of the Hartree equation (1.39). Thus the problem of proving the convergence towards the Hartree dynamics in the sense $\gamma_{N,t}^{(1)} \to |\varphi_t\rangle\langle\varphi_t|$ essentially reduces to showing the uniqueness of the solution of the infinite hierarchy.

This scheme was later extended to potentials with Coulomb singularities in [EY01] (and in [ES07] to bosons with relativistic dispersion relation).

In [ESY06b, ESY10, ESY07, ESYS09], the same strategy was then applied to analyze the dynamics in the Gross-Pitaevskii regime (1.15) and to obtain a rigorous derivation of the Gross-Pitaevskii equation (1.16).

The BBGKY hierarchy nicely shows the effect of correlations in the dynamical setting, as we will discuss in the rest of this subsection. Writing (1.15) as

$$H_N = \sum_{j=1}^{N} -\Delta_{x_j} + \frac{1}{N}\sum_{i<j}^{N} N^3 V(N(x_i - x_j)), \tag{2.1}$$

one can formally interpret the Gross-Pitaevskii regime as a very singular mean-field scaling, where the interaction potential $N^3V(N.)$ converges to a delta distribution as $N \to \infty$. However, as explained on the level of energies (see Eq. (1.14) and the discussion following it), unlike in the mean-field regime correlations play a crucial role in the Gross-Pitaevskii regime. To understand the role of correlations for the dynamics, let us consider the evolution of the one-particle reduced density $\gamma_{N,t}^{(1)}$ according to the BBGKY hierarchy:

$$\begin{aligned} &i\partial_t \gamma_{N,t}^{(1)}(x,x') \\ &= \left(-\Delta_x + \Delta_{x'}\right)\gamma_{N,t}^{(1)}(x,x') \\ &\quad + \int \mathrm{d}x_2\, \big((N-1)N^2V(N(x-x_2)) - (N-1)N^2V(N(x'-x_2))\big)\,\gamma_{N,t}^{(2)}(x,x_2,x',x_2). \end{aligned} \tag{2.2}$$

Assuming that the initial data exhibits complete condensation and that condensation is preserved by the time evolution, we expect $\gamma_{N,t}^{(1)}$ and $\gamma_{N,t}^{(2)}$ to be approximately factorized. In $\gamma_{N,t}^{(2)}$, however, one also wants to take into account the two-particle correlations. Describing the correlations through the solution f of the zero-energy scattering equation (1.10), we use the ansatz

$$\begin{aligned} \gamma_{N,t}^{(1)}(x,x') &\simeq \varphi_t(x)\overline{\varphi}_t(x'), \\ \gamma_{N,t}^{(2)}(x_1,x_2,x_1',x_2') &\simeq f(N(x_1-x_2))f(N(x_1'-x_2'))\,\varphi_t(x_1)\varphi_t(x_2)\overline{\varphi}_t(x_1')\overline{\varphi}_t(x_2'). \end{aligned} \tag{2.3}$$

Plugging this into (2.2), we obtain a new non-linear equation for φ_t (we call it the modified Gross-Pitaevskii equation), given by

$$i\partial_t\varphi_t = -\Delta\varphi_t + \left(N^2(N-1)V(N.)f(N.) * |\varphi_t|^2\right)\varphi_t. \tag{2.4}$$

Since $8\pi a_0 = \int Vf\mathrm{d}x$, we formally have $N^2(N-1)V(Nx)f(Nx) \to 8\pi a_0\delta(x)$ as $N \to \infty$. Therefore, in the limit, φ_t should be a solution of the Gross-Pitaevskii equation (1.16), complementing the results for the ground state energy (c. f. (1.14)).

The presence of the factor $f(N.)$ is crucial in this argument to understand the emergence of the scattering length in the Gross-Pitaevskii equation. We conclude that any derivation of the Gross-Pitaevskii equation must take into account the correlation structure. In fact, understanding the correlations and adapting the techniques of [S80, EY01, ES07] to deal with them was one of the main challenges in [ESY06a, ESY06b, ESY10, ESY07, ESYS09].

2.1.2. Strategy and main results

Before stating the main result of this Chapter, let us discuss the strategy followed.

In view of Section 1.4 we intend to use coherent states to obtain a derivation of the Gross-Pitaevskii equation (1.16) and bounds on the rate of the convergence. Recall the approach to the mean-field regime explained in Section 1.4. From (1.46), we notice that there are two contributions to the generator $\mathcal{L}_N(t)$, one arising from the derivative of the Weyl operator $W^*(\sqrt{N}\varphi_t)$, the other from the derivative of $e^{-i(t-s)\mathcal{H}_N}$:

$$\mathcal{L}_N(t) = \left(i\partial_t W^*(\sqrt{N}\varphi_t)\right) W(\sqrt{N}\varphi_t) + W^*(\sqrt{N}\varphi_t)\mathcal{H}_N W(\sqrt{N}\varphi_t).$$

The second contribution, given by $W^*(\sqrt{N}\varphi_t)\mathcal{H}_N W(\sqrt{N}\varphi)$, can be computed recalling that Weyl operators act as shifts on creation and annihilation operators (see (1.40)). It turns out that this contribution contains a term, linear in creation and annihilation operators, which has the form

$$\sqrt{N}\int \mathrm{d}x \left[-\Delta\varphi_t(x) + (V * |\varphi_t|^2)(x)\varphi_t(x)\right] a_x^* + \text{h.c.} \tag{2.5}$$

This term is large (of order $N^{1/2}$) and does not commute with the number operator. With such a term in the generator, it would be impossible to show uniform (in N) bounds for the growth of the number of particles

$$\left\langle U_N(t,0)\Omega, \mathcal{N} U_N(t,0)\Omega\right\rangle.$$

In the mean-field regime however, (2.5) is exactly canceled by the contribution proportional to the derivative of $W^*(\sqrt{N}\varphi_t)$, which contains the term

$$-\sqrt{N}\int \mathrm{d}x\,(i\partial_t\varphi_t(x))a_x^* - \text{h.c.} = -\sqrt{N}\int \mathrm{d}x \left[-\Delta\varphi_t(x) + (V * |\varphi_t|^2)(x)\varphi_t(x)\right] a_x^* - \text{h.c.}$$

where we used the Hartree equation (1.39). As a result, the generator $\mathcal{L}_N(t)$ in (1.46) contains only terms which, at least formally, are order one or smaller.

To adapt this approach to the Gross-Pitaevskii regime, we lift the Hamiltonian to Fock space $\mathcal{F}$ as

$$\mathcal{H}_N = \int \mathrm{d}x\, \nabla_x a_x^* \nabla_x a_x + \frac{1}{2}\int \mathrm{d}x\mathrm{d}y N^2 V(N(x-y)) a_x^* a_y^* a_y a_x \tag{2.6}$$

and, following (1.41), we naively introduce the fluctuation dynamics

$$\mathcal{U}^{\text{GP}}(t,s) = W^*(\sqrt{N}\varphi_t^{(N)}) e^{-i(t-s)\mathcal{H}_N} W(\sqrt{N}\varphi_t^{(N)}). \tag{2.7}$$

As discussed in Subsection 2.1.1, we choose $\varphi_t^{(N)}$ to solve the modified Gross-Pitaevskii equation[2]

$$i\partial_t\varphi_t^{(N)} = -\Delta\varphi_t^{(N)} + \left(N^3 V(N.) f(N.) * |\varphi_t^{(N)}|^2\right)\varphi_t^{(N)} \tag{2.8}$$

[2]From now on we use the notation $\varphi_t^{(N)}$ to distinguish the solution of the modified Gross-Pitaevskii equation (2.8) from the solution φ_t of the Gross-Pitaevskii equation (1.16).

where f is the solution of the zero-energy scattering equation (1.10). Since the solution of the modified Gross-Pitaevskii equation (2.8) can be shown to converge towards the solution of the Gross-Pitaevskii equation (1.16) with an error of order N^{-1} (see Proposition 2.3.1 (iv)), control of the fluctuations around the modified Gross-Pitaevskii equation also implies control of the fluctuations around the Gross-Pitaevskii equation. Let $\mathcal{L}_N^{\mathrm{GP}}(t)$ denote the generator of (2.7), given by

$$\mathcal{L}_N^{\mathrm{GP}}(t) = \left(i\partial_t W^*(\sqrt{N}\varphi_t^{(N)})\right) W(\sqrt{N}\varphi_t^{(N)}) + W^*(\sqrt{N}\varphi_t^{(N)})\mathcal{H}_N W(\sqrt{N}\varphi_t^{(N)}). \tag{2.9}$$

As in the mean-field regime, the term $W^*(\sqrt{N}\varphi_t^{(N)})\mathcal{H}_N W(\sqrt{N}\varphi_t^{(N)})$ contains a large contribution which is linear in creation and annihilation operators and given by

$$\sqrt{N}\int \mathrm{d}x \left[-\Delta\varphi_t^{(N)}(x) + (N^3V(N.) * |\varphi_t^{(N)}|^2)(x)\varphi_t^{(N)}(x)\right] a_x^* + \mathrm{h.c.}$$

On the other hand, the term $(i\partial_t W^*(\sqrt{N}\varphi_t^{(N)}))W(\sqrt{N}\varphi_t^{(N)})$ contains the linear summand

$$\begin{aligned} &-\sqrt{N}\int \mathrm{d}x\big[(i\partial_t\varphi_t^{(N)}(x))a_x^* + \mathrm{h.c.}\big] \\ &= -\sqrt{N}\int \mathrm{d}x \left[-\Delta\varphi_t^{(N)}(x) + (N^3V(N.)f(N.)|\varphi_t^{(N)}(x)|^2\varphi_t^{(N)}(x)\right] a_x^* - \mathrm{h.c.} \end{aligned}$$

In contrast to the mean-field regime discussed above, here there is no complete cancellation between the two large linear terms (because of the factor f in the second term). Hence, the generator $\mathcal{L}_N^{\mathrm{GP}}(t)$ of (2.7) contains a large contribution which is linear in the creation and annihilation operators and of the form

$$\sqrt{N}\int \mathrm{d}x \left(N^3V(N.)(1-f(N.)) * |\varphi_t^{(N)}|^2\right)(x)\left(\varphi_t^{(N)}(x)a_x^* + \mathrm{h.c.}\right). \tag{2.10}$$

Due to this term it seems impossible to obtain a uniform (in N) bound on the growth of the number of particles w. r. t. the fluctuation dynamics (2.7).

From a physical point of view, the reason for this failure is that we are trying to control fluctuations around the wrong evolution. When we approximate $e^{-it\mathcal{H}_N}W(\sqrt{N}\varphi)\psi$ by an evolved coherent state $W(\sqrt{N}\varphi_t^{(N)})\psi$, we completely neglect the correlation structure developed by the many-body evolution. As a result, fluctuations around the coherent approximation $W(\sqrt{N}\varphi_t^{(N)})\psi$ are too strong to be bounded uniformly in N. Since correlations are in first order an effect of two-body interactions, we are going to approximate them using the unitary operator

$$T(k) = \exp\left(\frac{1}{2}\int \mathrm{d}x\mathrm{d}y\left(k(x,y)a_x^*a_y^* - \overline{k}(x,y)a_x a_y\right)\right)$$

for an appropriate $k \in L^2(\mathbb{R}^3 \times \mathbb{R}^3)$, which will be interpreted as the integral kernel of a Hilbert-Schmidt operator (again denoted by k) on $L^2(\mathbb{R}^3)$. Recall from Section 1.5 that the operator $T(k)$ acts on creation and annihilation operators as a Bogoliubov transformation

$$\begin{aligned} T^*(k)a(f)T(k) &= a(\mathrm{ch}(k)(f)) + a^*(\mathrm{sh}(k)(\overline{f})), \\ T^*(k)a^*(f)T(k) &= a^*(\mathrm{ch}(k)(f)) + a(\mathrm{sh}(k)(\overline{f})), \end{aligned}$$

where ch(k) and sh(k) are the bounded operators on $L^2(\mathbb{R}^3)$ defined by the absolutely convergent series (where products of k and $\overline{k}$ are in the sense of operators)

$$\mathrm{ch}(k) = \sum_{n\geq 0} \frac{1}{(2n)!}(k\overline{k})^n \qquad \text{and} \qquad \mathrm{sh}(k) = \sum_{n\geq 0} \frac{1}{(2n+1)!}(k\overline{k})^n k.$$

(For a heuristic picture, it is often sufficient to think of the leading terms only, i. .e. $\mathrm{ch}(k) \simeq \mathbb{1}$ and $\mathrm{sh}(k) \simeq k$, and in fact we will treat the higher powers as error terms. In particular

$$T^* a_x^* T \simeq a_x^* + a(k(,x)),$$

showing that the contribution of the creation operator is singular while the annihilation operator is regularized by k.)

Inspired by the discussion in Section 2.1.1, where correlations were successfully described by the solution of the zero-energy scattering equation, we define the time-dependent kernel

$$k_t(x,y) = -Nw(N(x-y))\varphi_t^{(N)}(x)\varphi_t^{(N)}(y), \tag{2.11}$$

where $\varphi_t^{(N)}$ is the solution of the modified Gross-Pitaevskii equation (2.8), and where

$$w(x) = 1 - f(x),$$

with f the solution of the zero-energy scattering equation (1.10). We will consider a initial data of the form $W(\sqrt{N}\varphi)T(k_0)\psi$, for $\psi \in \mathcal{F}$ with bounded number of particles and bounded energy (think of the vacuum, $\psi = \Omega$), and we will approximate its time evolution by $W(\sqrt{N}\varphi_t)T(k_t)\psi$, leading to the fluctuation dynamics

$$\mathcal{U}(t,s) = T^*(k_t)W^*(\sqrt{N}\varphi_t)e^{-i(t-s)\mathcal{H}_N}W(\sqrt{N}\varphi_s)T(k_s). \tag{2.12}$$

In this way, the approximating dynamics takes into account the correlation structure and we expect that the fluctuations are bounded. Indeed, we will show in Section 2.4 that it is possible to obtain a uniform (in N) control for the growth of the number of particles

$$\langle \mathcal{U}(t,0)\Omega, \mathcal{N}\mathcal{U}(t,0)\Omega \rangle.$$

To understand this, notice that the evolution $\mathcal{U}(t,s)$ has the generator

$$\begin{aligned}\mathcal{L}_N(t) = T^*(k_t)\Big[\Big(i\partial_t W^*(\sqrt{N}\varphi_t^{(N)})\Big)W(\sqrt{N}\varphi_t^{(N)}) + W^*(\sqrt{N}\varphi_t^{(N)})\mathcal{H}_N W(\sqrt{N}\varphi_t^{(N)})\Big]T(k_t)\\ + \left(i\partial_t T^*(k_t)\right)T(k_t).\end{aligned}$$

We will show that the summand $\left(i\partial_t T^*(k_t)\right)T(k_t)$ does not play a role, see Proposition 2.6.10. Notice that the first line in the generator is of the same form as the generator (2.9), just conjugated with the Bogoliubov transformation $T(k_t)$. In particular, the large linear (in creation/annihilation operators) contribution (2.10) still appears, but it is compensated by a contribution arising from conjugating the cubic (in creation/annihilation operators) term in $W^*(\sqrt{N}\varphi_t^{(N)})\mathcal{H}_N W(\sqrt{N}\varphi_t^{(N)})$ with the Bogoliubov transformation. More precisely, after conjugating with the Bogoliubov transformation, some of the cubic terms will not be in normal-order. By the canonical commutation relations, bringing them into normal-order produces terms which are linear in creation and annihilation operators; some of these terms cancel exactly the large contribution (2.10). Other important cancellations will emerge between the quadratic and the non-normal-ordered quartic terms; see Section 2.6 for the details. The control of the growth of the number of particles w. r. t. (2.12) will imply convergence of the one-particle reduced density matrix associated with the fully evolved Fock space vector $e^{-i\mathcal{H}_N t}W(\sqrt{N}\varphi_t)T(k_t)\psi$ towards the orthogonal projection onto the solution of the Gross-Pitaevskii equation (1.16), with a bound on the rate of the convergence.

The main theorem. Recall that the one-particle reduced density associated with a Fock space vector Ψ is defined by the integral kernel

$$\gamma_\Psi^{(1)}(x,y) = \frac{1}{\langle \Psi, \mathcal{N}\Psi\rangle} \left\langle \Psi, a_y^* a_x \Psi \right\rangle . \tag{2.13}$$

We are now ready to state our main result.

Theorem 2.1.1. *Let $\varphi \in H^4(\mathbb{R}^3)$, with $\|\varphi\|_2 = 1$. Let $\mathcal{H}_N$ be the Hamilton operator defined in equation (2.6), with a non-negative and spherically symmetric interaction potential $V \in L^1 \cap L^3(\mathbb{R}^3, (1+|x|^6)dx)$. Let $\psi \in \mathcal{F}$ (possibly depending on N) be such that*

$$\langle \psi, \mathcal{N}\psi\rangle, \frac{1}{N}\langle \psi, \mathcal{N}^2\psi\rangle, \langle \psi, \mathcal{H}_N\psi\rangle \leq D \tag{2.14}$$

for a constant $D > 0$. Let $\gamma_{N,t}^{(1)}$ denote the one-particle reduced density associated with the evolved vector $e^{-i\mathcal{H}_N t}W(\sqrt{N}\varphi)T(k_0)\psi$. Then there exist constants $C, c_1, c_2 > 0$, depending only on $V, \|\varphi\|_{H^4}$ and on the constant D appearing in (2.14), such that

$$\operatorname{tr}\left|\gamma_{N,t}^{(1)} - |\varphi_t\rangle\langle\varphi_t|\right| \leq \frac{C\exp(c_1\exp(c_2|t|))}{N^{1/2}} \tag{2.15}$$

for all $t \in \mathbb{R}$ and $N \in \mathbb{N}$. Here φ_t denotes the solution of the time-dependent Gross-Pitaevskii equation

$$i\partial_t\varphi_t = -\Delta\varphi_t + 8\pi a_0|\varphi_t|^2\varphi_t \tag{2.16}$$

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

Remarks.

(i) Let us point out that we insert the correct correlation structure in the initial data. Our result implies the approximate stability of vectors of the form $W(\sqrt{N}\varphi)T(k_0)\psi$ with respect to the many-body evolution (in the sense that the evolution of $W(\sqrt{N}\varphi)T(k_0)\psi$ has approximately the same form, just with evolved φ_t, up to a small error). It does not imply, on the other hand, that the correlation structure is produced by the time-evolution. This is in contrast with the results of [ESY06b, ESY10, ESY07, ESYS09], which can also be applied to completely factorized initial data. It remains unclear, however, if it is possible to obtain convergence with a $N^{-1/2}$ rate (or with any rate) for initial data with no correlations (the problem of the creation of correlations was studied in [EMS06]).

(ii) Initial data of the form $W(\sqrt{N}\varphi)T(k_0)\psi$, with ψ satisfying (2.14), arise naturally as approximation for the ground state of the Hamiltonian

$$\mathcal{H}_N^{\text{trap}} = \int \mathrm{d}x\, a_x^* \left(-\Delta_x + V_{\text{ext}}(x)\right) a_x + \frac{1}{2}\int \mathrm{d}x\mathrm{d}y\, N^2V(N(x-y))a_x^*a_y^*a_ya_x\,,$$

describing a Bose gas trapped by a confining potential V_{ext}, when the chemical potential is tuned so that the expected number of particles is N (the number of particles in $W(\sqrt{N}\varphi)T(k_0)\psi$ concentrates around N, up to errors of order $\sqrt{N}$). Hence, $W(\sqrt{N}\varphi)T(k_0)\psi$ models the state prepared in experiments by cooling the trapped Bose gas to very low temperatures. In fact, combining the results of Propositions 2.6.1, 2.6.3, 2.6.5 and 2.6.6, and assuming $\psi \in \mathcal{F}$ to satisfy (2.14) (with $\mathcal{H}_N$ replaced by $\mathcal{H}_N^{\text{trap}}$), one can easily show that

$$\begin{aligned}&\left\langle W(\sqrt{N}\varphi)T(k_0)\psi, \mathcal{H}_N^{\text{trap}} W(\sqrt{N}\varphi)T(k_0)\psi \right\rangle \\ &\qquad = N\left[\int \mathrm{d}x \, \left(|\nabla\varphi(x)|^2 + V_{\text{ext}}(x)|\varphi(x)|^2 + 4\pi a_0|\varphi(x)|^4\right)\right] + O(\sqrt{N}) \\ &\qquad = N\mathcal{E}_{\text{GP}}(\varphi) + O(\sqrt{N})\end{aligned}$$

with the Gross-Pitaevskii energy functional defined in (1.14). Choosing φ as the normalized minimizer of $\mathcal{E}_{\text{GP}}$, it follows from [LSY00] that $W(\sqrt{N}\varphi)T(k_0)\psi$ has, in leading order, the energy of the ground state.

(iii) The time dependence on the r. h. s. of (2.15) deteriorates fast for large t. This however is just a consequence of the fact that, in general, high Sobolev norms of the solution of (2.16) can grow exponentially fast. Assuming a uniform bound for $\|\varphi_t\|_{H^4}$, the time dependence on the r. h. s. of (2.15) can be replaced by $C\exp(K|t|)$.

(iv) To simplify a little bit the computations, we did not include an external potential in the Hamiltonian (2.6) generating the evolution on the Fock space. In contrast to [ESY06b, ESY10, ESY07, ESYS09], the approach presented in this paper can be extended with no additional complication to Hamilton operators with external potential. This remark is important to describe experiments where the evolution of the condensate is observed after tuning the traps, rather than switching them off.

(v) The convergence (2.15) and the fact that the limit is a rank-one projection immediately implies convergence of the higher order reduced density $\gamma_{N,t}^{(k)}$ associated with the evolved vector $\Psi_{N,t} = e^{-i\mathcal{H}_N t}W(\sqrt{N}\varphi)T(k_0)\psi$. Following the arguments in [KP10, Section 2], the bound (2.15) implies that, for every $k \in \mathbb{N}$,

$$\operatorname{tr}\left|\gamma_{N,t}^{(k)} - |\varphi_t\rangle\langle\varphi_t|^{\otimes k}\right| \le C\frac{k^{1/2}}{N^{1/4}}\exp\left(\frac{c_1}{2}\exp(c_2|t|)\right).$$

To obtain bounds for the convergence of the k-particle reduced density with the same $N^{-1/2}$ rate as in (2.15), following the same approach used below to study $\gamma_{N,t}^{(1)}$ would require to control the growth of higher powers of the number of particle operator with respect to the fluctuation dynamics (2.12). This may be doable, but the analysis becomes more involved.

(vi) Theorem 2.1.1 and the method used in its proof can also be applied to deduce the convergence towards the Gross-Pitaevskii dynamics for certain initial data with exact number of particles. In Appendix 2.C, we consider initial N-particle wave functions of the form $P_N W(\sqrt{N}\varphi)T(k_0)\psi$, for $\psi \in \mathcal{F}$ satisfying (2.14), assuming that we have $\|P_N W(\sqrt{N}\varphi)T(k_0)\psi\| \gg N^{-1/2}$ for large N (it is explained in Appendix 2.C why this is a reasonable condition). Here P_N denotes the orthogonal projection onto the

N-particle sector of $\mathcal{F}$. It remains to be understood which class of N-particle vectors can be written as $P_N W(\sqrt{N}\varphi)T(k_0)\psi$, for a $\psi \in \mathcal{F}$ satisfying (2.14).

2.2. Lifting the evolution to Fock space

To define an evolution on Fock space, we lift the Hamilton operator to Fock space like in Section 1.3. We define

$$(\mathcal{H}_N\psi)^{(n)} = \mathcal{H}_N^{(n)}\psi^{(n)}$$

with the operator on the n-th sector defined as

$$\mathcal{H}_N^{(n)} = \sum_{j=1}^{n} -\Delta_{x_j} + \sum_{i<j}^{n} N^2 V(N(x_i - x_j)).$$

Note that the subscript N in the notation $\mathcal{H}_N$ is not related to the number of particles (which is not fixed on Fock space), but only reflects the scaling of the interaction potential. Of course, we will relate the number of particles in the initial Fock space vector to N by choosing the initial Fock space vector to have expected number of particles close to N; otherwise, there would be no relation with the regime discussed in Section 2.1. Since $\mathcal{H}_N$ commutes with $\mathcal{N}$, the evolution generated by $\mathcal{H}_N$ leaves each n-particle sector invariant and we have

$$e^{-i\mathcal{H}_N t}(0,\dots,0,\psi_N,0,\dots) = (0,\dots,0,e^{-iH_N t}\psi_N,0,\dots)$$

where H_N is the N-particle Hamiltonian defined in (1.15). In this sense, the N-body dynamics is embedded in the Fock space representation.

As discussed in Section 1.3, the Hamilton operator $\mathcal{H}_N$ can be written as

$$\mathcal{H}_N = \int \mathrm{d}x\, \nabla_x a_x^* \nabla_x a_x + \frac{1}{2}\int \mathrm{d}x\mathrm{d}y\, N^2 V(N(x-y)) a_x^* a_y^* a_y a_x. \tag{2.17}$$

The first term in the Hamiltonian is the kinetic energy; since it will play an important role in our analysis, we introduce the notation

$$\mathcal{K} = \int \mathrm{d}x\, \nabla_x a_x^* \nabla a_x.$$

Note that, like $\mathcal{H}_N$, $\mathcal{K}$ leaves every n-particle sector invariant, and for $\psi \in \mathcal{F}$

$$(\mathcal{K}\psi)^{(n)} = \sum_{j=1}^{n} -\Delta_{x_j}\psi^{(n)}.$$

The kinetic energy operator can also be written as $\mathcal{K} = \mathrm{d}\Gamma(-\Delta)$.

2.2.1. Bogoliubov transformations implementing correlations

As explained before, we are interested in Bogoliubov transformations implemented by operator exponentials with exponent quadratic in creation and annihilation operators. We think of these Bogoliubov transformations as implementing two-particle correlations. We will now give a rigorous discussion of the Bogoliubov transformations we use.

For a kernel $k \in L^2(\mathbb{R}^3 \times \mathbb{R}^3)$ with $k(x,y) = k(y,x)$, we define the operator

$$T(k) = \exp\left(\frac{1}{2}\int \mathrm{d}x\mathrm{d}y \, \left(k(x,y)a_x^* a_y^* - \overline{k}(x,y)a_x a_y\right)\right) \tag{2.18}$$

acting on the Fock space $\mathcal{F}$.

Lemma 2.2.1. *Let $k \in L^2(\mathbb{R}^3 \times \mathbb{R}^3)$ be symmetric, in the sense that $k(x,y) = k(y,x)$.*

(i) The operator $T(k)$ is unitary on $\mathcal{F}$ and

$$T(k)^* = T(k)^{-1} = T(-k).$$

(ii) For every $f, g \in L^2(\mathbb{R}^3)$, we have

$$T(k)^* A(f,g) T(k) = A(\nu_k(f,g)) \tag{2.19}$$

where $\nu_k : L^2(\mathbb{R}^3) \oplus L^2(\mathbb{R}^3) \to L^2(\mathbb{R}^3) \oplus L^2(\mathbb{R}^3)$ is the Bogoliubov transformation defined by the matrix

$$\nu_k = \begin{pmatrix} ch(k) & sh(k) \\ sh(\overline{k}) & ch(\overline{k}) \end{pmatrix}.$$

Here $ch(k), sh(k) : L^2(\mathbb{R}^3) \to L^2(\mathbb{R}^3)$ are the bounded operators defined by

$$ch(k) = \sum_{n \geq 0} \frac{1}{(2n)!}(k\overline{k})^n \quad \text{and} \quad sh(k) = \sum_{n \geq 0} \frac{1}{(2n+1)!}(k\overline{k})^n k,$$

where products of k and $\overline{k}$ have to be understood in the sense of operators.

(iii) We decompose

$$ch(k) = 1 + p(k), \quad sh(k) = k + r(k), \tag{2.20}$$

where 1 denotes the identity operator on $L^2(\mathbb{R}^3)$. Then $p(k)$ and $r(k)$ (and therefore $sh(k)$) are Hilbert-Schmidt operators, with

$$\|p(k)\|_2 \leq e^{\|k\|_2}, \quad \|r(k)\|_2 \leq e^{\|k\|_2}, \quad \|sh(k)\|_2 \leq e^{\|k\|_2}. \tag{2.21}$$

(Here $\|p(k)\|_2$ denotes the $L^2(\mathbb{R}^3 \times \mathbb{R}^3)$ norm of the kernel $p(k)(x,y)$, which agrees with the Hilbert-Schmidt norm of the operator $p(k)$.)

(iv) Suppose now that $k \in L^2(\mathbb{R}^3 \times \mathbb{R}^3)$ is s.t. $\nabla_1 k \in L^2(\mathbb{R}^3 \times \mathbb{R}^3)$. Then, by symmetry, also $\nabla_2 k \in L^2(\mathbb{R}^3 \times \mathbb{R}^3)$. (We use the notation $(\nabla_1 k)(x,y) = \nabla_x k(x,y)$ and $(\nabla_2 k)(x,y) = \nabla_y k(x,y)$; note that $\nabla_1 k$ and $\nabla_2 k$ are the integral kernels of the operator products ∇k and $-k\nabla$.) Moreover

$$\|\nabla_1 p(k)\|_2, \|\nabla_1 r(k)\|_2 \leq e^{\|k\|_2}\|\nabla_1(k\overline{k})\|_2,$$
$$\|\nabla_2 p(k)\|_2, \|\nabla_2 r(k)\|_2 \leq e^{\|k\|_2}\|\nabla_2(\overline{k}k)\|_2.$$

(v) If the kernel k depends on a parameter t (later, it will depend on time), and if derivatives w. r. t. t are denoted by a dot, we have

$$\|\dot{p}(k)\|_2, \|\dot{r}(k)\|_2 \leq \|\dot{k}\|_2 \, e^{\|k\|_2}$$

and

$$\|\nabla_1 \dot{p}(k)\|_2, \|\nabla_1 \dot{r}(k)\|_2 \leq C e^{\|k\|_2}\left(\|\dot{k}\|_2\|\nabla_1(k\overline{k})\|_2 + \|\nabla_1(\dot{k}\overline{k})\|_2 + \|\nabla_1(k\dot{\overline{k}})\|_2\right),$$
$$\|\nabla_2 \dot{p}(k)\|_2, \|\nabla_2 \dot{r}(k)\|_2 \leq C e^{\|k\|_2}\left(\|\dot{k}\|_2\|\nabla_2(k\overline{k})\|_2 + \|\nabla_2(\dot{k}\overline{k})\|_2 + \|\nabla_2(k\dot{\overline{k}})\|_2\right).$$

Proof. (i) is clear. To prove (ii), we observe that, setting

$$B = \frac{1}{2}\int \mathrm{d}x\mathrm{d}y \, \left(k(x,y)a_x^* a_y^* - \overline{k}(x,y)a_x a_y\right),$$

we have, for any $f, g \in L^2(\mathbb{R}^3)$,

$$\begin{aligned} e^{-B}A(f,g)e^{B} &= A(f,g) + \int_0^1 \mathrm{d}\lambda_1 \frac{d}{d\lambda_1} e^{-\lambda_1 B} A(f,g) e^{\lambda_1 B} \\ &= A(f,g) - \int_0^1 \mathrm{d}\lambda_1 \, e^{-\lambda_1 B}[B, A(f,g)]e^{\lambda_1 B}. \end{aligned}$$

Iterating, we find a BCH formula with error term

$$\begin{aligned} e^{-B}A(f,g)e^{B} &= A(f,g) + \sum_{j=1}^{n} \frac{(-1)^j}{j!} \, \mathrm{ad}_B^j(A(f,g)) \\ &\quad + (-1)^{n+1} \int_0^1 \mathrm{d}\lambda_1 \int_0^{\lambda_1} \mathrm{d}\lambda_2 \ldots \int_0^{\lambda_n} \mathrm{d}\lambda_{n+1} \, e^{-\lambda_{n+1}B} \mathrm{ad}_B^{n+1}(A(f,g)) \, e^{\lambda_{n+1}B} \end{aligned} \tag{2.22}$$

where $\mathrm{ad}_B^1(C) = [B, C]$ and $\mathrm{ad}_B^{n+1}(C) = [B, \mathrm{ad}_B^n(C)]$. A simple computation shows that

$$\mathrm{ad}_B^1(A(f,g)) = [B, A(f,g)] = -A\left(\begin{pmatrix} 0 & k \\ \overline{k} & 0 \end{pmatrix}\begin{pmatrix} f \\ g \end{pmatrix}\right)$$

and therefore that

$$\mathrm{ad}_B^j(A(f,g)) = (-1)^j A\left(\begin{pmatrix} 0 & k \\ \overline{k} & 0 \end{pmatrix}^j \begin{pmatrix} f \\ g \end{pmatrix}\right).$$

We have

$$\begin{pmatrix} 0 & k \\ \overline{k} & 0 \end{pmatrix}^{2m} = \begin{pmatrix} (k\overline{k})^m & 0 \\ 0 & (\overline{k}k)^m \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} 0 & k \\ \overline{k} & 0 \end{pmatrix}^{2m+1} = \begin{pmatrix} 0 & (k\overline{k})^m k \\ (\overline{k}k)^m \overline{k} & 0 \end{pmatrix}$$

for every $m \in \mathbb{N}$ (the products of ks and $\overline{k}$s are in the sense of operators, which means in terms of integral kernels $(k_1k_2)(x,y) = \int \mathrm{d}z \, k_1(x,z)k_2(z,y)$). Inserting all this in (2.22), we obtain (2.19), if we can show that the error converges to zero. We claim, more precisely, that the error term on the r. h. s. of (2.22) vanishes, as $n \to \infty$, when applied on the domain $D(\mathcal{N}^{1/2})$. To prove this claim, we start by observing that

$$\|(\mathcal{N}+1)^{1/2} e^{-\lambda B} (\mathcal{N}+1)^{-1/2}\| \leq e^{|\lambda| \|k\|_2} \tag{2.23}$$

for every $\lambda \in \mathbb{R}$. Assuming for example, that n is odd, (2.23) implies that

$$\begin{aligned} &\left\| \int_0^1 \mathrm{d}\lambda_1 \int_0^{\lambda_1} \mathrm{d}\lambda_2 \ldots \int_0^{\lambda_n} \mathrm{d}\lambda_{n+1} \, e^{-\lambda_{n+1}B} \mathrm{ad}_B^{n+1}(A(f,g)) \, e^{\lambda_{n+1}B} (\mathcal{N}+1)^{-1/2} \right\| \\ &\quad \leq \frac{e^{\|k\|_2}}{(n+1)!} \|A\left((k\overline{k})^{(n+1)/2} f, (\overline{k}k)^{(n+1)/2} g\right) (\mathcal{N}+1)^{-1/2}\| \\ &\quad \leq (\|f\|_2 + \|g\|_2) \, e^{\|k\|_2} \, \frac{\|(k\overline{k})^{(n+1)/2}\|_2}{(n+1)!} \leq C \frac{\|k\|_2^n}{(n+1)!} \end{aligned}$$

which vanishes as $n \to \infty$. The case n even can be treated similarly. To prove (2.23), we observe that

$$\begin{aligned}\frac{d}{d\lambda}&\|(\mathcal{N}+1)^{1/2}e^{-\lambda B}\psi\|^2\\ &= \langle e^{-\lambda B}\psi, [B,\mathcal{N}]\; e^{-\lambda B}\psi\rangle\\ &= -\int \mathrm{d}x\mathrm{d}y\, k(x,y)\langle e^{-\lambda B}\psi, a_x^* a_y^*\, e^{-\lambda B}\psi\rangle - \int \mathrm{d}x\mathrm{d}y\, \overline{k}(x,y)\langle e^{-\lambda B}\psi, a_x a_y\, e^{-\lambda B}\psi\rangle\\ &\le 2\int \mathrm{d}x\, \|a_x e^{-\lambda B}\psi\|\, \|a^*(k(x,.))e^{-\lambda B}\psi\|\\ &\le 2\|k\|_2\, \|(\mathcal{N}+1)^{1/2}e^{-\lambda B}\psi\|^2.\end{aligned}$$

Grönwall's Lemma implies (2.23).

To prove (iii), we notice that

$$\|p(k)\|_2 = \left\|\sum_{n\ge1}\frac{(k\overline{k})^n}{(2n)!}\right\|_2 \le \sum_{n\ge1}\frac{\|(k\overline{k})^n\|_2}{(2n)!} \le \sum_{n\ge1}\frac{\|k\|_2^{2n}}{(2n)!} \le e^{\|k\|_2}$$

where we used that, by Cauchy-Schwarz, for any two kernels $K_1, K_2 \in L^2(\mathbb{R}^3\times\mathbb{R}^3)$

$$\begin{aligned}\|K_1K_2\|_2^2 &= \int \mathrm{d}x\mathrm{d}y\left|\int \mathrm{d}z\, K_1(x,z)K_2(z,y)\right|^2\\ &= \int \mathrm{d}x\mathrm{d}y\mathrm{d}z_1\mathrm{d}z_2\, K_1(x,z_1)\overline{K}_1(x,z_2)K_2(z_1,y)\overline{K}_2(z_2,y)\\ &\le \int \mathrm{d}x\mathrm{d}y\mathrm{d}z_1\mathrm{d}z_2\, |K_1(x,z_1)|^2\, |K_2(z_2,y)|^2\\ &= \|K_1\|_2^2\, \|K_2\|_2^2.\end{aligned} \tag{2.24}$$

The bounds for $r(k)$ and $\mathrm{sh}(k)$ can be proven similarly.

To show (iv) we write, using the fact that the series for $p(k)$, $r(k)$ and $\mathrm{sh}(k)$ are absolutely convergent,

$$\begin{aligned}\nabla_1 p(k) &= \nabla_1(k\overline{k})\left[\sum_{n=1}^{\infty}\frac{1}{(2n)!}(k\overline{k})^{n-1}\right],\\ \nabla_1 r(k) &= \nabla_1(k\overline{k})\left[\sum_{n=1}^{\infty}\frac{1}{(2n+1)!}(k\overline{k})^{n-1}k\right].\end{aligned}$$

Applying (2.24), we find the desired bounds. The bounds for the derivative ∇_2 can be obtained similarly.

Finally, to show (v), we remark that

$$\|\dot{p}(k)\|_2 \le \sum_{n\ge1}\frac{1}{(2n)!}2n\|\dot{k}\|_2\|k\|_2^{2n-1} \le \|\dot{k}\|_2\, e^{\|k\|_2}.$$

The bound for $\dot{r}(k)$ can be proven analogously. From the product rule, we also find that

$$\begin{aligned}\|\nabla_1\dot{p}(k)\|_2 &\le \sum_{n=2}^{\infty}\frac{n-1}{(2n)!}\,\|k\|_2^{2(n-2)}\|\partial_t(k\overline{k})\|_2\,\|\nabla_1(k\overline{k})\|_2 + \sum_{n=1}^{\infty}\frac{1}{(2n)!}\,\|k\|_2^{2(n-1)}\|\nabla_1\partial_t(k\overline{k})\|_2\\ &\le e^{\|k\|_2}\left(\|\dot{k}\|_2\,\|\nabla_1(k\overline{k})\|_2 + \|\nabla_1(k\dot{\overline{k}})\|_2 + \|\nabla_1(\dot{k}\overline{k})\|_2\right).\end{aligned}$$

The other bounds are shown similarly. □

2.3. Construction of the fluctuation dynamics

In this section, we will construct an approximation to the full many-body evolution of initial data of the form $W(\sqrt{N}\varphi)T(k_0)\psi$, as considered in Theorem 2.1.1. Our approximation will consist of two parts. First of all, the evolution of a (approximately) coherent state will be approximated by a coherent state with evolved one-particle wave function. We will take care of the correlation structure later.

For a given $\varphi \in H^1(\mathbb{R}^3)$, we define $\varphi_t^{(N)}$ as the solution of the modified Gross-Pitaevskii equation

$$i\partial_t \varphi_t^{(N)} = -\Delta\varphi_t^{(N)} + \left(N^3 f(N.)V(N.) * |\varphi_t^{(N)}|^2\right)\varphi_t^{(N)}, \tag{2.25}$$

where f denotes the solution of the zero-energy scattering equation (1.10). As will become clear later on, it is more convenient to work with the solution $\varphi_t^{(N)}$ of the modified Gross-Pitaevskii equation (2.25), rather than directly with the solution φ_t of the Gross-Pitaevskii equation (2.16). Since $N^3 f(Nx)V(Nx) \to 8\pi a_0 \delta(x)$, the solution $\varphi_t^{(N)}$ converges towards the solution φ_t, as $N \to \infty$. This is proven, together with other important properties of the solutions of the Gross-Pitaevskii and modified Gross-Pitaevskii equation, in the next proposition.

Proposition 2.3.1. *Let $V \in L^1 \cap L^3(\mathbb{R}^3, (1+|x|^6)dx)$ be non-negative and spherically symmetric. Let f denote the solution of the zero-energy scattering equation (1.10), with boundary condition $f(x) \to 1$ as $|x| \to \infty$. Then, by Lemma 2.3.2 below, $0 \le f \le 1$ and therefore $Vf \ge 0$ with $Vf \in L^1 \cap L^3(\mathbb{R}^3, (1+|x|^6)dx)$. Let $\varphi \in H^1(\mathbb{R}^3)$, with $\|\varphi\|_2 = 1$.*

(i) Well-posedness. There exist unique global solutions $\varphi_{(.)}$ and $\varphi_{(.)}^{(N)} \in C(\mathbb{R}, H^1(\mathbb{R}^3))$ of the Gross-Pitaevskii equation (2.16) and of the modified Gross-Pitaevskii equation (2.25), respectively, with initial data φ. These solutions are such that $\|\varphi_t\|_2 = \|\varphi_t^{(N)}\|_2 = 1$ for all $t \in \mathbb{R}$. Moreover, there exists a constant $C > 0$ such that

$$\|\varphi_t\|_{H^1}, \|\varphi_t^{(N)}\|_{H^1} \le C \tag{2.26}$$

for all $t \in \mathbb{R}$.

(ii) Propagation of higher regularity. If we make the additional assumption that $\varphi \in H^n(\mathbb{R}^3)$, for some integer $n \ge 2$, then $\varphi_t, \varphi_t^{(N)} \in H^n(\mathbb{R}^3)$ for every $t \in \mathbb{R}$. Moreover there exists a constant $C > 0$ depending on $\|\varphi\|_{H^n}$ and on n, and a constant $K > 0$, depending only on $\|\varphi\|_{H^1}$ and n, such that

$$\|\varphi_t\|_{H^n}, \|\varphi_t^{(N)}\|_{H^n} \le Ce^{K|t|} \tag{2.27}$$

for all $t \in \mathbb{R}$.

(iii) Regularity of time derivatives. Suppose $\varphi \in H^4(\mathbb{R}^3)$. Then there exist a constant $C > 0$, depending on $\|\varphi\|_{H^4}$, and a constant $K > 0$, depending only on $\|\varphi\|_{H^1}$, such that

$$\|\dot{\varphi}_t^{(N)}\|_{H^2}, \|\ddot{\varphi}_t^{(N)}\|_2 \le Ce^{K|t|}$$

for all $t \in \mathbb{R}$.

(iv) *Comparison of dynamics. Suppose now* $\varphi \in H^2(\mathbb{R}^3)$. *Then there exist constants* $C, c_1, c_2 > 0$, *depending on* $\|\varphi\|_{H^2}$ *(*c_2 *actually depends only on* $\|\varphi\|_{H^1}$*) such that*

$$\|\varphi_t^{(N)} - \varphi_t\|_2 \leq \frac{C \exp(c_1 \exp(c_2|t|))}{N}$$

for all $t \in \mathbb{R}$.

The proof of Proposition 2.3.1 can be found in Appendix 2.A.

Using the solution $\varphi_t^{(N)}$ of (2.25), we are going to approximate the coherent part of the evolution. As explained in the introduction, however, this approximation is not good enough. The many-body evolution develops a singular correlation structure, which is completely absent in the evolved coherent state. As a consequence, fluctuations around the coherent approximation are too strong to be controlled. To solve this problem, we have to produce a better approximation of the many-body evolution, in particular an approximation which takes into account the short-scale correlation structure. To reach this goal, we are going to multiply the Weyl operator $W(\sqrt{N}\varphi_t^{(N)})$, which generates the coherent approximation to the many-body dynamics, by a Bogoliubov transformation $T(k)$ having the form (2.18). The kernel $k \in L^2(\mathbb{R}^3 \times \mathbb{R}^3)$ has to be chosen so that $T(k)$ creates the correct correlations among the particles. Since correlations are, in good approximation, two-body effects, we can describe them through the solution f of the zero-energy scattering equation (1.10). We write

$$f(x) = 1 - w(x) \tag{2.28}$$

with $\lim_{|x|\to\infty} w(x) = 0$. The scattering length of V is defined as

$$8\pi a_0 = \int \mathrm{d}x\, V(x) f(x).$$

Equivalently, a_0 is given by

$$a_0 = \lim_{|x|\to\infty} w(x)|x|.$$

Note that, if V has compact support inside $\{x \in \mathbb{R}^3 : |x| < R\}$, then $a_0 \leq R$ and $w(x) = a_0/|x|$ for $|x| > R$. In general, under our assumptions on V, one can prove the following properties of the function w.

Lemma 2.3.2. *Let* $V \in L^1 \cap L^3(\mathbb{R}^3, (1+|x|^6)dx)$ *be spherically symmetric, with* $V \geq 0$. *Denote by* f *the solution of the zero-energy scattering equation (1.10) and let* $w = 1 - f$. *Then*

$$0 \leq w(x) \leq 1 \quad \text{for all } x \in \mathbb{R}^3.$$

Moreover, there is a constant $C > 0$ *such that*

$$w(x) \leq \frac{C}{|x|+1} \qquad \text{and} \qquad |\nabla w(x)| \leq \frac{C}{|x|^2+1}. \tag{2.29}$$

Proof. Standard arguments show that $0 \leq f(x) \leq 1$ holds for every $x \in \mathbb{R}^3$ ($f(x) \leq 1$ follows from $V \geq 0$, because of the monotonic dependence of f on the potential; see [LSSY05, Appendix C]). This implies that $0 \leq w(x) \leq 1$ for all $x \in \mathbb{R}^3$. From the zero-energy scattering equation, we have $-\Delta w = Vf/2$. This implies that

$$w(x) = C \int \mathrm{d}y\, \frac{1}{|x-y|} V(y) f(y) \qquad \text{and} \qquad \nabla w(x) = C \int \mathrm{d}y \frac{x-y}{|x-y|^3} V(y) f(y)$$

for an appropriate constant $C \in \mathbb{R}$. Using $|x| \leq |x-y| + |y|$, the fact that $f \leq 1$, and the Hardy-Littlewood-Sobolev inequality, we find

$$\begin{aligned}|(1+|x|)w(x)| &\leq C \int \mathrm{d}y \left(\frac{1}{|x-y|} + 1 + \frac{|y|}{|x-y|} \right) V(y) f(y) \\ &\leq C(\|V\|_{3/2} + \|V\|_{L^1} + \||y|V(y)\|_{3/2})\end{aligned}$$

and, analogously,

$$\begin{aligned}\left|(1+|x|^2)w(x)\right| &\leq C \int \mathrm{d}y \left(\frac{1}{|x-y|^2} + 1 + \frac{|y|^2}{|x-y|^2} \right) V(y) f(y) \\ &\leq C \left(\|V\|_3 + \|V\|_1 + \||y|^2 V\|_3 \right).\end{aligned}$$

The right hand side of the last two equations is bounded under the assumption $V \in L^1 \cap L^3((1+|x|^6)dx)$. □

The zero-energy scattering equation for the rescaled potential $N^2 V(Nx)$ is solved by $f(Nx)$. We define $w(Nx) = 1 - f(Nx)$. Clearly

$$\lim_{|x| \to \infty} w(Nx)|x| = \frac{a_0}{N},$$

showing that the scattering length of $N^2 V(Nx)$ is a_0/N. Equivalently, this follows from $\int \mathrm{d}x \, N^2 V(Nx) f(Nx) = 8\pi a_0 / N$.

It follows immediately from Lemma 2.3.2 that $0 < w(Nx) < c$ for some $c < 1$ and for all $x \in \mathbb{R}^3$, and that there exists C with

$$w(Nx) \leq \frac{C}{N|x|+1} \qquad \text{and} \qquad |\nabla_x w(Nx)| \leq C \frac{N}{N^2|x|^2+1}. \tag{2.30}$$

We will use the solution $f(Nx)$ of the scaled zero-energy scattering equation to approximate the correlations among the particles, arising on the microscopic scale. It is however important to keep in mind that these correlations are also modulated on the macroscopic scale. We describe the macroscopic variation by the solution $\varphi_t^{(N)}$ of the modified Gross-Pitaevskii equation (2.25). We define therefore the kernel[3]

$$k_t(x,y) = -Nw(N(x-y)) \varphi_t^{(N)}(x) \varphi_t^{(N)}(y) \tag{2.31}$$

and the corresponding unitary operator

$$T(k_t) = \exp\left(\frac{1}{2} \int \mathrm{d}x \mathrm{d}y \, \left(k_t(x,y) a_x^* a_y^* - \overline{k}_t(x,y) a_x a_y \right) \right).$$

In the next lemma, we collect several bounds for the kernel k_t which will be useful in the following.

Lemma 2.3.3. *Let $w(Nx) = 1 - f(Nx)$, where f solves the zero-energy scattering equation (1.10). Let*

$$k(x,y) = -Nw(N(x-y)) \varphi(x) \varphi(y)$$

with $\varphi \in H^1(\mathbb{R}^3)$. (This lemma holds for general φ, not requiring it to be a solution of the modified Gross-Pitaevskii equation. Nevertheless, the application is to the solution of the modified Gross-Pitaevskii equation, and so in view of (2.26) *we treat $\|\varphi\|_{H^1}$ as a constant.)*

[3] Some typos in the following part of the section in [BdS12] were corrected here.

(i) *There exists a constant C, depending only on $\|\varphi\|_{H^1}$ such that*

$$\begin{aligned}\|k\|_2 &\leq C,\\ \|\nabla_1 k\|_2, \|\nabla_2 k\|_2 &\leq C\sqrt{N},\\ \|\nabla_1(k\bar{k}_t)\|_2, \|\nabla_2(k\bar{k}_t)\|_2 &\leq C.\end{aligned}$$

Defining $p(k)$ and $r(k)$ as in (2.20), so that $ch(k) = 1 + p(k)$ and $sh(k) = k + r(k)$, it follows from Lemma 2.2.1, part (iii) and (iv), that

$$\begin{aligned}\|p(k)\|_2, \|r(k)\|_2, \|sh(k)\|_2 &\leq C,\\ \|\nabla_1 p(k)\|_2, \|\nabla_2 p(k)\|_2 &\leq C,\\ \|\nabla_1 r(k)\|_2, \|\nabla_2 r(k)\|_2 &\leq C.\end{aligned}$$

(ii) *For almost all $x, y \in \mathbb{R}^3$, we have the pointwise bounds*

$$\begin{aligned}|k(x,y)| &\leq \min\left(N|\varphi(x)||\varphi(y)|, \frac{1}{|x-y|}|\varphi(x)||\varphi(y)|\right),\\ |r(k)(x,y)| &\leq C|\varphi(x)||\varphi(y)|,\\ |p(k)(x,y)| &\leq C|\varphi(x)||\varphi(y)|\,.\end{aligned}$$

(iii) *Suppose further that $\varphi \in H^2(\mathbb{R}^3)$. Then*

$$\sup_{x\in\mathbb{R}^3}\|k(.,x)\|_2,\ \sup_{x\in\mathbb{R}^3}\|p(k)(.,x)\|_2,\ \sup_{x\in\mathbb{R}^3}\|r(k)(.,x)\|_2,\ \sup_{x\in\mathbb{R}^3}\|sh(k)(.,x)\|_2 \leq C\|\varphi\|_{H^2}.$$

The proof can be found in Appendix 2.B. We will also need bounds on the time derivative of the kernels k_t, $p(k_t)$, $r(k_t)$. These are collected in the following lemma.

Lemma 2.3.4. *Let $\varphi \in H^4(\mathbb{R}^3)$, and $\varphi_t^{(N)} \in H^4(\mathbb{R}^3)$ be the solution of (2.25), with initial data φ. Let $w(Nx) = 1 - f(Nx)$, where f is the solution of the zero-energy scattering equation (1.10). Let the kernel k_t be defined as in (2.31), so that*

$$\dot{k}_t(x,y) = -Nw(N(x-y))\left(\dot{\varphi}_t^{(N)}(x)\varphi_t^{(N)}(y) + \varphi_t^{(N)}(x)\dot{\varphi}_t^{(N)}(y)\right). \tag{2.32}$$

Then there are constants $C, K > 0$, where C depends on the $\|\varphi\|_{H^4}$ and K only on $\|\varphi\|_{H^1}$ such that the following bounds hold:

(i)
$$\|\dot{k}_t\|_2, \|\ddot{k}_t\|_2, \|\dot{p}(k_t)\|_2, \|\dot{r}(k_t)\|_2 \leq Ce^{K|t|},$$

(ii)
$$\|\nabla_1\dot{p}(k)\|_2, \|\nabla_2\dot{p}(k)\|_2, \|\nabla_1\dot{r}(k)\|_2, \|\nabla_2\dot{r}(k)\|_2 \leq Ce^{K|t|},$$

(iii)
$$\sup_x\|\dot{k}_t(.,x)\|_2,\ \sup_x\|\dot{p}(k_t)(.,x)\|_2,\ \sup_x\|\dot{r}(k_t)(.,x)\|_2,\ \sup_x\|\dot{sh}(k_t)(.,x)\|_2 \leq Ce^{K|t|}.$$

The proof can be found in Appendix 2.B.

As explained in the introduction, we are going to approximate the many-body evolution

$$e^{-i\mathcal{H}_N t} W(\sqrt{N}\varphi)T(k_0)\psi$$

of a initial data which is almost coherent but has the correct short-scale structure, with the Fock space vector $W(\sqrt{N}\varphi_t^{(N)})T(k_t)\psi$, which is again almost coherent and has again the correct short-scale structure. Here $\varphi_t^{(N)}$ is the solution to the Gross-Pitaevskii equation with initial data $\varphi_0^{(N)} = \varphi$ (the same φ appearing in the Weyl operator of the initial data). (We remark that in this ansatz the correlation structure, modeled by the time-independent $-Nw(N(x-y))$ in (2.31), is static.) This leads us to the fluctuation dynamics, defined as the two-parameter group of unitary transformations

$$\mathcal{U}(t,s) := T^*(k_t)W^*(\sqrt{N}\varphi_t^{(N)})e^{-i\mathcal{H}_N(t-s)}W(\sqrt{N}\varphi_s^{(N)})T(k_s) \tag{2.33}$$

where $\mathcal{U}(s,s) = 1$ for all $s \in \mathbb{R}$.

The fluctuation dynamics satisfies the Schrödinger-type equation

$$i\partial_t \mathcal{U}(t,s) = \mathcal{L}_N(t)\mathcal{U}(t,s)$$

with the time-dependent generator

$$\begin{aligned}\mathcal{L}_N(t) = {} & T^*(k_t)\left[i\partial_t W^*(\sqrt{N}\varphi_t^{(N)})\right] W(\sqrt{N}\varphi_t^{(N)})T(k_t) \\ & + T^*(k_t)W^*(\sqrt{N}\varphi_t^{(N)})\mathcal{H}_N W(\sqrt{N}\varphi_t^{(N)})T(k_t) + \left[i\partial_t T^*(k_t)\right]T(k_t).\end{aligned}$$

The next theorem, whose proof is deferred to Section 2.6, is the main technical ingredient of this paper. It contains important estimates for the generator $\mathcal{L}_N(t)$, which will be used in the next section to control the growth of the expectation of the number of particles operator with respect to the fluctuation dynamics $\mathcal{U}(t,s)$.

Theorem 2.3.5. *Define the time-dependent constant (of order N; the precise form is not of importance[4])*

$$\begin{aligned} C_N(t) := {} & \mathcal{L}_{0,N}^{(0)}(t) + \int dx\,dy\,|\nabla_x sh(k_t)(y,x)|^2 \\ & + \int dx\,dy (N^3 V(N.) * |\varphi_t^{(N)}|^2)(x)\,|sh(k_t)(y,x)|^2 \\ & + \int dx\,dy\,dz\, N^3 V(N(x-y))\varphi_t^{(N)}(x)\overline{\varphi}_t^{(N)}(y) sh(\overline{k}_t)(z,x)\, sh(k_t)(z,y) \\ & + \mathrm{Re} \int dx\,dy\,dz\, N^3 V(N(x-y))\varphi_t^{(N)}(x)\varphi_t^{(N)}(y) sh(\overline{k}_t)(z,x) ch(k_t)(z,y) \\ & + \int dx\,dy N^2 V(N(x-y)) \\ & \qquad \times \left[\left| \int dz\, sh(\overline{k}_t)(z,x)\, ch(z,y)\right|^2 + \left|\int dz\, sh(\overline{k}_t)(z,x)\, sh(z,y)\right|^2 \right. \\ & \qquad \left. + \int dz_1 dz_2\, sh(\overline{k}_t)(z_1,x)\, sh(k_t)(z_1,y) sh(\overline{k}_t)(z_2,x)\, sh(k_t)(z_2,y)\right] \end{aligned} \tag{2.34}$$

[4]In fact, $C_N(t)$ just collects all terms of the generator $\mathcal{L}_N(t)$ which are constant in the sense that they do not contain creation or annihilation operators. The form of these terms does not matter for our study of the dynamics. However, if one attempts to use initial data without the squeezing operator $T(k_0)$, $C_N(t)$ causes the constant of $t = 0$ in Grönwall's lemma to be of order N, which is too large.

and define the generator without constant terms by

$$\widetilde{\mathcal{L}}_N(t) := \mathcal{L}_N(t) - C_N(t). \tag{2.35}$$

Then we have, for some $K > 0$ depending only on $\|\varphi\|_{H^1}$,

$$\widetilde{\mathcal{L}}_N(t) \geq \frac{1}{2}\mathcal{H}_N - C\,\frac{\mathcal{N}^2}{N} - Ce^{K|t|}\,(\mathcal{N}+1) \tag{2.36}$$

and

$$\widetilde{\mathcal{L}}_N(t) \leq \frac{3}{2}\mathcal{H}_N + C\,\frac{\mathcal{N}^2}{N} + Ce^{K|t|}\,(\mathcal{N}+1)\,. \tag{2.37}$$

Moreover,

$$\pm\left[\mathcal{N}, \widetilde{\mathcal{L}}_N(t)\right] \leq \mathcal{H}_N + C\frac{\mathcal{N}^2}{N} + Ce^{K|t|}(\mathcal{N}+1) \tag{2.38}$$

and

$$\pm\dot{\widetilde{\mathcal{L}}}_N(t) \leq \mathcal{H}_N + Ce^{K|t|}\left(\frac{\mathcal{N}^2}{N} + \mathcal{N} + 1\right). \tag{2.39}$$

The proof of Theorem 2.3.5 can be found in Subsection 2.6.6. The preceding parts of Section 2.6 provide the necessary explicit estimates of the terms of the generator $\mathcal{L}_N(t)$ of the dynamics $\mathcal{U}(t,s)$.

2.4. Growth of fluctuations

The goal of this section is to prove a bound, uniform in N, for the growth of the expectation of the number of particles operator with respect to the fluctuation dynamics. The properties of the generator $\mathcal{L}_N(t)$ of the fluctuation dynamics, as established in Theorem 2.3.5, play a crucial role.

Theorem 2.4.1. *Suppose $\psi \in \mathcal{F}$ (possibly depending on N) with $\|\psi\| = 1$ is such that*

$$\left\langle \psi, \left(\frac{\mathcal{N}^2}{N} + \mathcal{N} + \mathcal{H}_N\right)\psi\right\rangle \leq C \tag{2.40}$$

for a constant $C > 0$. Let $\varphi \in H^4(\mathbb{R}^3)$, and let $\varphi_t^{(N)}$ be the solution of the modified Gross-Pitaevskii equation (2.25) with initial data φ. Let $\mathcal{U}(t,s)$ be the fluctuation dynamics defined in (2.33). Then there exist constants $C, c_1, c_2 > 0$ such that

$$\langle \psi, \mathcal{U}^*(t,0)\mathcal{N}\mathcal{U}(t,0)\psi\rangle \leq C\exp(c_1\exp(c_2|t|)).$$

The strategy to prove Theorem 2.4.1 consists in applying Grönwall's inequality. The derivative of the expectation of $\mathcal{N}$ is given by the expectation of the commutator $i[\mathcal{N}, \mathcal{L}_N(t)]$, where $\mathcal{L}_N(t)$ is the generator (2.51) of the fluctuation dynamics[5]. By (2.38), this commutator is bounded in terms of the energy, of $(\mathcal{N}+1)$, and of $\mathcal{N}^2/N$. The growth of the energy is controlled with the help of (2.39). What remains to be done in order to apply Grönwall's inequality is to bound the term $\mathcal{N}^2/N$. In the next proposition, we show that the expectation of $\mathcal{N}^2/N$ at time t can be controlled by its expectation at time $t = 0$ (a harmless constant, by assumption (2.40)) and by the expectation of $(\mathcal{N}+1)$ (which fits well in the scheme of Grönwall's inequality).

[5] clearly the constant (2.34) can be ignored in this argument

Proposition 2.4.2. *Let the fluctuation dynamics $\mathcal{U}(t,s)$ be defined as in (2.33). Then there exists a constant $C > 0$ such that*

$$\mathcal{U}^*(t,0)\mathcal{N}^2\,\mathcal{U}(t,0) \leq C\big(N\,\mathcal{U}^*(t,0)\mathcal{N}\,U(t,0) + N(\mathcal{N}+1) + (\mathcal{N}+1)^2\big).$$

The next lemma is useful in the proof of Proposition 2.4.2.

Lemma 2.4.3. *Let $k_t \in L^2(\mathbb{R}^3 \times \mathbb{R}^3)$ be as defined in (2.31). Then there exists a constant C, depending only on $\|k_t\|_2$, such that*

$$T^*(k_t)\,\mathcal{N}\,T(k_t) \leq C(\mathcal{N}+1), \tag{2.41}$$

$$T^*(k_t)\,\mathcal{N}^2\,T(k_t) \leq C(\mathcal{N}+1)^2 \tag{2.42}$$

for all $t \in \mathbb{R}$.

Proof. We use the decomposition $\mathrm{ch}(k_t) = 1 + p(k_t)$ and the shorthand notation $c_x(z) = \mathrm{ch}(k_t)(z,x)$, $p_x(z) = p(k_t)(z,x)$ and $s_x(z) = \mathrm{sh}(k_t)(z,x)$. We have

$$\begin{aligned}
\langle \psi, T^*(k_t)\mathcal{N}T(k_t)\psi\rangle &= \int \mathrm{d}x\,\langle \psi, (a^*(c_x) + a(s_x))(a(c_x) + a^*(s_x))\psi\rangle \\
&= \int \mathrm{d}x\,\|(a_x + a(p_x) + a^*(s_x))\psi\|^2 \\
&\leq C\int \mathrm{d}x\,\|a_x\psi\|^2 + \int \mathrm{d}x\,\|a(p_x)\psi\|^2 + \int \mathrm{d}x\,\|a^*(s_x)\psi\|^2 \\
&\leq C(1 + \|p(k_t)\|_2^2 + \|\mathrm{sh}(k_t)\|_2^2)\|(\mathcal{N}+1)^{1/2}\psi\|,
\end{aligned}$$

and (2.41) follows by Lemma 2.2.1 (since $\|p(k_t)\|_2, \|\mathrm{sh}(k_t)\|_2 \leq e^{\|k_t\|_2}$). To prove (2.42), we observe that

$$\begin{aligned}
&\langle \psi, T^*(k_t)\mathcal{N}^2T(k_t)\psi\rangle = \int \mathrm{d}x dy\,\langle \psi, T^*(k_t)a_x^*a_xa_y^*a_yT(k_t)\psi\rangle \\
&= \int \mathrm{d}x\,\langle \psi, T^*(k_t)a_x^*\mathcal{N}a_xT(k_t)\psi\rangle + \langle \psi, T^*(k_t)\mathcal{N}T(k_t)\psi\rangle \\
&= \int \mathrm{d}x\,\langle (a(c_x) + a^*(s_x))\psi, T^*(k)\mathcal{N}T(k)(a(c_x) + a^*(s_x))\psi\rangle + \langle \psi, T^*(k_t)\mathcal{N}T(k_t)\psi\rangle.
\end{aligned}$$

Then, applying (2.41), we obtain

$$\begin{aligned}
&\langle \psi, T^*(k_t)\mathcal{N}^2T(k_t)\psi\rangle \\
&\leq C\int \mathrm{d}x\,\|(\mathcal{N}+1)^{1/2}(a(c_x) + a^*(s_x))\psi\|^2 + C\langle \psi, (\mathcal{N}+1)\psi\rangle \\
&\leq C\int \mathrm{d}x\,(\|a_x\mathcal{N}^{1/2}\psi\|^2 + \|a(p_x)\mathcal{N}^{1/2}\psi\|^2 + \|a^*(s_x)(\mathcal{N}+2)^{1/2}\psi\|^2) + C\langle \psi, (\mathcal{N}+1)\psi\rangle \\
&\leq C(1 + \|p(k_t)\|_2^2 + \|\mathrm{sh}(k_t)\|_2^2)\langle \psi, (\mathcal{N}+1)^2\psi\rangle.
\end{aligned}$$

The bounds from Lemma 2.2.1 imply (2.42). □

Proof of Proposition 2.4.2. From Lemma 2.4.3, we find

$$\langle \psi, \mathcal{U}^*(t,0)\mathcal{N}^2\mathcal{U}(t,0)\psi\rangle \leq C\langle \psi, \mathcal{U}^*(t,0)T^*(k_t)\mathcal{N}^2T(k_t)\mathcal{U}(t,0)\psi\rangle. \tag{2.43}$$

We now show how to bound the r. h. s. of the last equation. Using the definition of the fluctuation dynamics $\mathcal{U}(t,0) = T^*(k_t)W^*(\sqrt{N}\varphi_t^{(N)})e^{-i\mathcal{H}_N t}W^*(\sqrt{N}\varphi)T(k_0)$, we find

$$\begin{aligned}
&\langle\psi,\mathcal{U}^*(t,0)T^*(k_t)\mathcal{N}^2T(k_t)\mathcal{U}(t,0)\psi\rangle \\
&= \langle\mathcal{N}\,T(k_t)\mathcal{U}(t,0)\psi, W^*(\sqrt{N}\varphi_t^{(N)})\,(\mathcal{N} - \sqrt{N}\phi(\varphi_t^{(N)}) + N)e^{-i\mathcal{H}_N t}W(\sqrt{N}\varphi)T(k_0)\psi\rangle \\
&= \langle\mathcal{N}\,T(k_t)\mathcal{U}(t,0)\psi, W^*(\sqrt{N}\varphi_t^{(N)})\,\mathcal{N}e^{-i\mathcal{H}_N t}W(\sqrt{N}\varphi)T(k_0)\psi\rangle \\
&\quad - \sqrt{N}\,\langle\mathcal{N}\,T(k_t)\mathcal{U}(t,0)\psi, W^*(\sqrt{N}\varphi_t^{(N)})\,\phi(\varphi_t^{(N)})e^{-i\mathcal{H}_N t}W(\sqrt{N}\varphi)T(k_0)\psi\rangle \\
&\quad + N\langle\psi,\mathcal{U}^*(t,0)T^*(k_t)\mathcal{N}T(k_t)\mathcal{U}(t,0)\psi\rangle
\end{aligned} \tag{2.44}$$

where we used the notation $\phi(f) = a(f) + a^*(f)$, and the property (1.40) to show that

$$W^*(\sqrt{N}\varphi_t^{(N)})\mathcal{N}W(\sqrt{N}\varphi_t^{(N)}) = \mathcal{N} - \sqrt{N}\phi(\varphi_t^{(N)}) + N.$$

In the first term on the r. h. s. of (2.44), we use now the fact that $\mathcal{N}$ commutes with $\mathcal{H}_N$. In the second term, on the other hand, we move the factor $\phi(\varphi_t^{(N)})$ back to the left of the Weyl operator $W(\sqrt{N}\varphi_t^{(N)})$, using that

$$W^*(\sqrt{N}\varphi_t^{(N)})\phi(\varphi_t^{(N)}) = \left(\phi(\varphi_t^{(N)}) + 2\sqrt{N}\right)\,W^*(\sqrt{N}\varphi_t^{(N)})\,.$$

We conclude that

$$\begin{aligned}
&\langle\psi,\mathcal{U}^*(t,0)T^*(k_t)\mathcal{N}^2T(k_t)\mathcal{U}(t,0)\psi\rangle \\
&= \langle\mathcal{N}\,T(k_t)\mathcal{U}(t,0)\psi, W^*(\sqrt{N}\varphi_t^{(N)})\,e^{-i\mathcal{H}_N t}W(\sqrt{N}\varphi)(\mathcal{N} + \sqrt{N}\phi(\varphi) + N)\,T(k_0)\psi\rangle \\
&\quad - \sqrt{N}\,\langle\mathcal{N}\,T(k_t)\mathcal{U}(t,0)\psi, \left(\phi(\varphi_t^{(N)}) + 2\sqrt{N}\right)W^*(\sqrt{N}\varphi_t^{(N)})\,e^{-i\mathcal{H}_N t}W(\sqrt{N}\varphi)T(k_0)\psi\rangle \\
&\quad + N\langle\psi,\mathcal{U}^*(t,0)T^*(k_t)\mathcal{N}T(k_t)\mathcal{U}(t,0)\psi\rangle \\
&= \langle\mathcal{N}\,T(k_t)\mathcal{U}(t,0)\psi, W^*(\sqrt{N}\varphi_t^{(N)})\,e^{-i\mathcal{H}_N t}W(\sqrt{N}\varphi)\mathcal{N}\,T(k_0)\psi\rangle \\
&\quad + \sqrt{N}\langle\mathcal{N}\,T(k_t)\mathcal{U}(t,0)\psi, W^*(\sqrt{N}\varphi_t^{(N)})\,e^{-i\mathcal{H}_N t}W(\sqrt{N}\varphi)\phi(\varphi)\,T(k_0)\psi\rangle \\
&\quad - \sqrt{N}\,\langle\mathcal{N}\,T(k_t)\mathcal{U}(t,0)\psi, \phi(\varphi_t^{(N)})W^*(\sqrt{N}\varphi_t^{(N)})\,e^{-i\mathcal{H}_N t}W(\sqrt{N}\varphi)T(k_0)\psi\rangle.
\end{aligned} \tag{2.45}$$

By Cauchy-Schwarz, we obtain

$$\begin{aligned}
&\langle\psi,\mathcal{U}^*(t,0)T^*(k_t)\mathcal{N}^2T(k_t)\mathcal{U}(t,0)\psi\rangle \\
&\qquad \le \|\mathcal{N}\,T(k_t)\mathcal{U}(t,0)\psi\| \\
&\qquad\qquad \times\left(\|\mathcal{N}\,T(k_0)\psi\rangle\| + \sqrt{N}\|\phi(\varphi)\,T(k_0)\psi\| + \sqrt{N}\|\phi(\varphi_t^{(N)})T(k_t)\mathcal{U}(t,0)\psi\|\right) \\
&\qquad \le \frac{1}{2}\|\mathcal{N}\,T(k_t)\mathcal{U}(t,0)\psi\|^2 \\
&\qquad\quad + C\left(\|\mathcal{N}\,T(k_0)\psi\|^2 + N\|\phi(\varphi)\,T(k_0)\psi\|^2 + N\|\phi(\varphi_t^{(N)})T(k_t)\mathcal{U}(t,0)\psi\|^2\right).
\end{aligned}$$

Subtracting the first term appearing on the r. h. s., and using the bound from Lemma 1.4.2 that $\|\phi(f)\psi\| \le 2\|f\|_2\|(\mathcal{N}+1)^{1/2}\psi\|$, we find that

$$\begin{aligned}
&\langle\psi,\mathcal{U}^*(t,0)T^*(k_t)\mathcal{N}^2T(k_t)\mathcal{U}(t,0)\psi\rangle \\
&\quad \le C\left(\|\mathcal{N}\,T(k_0)\psi\|^2 + N\|(\mathcal{N}+1)^{1/2}T(k_0)\psi\|^2 + N\|(\mathcal{N}+1)^{1/2}T(k_t)\mathcal{U}(t,0)\psi\|^2\right).
\end{aligned}$$

By Lemma 2.4.3 we conclude that

$$\begin{aligned}\langle \psi, \mathcal{U}^*(t,0)T^*(k_t)\mathcal{N}^2 T(k_t)\mathcal{U}(t,0)\psi\rangle \\ \leq CN\|\mathcal{N}^{1/2}\mathcal{U}(t,0)\psi\|^2 + C\|\mathcal{N}\psi\|^2 + CN\|(\mathcal{N}+1)^{1/2}\psi\|^2.\end{aligned}$$

With (2.43), this concludes the proof of the proposition. □

We are now ready to show Theorem 2.4.1. The basic idea is to apply the Grönwall lemma. Unfortunately we can not control $\frac{d}{dt}\langle\psi, \widetilde{\mathcal{U}}^*(t,0)\mathcal{N}\widetilde{\mathcal{U}}(t,0)\psi\rangle$ with $\langle\psi, \widetilde{\mathcal{U}}^*(t,0)\mathcal{N}\widetilde{\mathcal{U}}(t,0)\psi\rangle$; however, we can bound it using $\tilde{\mathcal{L}}_N(t) + \mathcal{N}$. Similarly we can bound the derivative of the expectation of $\tilde{\mathcal{L}}_N(t)$ using $\tilde{\mathcal{L}}_N(t) + \mathcal{N}$. Consequently, we can bound the derivative of the expectation value of $\tilde{\mathcal{L}}_N(t) + \mathcal{N}$ using $\tilde{\mathcal{L}}_N(t) + \mathcal{N}$, and thus apply the Grönwall lemma. We then use a lower bound for $\tilde{\mathcal{L}}_N(t)$ to derive a bound for the expectation of $\mathcal{N}$. The precise calculation looks a bit more complicated since we have to keep track of the constants (and the exponential factors).

Proof of Theorem 2.4.1. Let $C_N(t)$ be defined as in (2.34) and define

$$\widetilde{\mathcal{U}}(t,s) = e^{i\int_s^t C_N(\tau)d\tau}\mathcal{U}(t,s).$$

Then $\widetilde{\mathcal{U}}(t,s)$ satisfies the Schrödinger type equation

$$i\partial_t\widetilde{\mathcal{U}}(t,s) = \widetilde{\mathcal{L}}_N(t)\widetilde{\mathcal{U}}(t,s), \quad \text{with } \widetilde{\mathcal{U}}(s,s) = 1$$

for all $s \in \mathbb{R}$, and with generator $\widetilde{\mathcal{L}}_N(t) = \mathcal{L}_N(t) - C_N(t)$, as defined in (2.35). On the other hand, since the two evolutions only differ by a phase, we have

$$\langle\psi, \mathcal{U}^*(t,0)\mathcal{N}\mathcal{U}(t,0)\psi\rangle = \langle\psi, \widetilde{\mathcal{U}}^*(t,0)\mathcal{N}\widetilde{\mathcal{U}}(t,0)\psi\rangle.$$

We now use the properties of $\widetilde{\mathcal{L}}_N(t)$, as established in (2.36)–(2.39). Eq. (2.36) implies

$$\mathcal{H}_N \leq 2\widetilde{\mathcal{L}}_N(t) + C\frac{\mathcal{N}^2}{N} + Ce^{K|t|}(\mathcal{N}+1). \tag{2.46}$$

From Proposition 2.4.2, we conclude that there exists a constant C_1 (which depends on $\langle\psi, (\mathcal{N}^2/N + \mathcal{N} + 1)\psi\rangle$), such that

$$0 \leq \left\langle\psi, \widetilde{\mathcal{U}}^*(t,0)\mathcal{H}_N\widetilde{\mathcal{U}}(t,0)\psi\right\rangle \leq \left\langle\psi, \widetilde{\mathcal{U}}^*(t,0)\left(2\widetilde{\mathcal{L}}_N(t) + C_1e^{K|t|}(\mathcal{N}+1)\right)\widetilde{\mathcal{U}}(t,0)\psi\right\rangle. \tag{2.47}$$

From (2.38), combined with (2.46) and Proposition 2.4.2, there exists moreover a constant $C_2 > 0$ (depending on $\langle\psi, (\mathcal{N}^2/N + \mathcal{N} + 1)\psi\rangle$) such that

$$\frac{d}{dt}\left\langle\psi, \widetilde{\mathcal{U}}^*(t,0)\mathcal{N}\widetilde{\mathcal{U}}(t,0)\psi\right\rangle \leq \left\langle\psi, \widetilde{\mathcal{U}}^*(t,0)\left(2\widetilde{\mathcal{L}}_N(t) + C_2e^{K|t|}(\mathcal{N}+1)\right)\widetilde{\mathcal{U}}(t,0)\psi\right\rangle.$$

We now estimate the growth of the expectation of the generator $\widetilde{\mathcal{L}}_N(t)$. Using (2.39) together with (2.46) and Proposition 2.4.2, we conclude that there exists a constant $C_3 > 0$ (again, depending on $\langle\psi, (\mathcal{N}^2/N + \mathcal{N} + 1)\psi\rangle$), with

$$\begin{aligned}\frac{d}{dt}\left\langle\psi, \widetilde{\mathcal{U}}^*(t,0)\widetilde{\mathcal{L}}_N(t)\widetilde{\mathcal{U}}(t,0)\psi\right\rangle &= \left\langle\psi, \widetilde{\mathcal{U}}^*(t,0)\dot{\widetilde{\mathcal{L}}}_N(t)\widetilde{\mathcal{U}}(t,0)\psi\right\rangle \\ &\leq \left\langle\psi, \widetilde{\mathcal{U}}^*(t,0)\left(2\widetilde{\mathcal{L}}_N(t) + C_3e^{K|t|}(\mathcal{N}+1)\right)\widetilde{\mathcal{U}}(t,0)\psi\right\rangle.\end{aligned}$$

We now fix $D := \max(C_1 + 1, C_2, C_3, K)$. Then, we have

$$\begin{aligned}
&\frac{d}{dt}\left\langle \psi, \widetilde{\mathcal{U}}^*(t,0)\left(\widetilde{\mathcal{L}}_N(t) + De^{K|t|}(\mathcal{N}+1)\right)\widetilde{\mathcal{U}}(t,0)\psi\right\rangle \\
&\quad\leq \left\langle \psi, \widetilde{\mathcal{U}}^*(t,0)\left[(2+2De^{K|t|})\widetilde{\mathcal{L}}_N(t) + (De^{K|t|} + DKe^{K|t|} + D^2e^{2K|t|})(\mathcal{N}+1)\right]\widetilde{\mathcal{U}}(t,0)\psi\right\rangle \\
&\quad\leq 4De^{K|t|}\left\langle \psi, \widetilde{\mathcal{U}}^*(t,0)\left(\widetilde{\mathcal{L}}_N(t) + De^{K|t|}(\mathcal{N}+1)\right)\widetilde{\mathcal{U}}(t,0)\psi\right\rangle.
\end{aligned}$$

By Grönwall's lemma, we conclude that

$$\begin{aligned}
&\left\langle \psi, \widetilde{\mathcal{U}}^*(t,0)\left(\widetilde{\mathcal{L}}_N(t) + De^{K|t|}(\mathcal{N}+1)\right)\widetilde{\mathcal{U}}(t,0)\psi\right\rangle \\
&\quad\leq e^{4\frac{D}{K}e^{K|t|}}\left\langle \psi, \left(\widetilde{\mathcal{L}}_N(0) + D(\mathcal{N}+1)\right)\psi\right\rangle \\
&\quad\leq e^{4\frac{D}{K}e^{K|t|}}\left\langle \psi, \left(\frac{3}{2}\mathcal{H}_N + C\frac{\mathcal{N}^2}{N} + C(\mathcal{N}+1)\right)\psi\right\rangle
\end{aligned}$$

where in the last inequality, we used the upper bound (2.37). From assumption (2.40) we then obtain

$$\left\langle \psi, \widetilde{\mathcal{U}}^*(t,0)\left(\widetilde{\mathcal{L}}_N(t) + De^{K|t|}(\mathcal{N}+1)\right)\widetilde{\mathcal{U}}(t,0)\psi\right\rangle \leq C\exp(c_1\exp(c_2|t|)). \tag{2.48}$$

Furthermore, from (2.47) we have

$$-\frac{C_1}{2}e^{K|t|}\langle \psi, \widetilde{\mathcal{U}}^*(t,0)(\mathcal{N}+1)\widetilde{\mathcal{U}}(t,0)\psi\rangle \leq \langle \psi, \widetilde{\mathcal{U}}^*(t,0)\widetilde{\mathcal{L}}_N(t)\widetilde{\mathcal{U}}(t,0)\psi\rangle.$$

Inserting this in (2.48) as a lower bound for $\widetilde{\mathcal{L}}_N(t)$ and recalling $D - C_1 \geq 1$, we obtain the intended bound for the expectation of $\mathcal{N}$. □

2.5. Proof of the main theorem

Using the bounds established in Theorem 2.4.1, we proceed now to prove our main result.

Proof of Theorem 2.1.1. Let $\Psi_{N,t} = e^{-i\mathcal{H}_N t}W(\sqrt{N}\varphi)T(k_0)\psi$. Recall that the one-particle reduced density matrix of $\Psi_{N,t}$ has the integral kernel

$$\gamma_{N,t}^{(1)}(x,y) = \frac{1}{\langle \Psi_{N,t}, \mathcal{N}\Psi_{N,t}\rangle}\langle \Psi_{N,t}, a_y^* a_x \Psi_{N,t}\rangle. \tag{2.49}$$

We start by computing the denominator. Since $\mathcal{H}_N$ commutes with the number of particles operator we find

$$\begin{aligned}
\langle \Psi_{N,t}, \mathcal{N}\Psi_{N,t}\rangle &= \langle \psi, T^*(k_0)W^*(\sqrt{N}\varphi)\mathcal{N}W(\sqrt{N}\varphi)T(k_0)\psi\rangle \\
&= \langle \psi, T^*(k_0)\left(\mathcal{N} - \sqrt{N}\phi(\varphi) + N\right)T(k_0)\psi\rangle \\
&= N + \left\langle \psi, T^*(k_0)\left(\mathcal{N} - \sqrt{N}\phi(\varphi)\right)T(k_0)\psi\right\rangle.
\end{aligned}$$

By Lemma 2.4.3

$$\langle \psi, T^*(k_0)\mathcal{N}T(k_0)\psi\rangle \leq C\langle \psi, (\mathcal{N}+1)\,\psi\rangle \leq C$$

and

$$|\langle\psi, T^*(k_0)\phi(\varphi)T(k_0)\psi\rangle| \leq C\langle\psi, T^*(k_0)(\mathcal{N}+1)^{1/2}T(k_0)\psi\rangle \leq C\langle\psi, (\mathcal{N}+1)\psi\rangle \leq C.$$

Hence, there exists $C > 0$ with

$$|\langle\Psi_{N,t}, \mathcal{N}\Psi_{N,t}\rangle - N| \leq CN^{1/2}. \tag{2.50}$$

On the other hand, with $\varphi_t^{(N)}$ denoting the solution of the modified Gross-Pitaevskii equation (2.25), the numerator of (2.49) can be written as

$$\begin{aligned}
&\langle\Psi_{N,t}, a_y^* a_x \Psi_{N,t}\rangle \\
&\quad = \langle\psi, T(k_0)W(\sqrt{N}\varphi)e^{it\mathcal{H}_N} a_y^* a_x e^{-i\mathcal{H}_N t} W(\sqrt{N}\varphi)T(k_0)\psi\rangle \\
&\quad = N\,\varphi_t(x)\overline{\varphi}_t(y) \\
&\qquad + \sqrt{N}\,\varphi_t(x)\,\langle\psi, T^*(k_0)W^*(\sqrt{N}\varphi)e^{it\mathcal{H}_N}\left(a_y^* - \sqrt{N}\overline{\varphi}_t^{(N)}(y)\right)e^{-i\mathcal{H}_N t}W(\sqrt{N}\varphi)T(k_0)\psi\rangle \\
&\qquad + \sqrt{N}\,\overline{\varphi}_t(y)\,\langle\psi, T^*(k_0)W^*(\sqrt{N}\varphi)e^{it\mathcal{H}_N}\left(a_x - \sqrt{N}\varphi_t^{(N)}(x)\right)e^{-i\mathcal{H}_N t}W(\sqrt{N}\varphi)T(k_0)\psi\rangle \\
&\qquad + \Big\langle\psi, T^*(k_0)W^*(\sqrt{N}\varphi)e^{it\mathcal{H}_N}\left(a_y^* - \sqrt{N}\overline{\varphi}_t^{(N)}(y)\right) \\
&\qquad\qquad\qquad \times \left(a_x - \sqrt{N}\varphi_t^{(N)}(x)\right)e^{-i\mathcal{H}_N t}W(\sqrt{N}\varphi)T(k_0)\psi\Big\rangle.
\end{aligned}$$

Recognizing that

$$\begin{aligned}
(a_y^* - \sqrt{N}\overline{\varphi}_t^{(N)}(y)) &= W(\sqrt{N}\varphi_t^{(N)})a_y^* W^*(\sqrt{N}\varphi_t^{(N)}) \\
(a_x - \sqrt{N}\varphi_t^{(N)}(x)) &= W(\sqrt{N}\varphi_t^{(N)})a_x W^*(\sqrt{N}\varphi_t^{(N)})
\end{aligned}$$

we obtain

$$\begin{aligned}
&\langle\Psi_{N,t}, a_y^* a_x \Psi_{N,t}\rangle \\
&\quad = N\varphi_t^{(N)}(x)\overline{\varphi}_t^{(N)}(y) \\
&\qquad + \sqrt{N}\,\varphi_t^{(N)}(x)\,\langle\psi, T^*(k_0)W^*(\sqrt{N}\varphi)e^{it\mathcal{H}_N}W(\sqrt{N}\varphi_t^{(N)}) \\
&\qquad\qquad \times a_y^* W^*(\sqrt{N}\varphi_t^{(N)})e^{-i\mathcal{H}_N t}W(\sqrt{N}\varphi)T(k_0)\psi\rangle \\
&\qquad + \sqrt{N}\,\overline{\varphi}_t^{(N)}(y)\langle\psi, T^*(k_0)W^*(\sqrt{N}\varphi)e^{it\mathcal{H}_N}W(\sqrt{N}\varphi_t^{(N)}) \\
&\qquad\qquad \times a_x W^*(\sqrt{N}\varphi_t^{(N)})e^{-i\mathcal{H}_N t}W(\sqrt{N}\varphi)T(k_0)\psi\rangle \\
&\qquad + \langle\psi, T^*(k_0)W^*(\sqrt{N}\varphi)e^{it\mathcal{H}_N}W(\sqrt{N}\varphi_t^{(N)})a_y^* a_x W^*(\sqrt{N}\varphi_t^{(N)})e^{-i\mathcal{H}_N t}W(\sqrt{N}\varphi)T(k_0)\psi\rangle.
\end{aligned}$$

Combining the last equation with (2.50) and inserting in (2.49), we have that

$$\begin{aligned}
&\left|\gamma_{N,t}^{(1)}(x,y) - \overline{\varphi}_t^{(N)}(y)\varphi_t^{(N)}(x)\right| \\
&\quad \leq \frac{C}{\sqrt{N}}|\varphi_t^{(N)}(x)||\varphi_t^{(N)}(y)| \\
&\qquad + \frac{1}{\sqrt{N}}|\varphi_t^{(N)}(y)|\,\|a_x\,W^*(\sqrt{N}\varphi_t^{(N)})e^{-i\mathcal{H}_N t}W(\sqrt{N}\varphi)T(k_0)\psi\| \\
&\qquad + \frac{1}{\sqrt{N}}|\varphi_t^{(N)}(x)|\,\|a_y\,W^*(\sqrt{N}\varphi_t^{(N)})e^{-i\mathcal{H}_N t}W(\sqrt{N}\varphi)T(k_0)\psi\| \\
&\qquad + \frac{1}{N}\|a_y\,W^*(\sqrt{N}\varphi_t^{(N)})e^{-i\mathcal{H}_N t}W(\sqrt{N}\varphi)T(k_0)\psi\| \\
&\qquad\qquad \times \|a_x\,W^*(\sqrt{N}\varphi_t^{(N)})e^{-i\mathcal{H}_N t}W(\sqrt{N}\varphi)T(k_0)\psi\|.
\end{aligned}$$

Taking the square and integrating over x, y, we find

$$\left\| \gamma_{N,t}^{(1)} - |\varphi_t^{(N)}\rangle\langle\varphi_t^{(N)}| \right\|_{\mathrm{HS}} \leq \frac{C}{\sqrt{N}} \|(\mathcal{N}+1)^{1/2}\, W^*(\sqrt{N}\varphi_t^{(N)}) e^{-i\mathcal{H}_N t} W(\sqrt{N}\varphi) T(k_0)\psi\|^2.$$

Lemma 2.4.3 implies that

$$\begin{aligned} \left\| \gamma_{N,t}^{(1)} - |\varphi_t^{(N)}\rangle\langle\varphi_t^{(N)}| \right\|_{\mathrm{HS}} &\leq \frac{C}{\sqrt{N}} \|(\mathcal{N}+1)^{1/2}\, T^*(k_t) W^*(\sqrt{N}\varphi_t^{(N)}) e^{-i\mathcal{H}_N t} W(\sqrt{N}\varphi) T(k_0)\psi\|^2 \\ &= \frac{C}{\sqrt{N}} \|(\mathcal{N}+1)^{1/2}\, \mathcal{U}(t,0)\psi\|^2 \end{aligned}$$

with the fluctuation dynamics $\mathcal{U}(t,s)$ defined in (2.33). From Theorem 2.4.1 we conclude that

$$\left\| \gamma_{N,t}^{(1)} - |\varphi_t^{(N)}\rangle\langle\varphi_t^{(N)}| \right\|_{\mathrm{HS}} \leq \frac{C \exp(c_1 \exp(c_2|t|))}{\sqrt{N}}.$$

By Lemma 1.A.1 this implies

$$\mathrm{tr}\, \left| \gamma_{N,t}^{(1)} - |\varphi_t^{(N)}\rangle\langle\varphi_t^{(N)}| \right| \leq \frac{C \exp(c_1 \exp(c_2|t|))}{\sqrt{N}}.$$

Theorem 2.1.1 now follows because, if φ_t denotes the solution of the Gross-Pitaevskii equation (2.16), Proposition 2.3.1 implies that

$$\mathrm{tr}\, \left| |\varphi_t\rangle\langle\varphi_t| - |\varphi_t^{(N)}\rangle\langle\varphi_t^{(N)}| \right| \leq 2\|\varphi_t - \varphi_t^{(N)}\|_2 \leq \frac{Ce^{c_1|t|}}{N}. \qquad \square$$

2.6. Key bounds on the generator of the fluctuation dynamics

In this section, we prove Theorem 2.3.5, concerning the generator $\mathcal{L}_N(t)$ of the fluctuation dynamics

$$\mathcal{U}(t,s) = T^*(k_t) W^*(\sqrt{N}\varphi_t^{(N)}) e^{-i\mathcal{H}_N(t-s)} W(\sqrt{N}\varphi_s^{(N)}) T(k_s)$$

as defined in (2.33). We write

$$\begin{aligned} \mathcal{L}_N(t) &= T^*(k_t) \left[i\partial_t W^*(\sqrt{N}\varphi_t^{(N)}) \right] W(\sqrt{N}\varphi_t^{(N)}) T(k_t) \\ &\quad + T^*(k_t) W^*(\sqrt{N}\varphi_t^{(N)}) \mathcal{H}_N W(\sqrt{N}\varphi_t^{(N)}) T(k_t) + [i\partial_t T^*(k_t)]\, T(k_t) \\ &= T^*(k_t) \mathcal{L}_N^{(0)}(t) T(k_t) + [i\partial_t T^*(k_t)]\, T(k_t) \end{aligned} \tag{2.51}$$

with

$$\mathcal{L}_N^{(0)}(t) = \left[i\partial_t W^*(\sqrt{N}\varphi_t^{(N)}) \right] W(\sqrt{N}\varphi_t^{(N)}) + W^*(\sqrt{N}\varphi_t^{(N)}) \mathcal{H}_N W(\sqrt{N}\varphi_t^{(N)}).$$

A simple computation shows that

$$\left[i\partial_t W^*(\sqrt{N}\varphi_t^{(N)}) \right] W(\sqrt{N}\varphi_t^{(N)}) = -a(\sqrt{N} i\partial_t \varphi_t^{(N)}) - a^*(\sqrt{N} i\partial_t \varphi_t^{(N)}) - N\langle \varphi_t^{(N)}, i\partial_t \varphi_t^{(N)} \rangle.$$

On the other hand, using (1.40), we find

$$\begin{aligned}
&W^*(\sqrt{N}\varphi_t^{(N)})\mathcal{H}_N W(\sqrt{N}\varphi_t^{(N)}) \\
&\quad = N\left[\|\nabla\varphi_t^{(N)}\|_2^2 + \frac{1}{2}\int \mathrm{d}x\,(N^3V(N.)*|\varphi_t^{(N)}|^2)(x)|\varphi_t^{(N)}(x)|^2\right] \\
&\qquad + \sqrt{N}\left[a^*\left((N^3V(N.)*|\varphi_t^{(N)}|^2)\varphi_t^{(N)}\right) + a\left((N^3V(N.)*|\varphi_t^{(N)}|^2)\varphi_t^{(N)}\right)\right] \\
&\qquad + \left[\int \mathrm{d}x\,\nabla_x a_x^*\nabla_x a_x + \int \mathrm{d}x\,(N^3V(N.)*|\varphi_t^{(N)}|^2)(x)a_x^*a_x\right. \\
&\qquad\quad + \int \mathrm{d}x\mathrm{d}y N^3V(N(x-y))\varphi_t^{(N)}(x)\overline{\varphi}_t^{(N)}(y)a_x^*a_y \\
&\qquad\quad \left.+ \frac{1}{2}\int \mathrm{d}x\mathrm{d}y N^3V(N(x-y))\left(\varphi_t^{(N)}(x)\varphi_t^{(N)}(y)a_x^*a_y^* + \overline{\varphi}_t^{(N)}(x)\overline{\varphi}_t^{(N)}(y)a_xa_y\right)\right] \\
&\qquad + \frac{1}{\sqrt{N}}\int \mathrm{d}x\mathrm{d}y\, N^3V(N(x-y))a_x^*\left(\varphi_t^{(N)}(y)a_y^* + \overline{\varphi}_t^{(N)}(y)a_y\right)a_x \\
&\qquad + \frac{1}{2N}\int \mathrm{d}x\mathrm{d}y N^3V(N(x-y))a_x^*a_y^*a_ya_x.
\end{aligned}$$

Combining the last two equations and using (2.25), we conclude that

$$\begin{aligned}
\mathcal{L}_N^{(0)}(t) &= N\int \mathrm{d}x\left(N^3V(N.)\Big(\frac{1}{2}-f(N.)\Big)*|\varphi_t^{(N)}|^2\right)(x)|\varphi_t^{(N)}(x)|^2 \\
&\quad + \sqrt{N}\left[a^*\left((N^3w(N.)V(N.)*|\varphi_t^{(N)}|^2)\varphi_t^{(N)}\right) + a\left((N^3w(N.)V(N.)*|\varphi_t^{(N)}|^2)\varphi_t^{(N)}\right)\right] \\
&\quad + \left[\int \mathrm{d}x\,\nabla_x a_x^*\nabla_x a_x + \int \mathrm{d}x\,(N^3V(N.)*|\varphi_t^{(N)}|^2)(x)a_x^*a_x\right. \\
&\qquad + \int \mathrm{d}x\mathrm{d}y N^3V(N(x-y))\varphi_t^{(N)}(x)\overline{\varphi}_t^{(N)}(y)a_x^*a_y \\
&\qquad \left.+ \frac{1}{2}\int \mathrm{d}x\mathrm{d}y N^3V(N(x-y))\left(\varphi_t^{(N)}(x)\varphi_t^{(N)}(y)a_x^*a_y^* + \overline{\varphi}_t^{(N)}(x)\overline{\varphi}_t^{(N)}(y)a_xa_y\right)\right] \\
&\quad + \frac{1}{\sqrt{N}}\int \mathrm{d}x\mathrm{d}y\, N^3V(N(x-y))a_x^*\left(\varphi_t^{(N)}(y)a_y^* + \overline{\varphi}_t^{(N)}(y)a_y\right)a_x \\
&\quad + \frac{1}{2N}\int \mathrm{d}x\mathrm{d}y N^3V(N(x-y))a_x^*a_y^*a_ya_x \\
&=: \mathcal{L}_{0,N}^{(0)}(t) + \mathcal{L}_{1,N}^{(0)}(t) + \mathcal{L}_{2,N}^{(0)}(t) + \mathcal{L}_{3,N}^{(0)}(t) + \mathcal{L}_{4,N}^{(0)}
\end{aligned}$$

where $\mathcal{L}_{j,N}^{(0)}(t)$, for $j = 0,1,2,3,4$, is the part of $\mathcal{L}_N^{(0)}(t)$ containing the products of exactly j creation and annihilation operators. Recall here that $w(x) = 1 - f(x)$, as defined in (2.28).

From (2.51), we find that the generator of the fluctuation dynamics is given by

$$\mathcal{L}_N(t) = \mathcal{L}_{0,N}^{(0)}(t) + \sum_{j=1}^{4} T^*(k_t)\mathcal{L}_{j,N}^{(0)}(t)T(k_t) + [i\partial_t T^*(k_t)]\,T(k_t). \tag{2.52}$$

In the next subsections, we study separately the different terms on the r. h. s. of (2.52). The final goal of this analysis, a proof of Theorem 2.3.5, will be reached in Subsection 2.6.6.

Remark. The reader is invited to convince himself first of the cancellations explained in Subsection 2.6.6 and of their necessity. For understanding the estimates of the remaining terms of the generator $\mathcal{L}_N(t)$ without going through all the technical estimates below, we recommend to think of $a^\sharp(c_x)$ as $a^\sharp_x$ and of $a^\sharp(s_x)$ as $a^\sharp(k_x)$, neglecting p and r. Expand the generator completely (which gives a large number of terms) and consider the individual terms as inside an expectation value of a general vector in Fock space. The goal is to obtain bounds on their expectation value in terms of

$$C_\varepsilon \mathcal{N}, \quad C_\varepsilon \frac{\mathcal{N}^2}{N}, \quad \varepsilon\mathcal{K} \quad \text{and} \quad \varepsilon \frac{1}{2}\int \mathrm{d}x\mathrm{d}y\, N^2 V(N(x-y)) a_x^* a_y^* a_y a_x,$$

where $\varepsilon > 0$ is to be chosen small later, and $C_\varepsilon > 0$ is a N-independent constant possibly diverging as $\varepsilon \to 0$. The terms originating from the kinetic energy contain derivatives but are few and can be estimated one at a time. For the other terms, we have the following receipe. First, the singular operator a_x^* has to be moved to the other argument of the scalar product as a_x. The operator $a^*(k_x)$ can be kept and will be estimated by Lemma 1.4.2. Also, we distribute the operators such that there are no more than two in either argument of the scalar product. We then estimate scalar products by the Cauchy-Schwarz inequality and use $\int \mathrm{d}x\mathrm{d}y V(x-y) f(x,y) g(x,y) \le \int \mathrm{d}x\mathrm{d}y V(x-y)|f(x,y)|^2 + \int \mathrm{d}x\mathrm{d}y V(x-y)|g(x,y)|^2$, if necessary with a weight ε and $1/\varepsilon$ inserted for the two summands. Finally, we can use $\sup_x \|k_x\|^2$, $\|\varphi_t^{(N)}\|_\infty$ and the L^1-norm of NV_N, which is N-independent. The procedure for $\dot{\widetilde{\mathcal{L}}}_N(t)$ is similar but due to the even larger number of terms tedious. (Actually, $\dot{\widetilde{\mathcal{L}}}_N(t)$ is less singular, because $a^*(\dot{c}_x) = a^*(\dot{p}_x)$, where $\dot{p}_x$ is in L^2.)

Notation. In the rest of this section, we will use the shorthand notation

$$c_x(y) = \mathrm{ch}(k_t)(y,x),\ s_x(y) = \mathrm{sh}(k_t)(y,x),\ p_x(y) = p(k_t)(y,x),\ r_x(y) = r(k_t)(y,x). \quad (2.53)$$

Moreover, $\|p\|_2, \|r\|_2, \|\mathrm{sh}\|_2$ will denote the L^2-norms of the kernels $p(k_t)(x,y)$, $r(k_t)(x,y)$, and $\mathrm{sh}(k_t)(x,y)$ over $\mathbb{R}^3 \times \mathbb{R}^3$ (in other words, they denote the Hilbert-Schmidt norms of the corresponding operators). The norms $\|p_x\|_2, \|r_x\|_2, \|\mathrm{sh}_x\|_2$, on the other hand, indicate norms over $\mathbb{R}^3$. Finally, the notation $\langle .,. \rangle$ will denote the L^2 inner product. We will abbreviate $T(k_t)$ by T.

2.6.1. Analysis of the linear terms $T^*\mathcal{L}^{(0)}_{1,N}(t)T$

Conjugating the linear term $\mathcal{L}^{(0)}_{N,1}(t)$ with T produces again linear terms. From Lemma 2.2.1, we obtain

$$\begin{aligned}
&T^*\mathcal{L}^{(0)}_{1,N}(t)T \qquad (2.54)\\
&= \sqrt{N}\int \mathrm{d}x\mathrm{d}y\, N^3 V(N(x-y)) w(N(x-y)) |\varphi_t^{(N)}(y)|^2 \left(\varphi_t^{(N)}(x) T^* a_x^* T + \overline{\varphi}_t^{(N)}(x) T^* a_x T\right)\\
&= \sqrt{N}\int \mathrm{d}x\mathrm{d}y\, N^3 V(N(x-y)) w(N(x-y)) |\varphi_t^{(N)}(y)|^2\, \varphi_t^{(N)}(x)\, (a^*(c_x) + a(s_x))\\
&\quad + \sqrt{N}\int \mathrm{d}x\mathrm{d}y\, N^3 V(N(x-y)) w(N(x-y)) |\varphi_t^{(N)}(y)|^2\, \overline{\varphi}_t^{(N)}(x)\, (a(c_x) + a^*(s_x)).
\end{aligned}$$

These terms are potentially dangerous because they are large (of order $\sqrt{N}$) and do not commute with the number of particles. We will see however that they cancel with contributions arising from the cubic part $\mathcal{L}^{(0)}_{3,N}(t)$.

2.6.2. Analysis of the quadratic terms $T^*\mathcal{L}^{(0)}_{2,N}(t)T$

We split $\mathcal{L}^{(0)}_{2,N}(t)$ into a kinetic and a non-kinetic part, writing

$$\mathcal{L}^{(0)}_{2,N}(t) = \mathcal{K} + \widehat{\mathcal{L}}^{(0)}_{2,N}(t),$$

with $\mathcal{K} = \int \mathrm{d}x\, \nabla_x a^*_x \nabla_x a_x$ being the kinetic energy operator, and we consider separately the effects of $\mathcal{K}$ and of the other quadratic terms collected in $\widehat{\mathcal{L}}^{(0)}_{2,N}(t)$.

Properties of the kinetic part $T^*\mathcal{K}T$

We have

$$\begin{aligned} T^*\mathcal{K}T =& \int \mathrm{d}x\, \nabla_x(a^*(c_x) + a(s_x))\, \nabla_x(a(c_x) + a^*(s_x)) \\ =& \int \mathrm{d}x \nabla_x a^*(c_x)\nabla_x a(c_x) + \int \mathrm{d}x \nabla_x a^*(c_x)\nabla_x a^*(s_x) \\ &+ \int \mathrm{d}x \nabla_x a(s_x)\nabla_x a(c_x) + \int \mathrm{d}x \nabla a^*(s_x)\nabla_x a(s_x) + \int \mathrm{d}x \|\nabla_x s_x\|_2^2. \end{aligned}$$

Following (2.20), we decompose $c_x(y) = \delta(x-y) + p_x(y)$ and $s_x(y) = k(x,y) + r_x(y)$. Hence

$$\begin{aligned} T^*\mathcal{K}T = \mathcal{K} &+ \int \mathrm{d}x\mathrm{d}y\, |\nabla_x \mathrm{sh}_{k_t}(y,x)|^2 + \\ &+ \int \mathrm{d}x \nabla_x a^*_x a(\nabla_x p_x) + \int \mathrm{d}x a^*(\nabla_x p_x)\nabla_x a_x + \int \mathrm{d}x a^*(\nabla_x p_x) a(\nabla_x p_x) \\ &+ \int \mathrm{d}x \nabla_x a^*_x a^*(\nabla_x k_x) + \int \mathrm{d}x a^*(\nabla_x p_x) a^*(\nabla_x k_x) + \int \mathrm{d}x \nabla_x a^*_x a^*(\nabla_x r_x) \\ &+ \int \mathrm{d}x a^*(\nabla_x p_x) a^*(\nabla_x r_x) + \int \mathrm{d}x\, a(\nabla_x k_x)\nabla_x a_x + \int \mathrm{d}x a(\nabla_x r_x)\nabla_x a_x \\ &+ \int \mathrm{d}x a(\nabla_x k_x) a(\nabla_x p_x) + \int \mathrm{d}x a(\nabla_x r_x) a(\nabla_x p_x) + \int \mathrm{d}x\, a^*(\nabla_x k_x) a(\nabla_x k_x) \\ &+ \int \mathrm{d}x\, a^*(\nabla_x r_x) a(\nabla_x k_x) + \int \mathrm{d}x\, a^*(\nabla_x k_x) a(\nabla_x r_x) + \int \mathrm{d}x\, a^*(\nabla_x r_x) a(\nabla_x r_x). \end{aligned} \tag{2.55}$$

The properties of $T^*\mathcal{K}T$ are summarized in the next proposition.

Proposition 2.6.1. *We have*

$$\begin{aligned} T^*\mathcal{K}T =& \int dx\, dy |\nabla_x sh_{k_t}(y,x)|^2 + \mathcal{K} \\ &+ N^3 \int dx\, dy (\Delta w)(N(x-y)) \left(\varphi^{(N)}_t(x)\varphi^{(N)}_t(y) a^*_x a^*_y + \overline{\varphi}^{(N)}_t(x)\overline{\varphi}^{(N)}_t(y) a_x a_y \right) \\ &+ \mathcal{E}_K(t) \end{aligned} \tag{2.56}$$

where the error $\mathcal{E}_K(t)$ is an operator such that for every $\delta > 0$ there exists a constant $C_\delta > 0$ with

$$\begin{aligned} \pm\, \mathcal{E}_K(t) &\leq \delta\mathcal{K} + C_\delta e^{K|t|}\, (\mathcal{N}+1), \\ \pm\, [\mathcal{N}, \mathcal{E}_K(t)] &\leq \delta\mathcal{K} + C_\delta e^{K|t|}\, (\mathcal{N}+1), \\ \pm\, \dot{\mathcal{E}}_K(t) &\leq \delta\mathcal{K} + C_\delta e^{K|t|}\, (\mathcal{N}+1). \end{aligned} \tag{2.57}$$

To prove Proposition 2.6.1, we will use the next lemma.

Lemma 2.6.2. *Let $j_1, j_2 \in L^2(\mathbb{R}^3 \times \mathbb{R}^3)$. Let $j_{i,x}(z) := j_i(z,x)$ for $i = 1, 2$. Then we have*

$$\left| \int dx \langle \psi, a^\sharp(j_{1,x}) a^\sharp(j_{2,x}) \psi \rangle \right| \leq C \|j_1\|_2 \|j_2\|_2 \, \|(\mathcal{N}+1)^{1/2}\psi\|^2. \tag{2.58}$$

Here and in the following $a^\sharp$ can be either the annihilation operator a or the creation operator a^*. Moreover, for every $\delta > 0$, there exists $C_\delta > 0$ such that

$$\begin{aligned} &\left| \int dx \langle \psi, \nabla_x a_x^* a^\sharp(j_{1,x}) \psi \rangle \right| \leq \delta \mathcal{K} + C_\delta \|j_1\|_2^2 \|(\mathcal{N}+1)^{1/2}\psi\|^2 \quad \textit{and, by conjugation} \\ &\left| \int dx \langle \psi, a^\sharp(j_{1,x}) \nabla_x a_x \psi \rangle \right| \leq \delta \mathcal{K} + C_\delta \|j_1\|_2^2 \, \|(\mathcal{N}+1)^{1/2}\psi\|^2. \end{aligned} \tag{2.59}$$

Terms where the argument of a creation and/or annihilation operator is the kernel $\nabla_x k_x$ (whose L^2-norm diverges as $N \to \infty$) can be handled with the following bounds. For every $\delta > 0$ there exists $C_\delta > 0$ s.t.

$$\begin{aligned} &\left| \int dx \langle \psi, a^*(\nabla_x k_x) a^\sharp(j_{1,x}) \psi \rangle \right| \leq \delta \mathcal{K} + C_\delta (1 + \|j_1\|_2^2) \|(\mathcal{N}+1)^{1/2}\psi\|^2 \quad \textit{and, by conjugation} \\ &\left| \int dx \langle \psi, a^\sharp(j_{1,x}) a(\nabla_x k_x) \psi \rangle \right| \leq \delta \mathcal{K} + C_\delta (1 + \|j_1\|_2^2) \|(\mathcal{N}+1)^{1/2}\psi\|^2. \end{aligned} \tag{2.60}$$

Moreover, we have

$$\left| \int dx \langle \psi, a^*(\nabla_x k_x) a(\nabla_x k_x) \psi \rangle \right| \leq C \|\mathcal{N}^{1/2}\psi\|^2. \tag{2.61}$$

To control the time derivative of $\mathcal{E}_K(t)$, we will also use the following bounds. For every $\delta > 0$ there exists $C_\delta > 0$ such that

$$\left| \int dx \langle \psi, a^*(\nabla_x \dot{k}_x) a^\sharp(j_{1,x}) \psi \rangle \right| \leq \delta \mathcal{K} + C_\delta e^{K|t|} (1 + \|j_1\|_2^2) \, \|(\mathcal{N}+1)^{1/2}\psi\|^2. \tag{2.62}$$

Moreover,

$$\left| \int dx \langle \psi, a^*(\nabla_x \dot{k}_x) a(\nabla_x k_x) \psi \rangle \right| \leq C e^{K|t|} \|\mathcal{N}^{1/2}\psi\|^2. \tag{2.63}$$

Proof. To prove (2.58), we compute

$$\begin{aligned} \left| \int \mathrm{d}x \langle \psi, a^\sharp(j_{1,x}) a^\sharp(j_{2,x}) \psi \rangle \right| &\leq \int \mathrm{d}x \|a^\sharp(j_{1,x})\psi\| \, \|a^\sharp(j_{2,x})\psi\| \\ &\leq \left(\int \mathrm{d}x \|j_{1,x}\|_2 \|j_{2,x}\|_2 \right) \|(\mathcal{N}+1)^{1/2}\psi\|^2 \\ &\leq \|j_1\|_2 \|j_2\|_2 \, \|(\mathcal{N}+1)^{1/2}\psi\|^2. \end{aligned}$$

Eq. (2.59), on the other hand, follows by

$$\begin{aligned} \left| \int \mathrm{d}x \langle \psi, \nabla_x a_x^* a^\sharp(j_{1,x}) \psi \rangle \right| &\leq \int \mathrm{d}x \|\nabla_x a_x \psi\| \, \|a^\sharp(j_{1,x})\psi\| \\ &\leq \delta \langle \psi, \mathcal{K}\psi \rangle + C_\delta \int \mathrm{d}x \|j_{1,x}\|_2^2 \, \|(\mathcal{N}+1)^{1/2}\psi\|^2 \\ &\leq \delta \langle \psi, \mathcal{K}\psi \rangle + C_\delta \|j_1\|_2^2 \, \|(\mathcal{N}+1)^{1/2}\psi\|^2. \end{aligned} \tag{2.64}$$

To show (2.60), we need to integrate by parts. We write

$$\int \mathrm{d}x a^*(\nabla_x k_x) a^\sharp(j_{1,x}) = \int \mathrm{d}x\mathrm{d}y\, \nabla_x k(y,x)\, a_y^* a^\sharp(j_{1,x})$$

and we observe that

$$\nabla_x k(y,x) = -\nabla_y k(y,x) - Nw(N(y-x))\left(\nabla\varphi_t^{(N)}(x)\varphi_t^{(N)}(y) + \varphi_t^{(N)}(x)\nabla\varphi_t^{(N)}(y)\right).$$

Hence

$$\begin{aligned}\int \mathrm{d}x a^*(\nabla_x k_x) a^\sharp(j_{1,x}) = &\int \mathrm{d}x\mathrm{d}y k(x,y)\, \nabla_y a_y^* a^\sharp(j_{1,x})\\ &- \int \mathrm{d}x\mathrm{d}y Nw(N(x-y))\nabla\varphi_t^{(N)}(x)\varphi_t^{(N)}(y)\, a_y^*\, a^\sharp(j_{1,x})\\ &- \int \mathrm{d}x\mathrm{d}y Nw(N(x-y))\nabla\varphi_t^{(N)}(y)\varphi_t^{(N)}(x)\, a_y^*\, a^\sharp(j_{1,x}).\end{aligned}$$

This implies, using Lemma 2.3.2 to bound $Nw(N(x-y))$,

$$\begin{aligned}&\Big|\int dx\langle\psi, a^*(\nabla_x k_x) a^\sharp(j_{1,x})\psi\rangle\Big|\\ &\le \int \mathrm{d}x\mathrm{d}y\, |k(x,y)|\|\nabla_y a_y\psi\|\, \|a^\sharp(j_{1,x})\psi\|\\ &\quad + C\int \mathrm{d}x\mathrm{d}y\, \frac{1}{|x-y|}\left(|\nabla\varphi_t^{(N)}(x)||\varphi_t^{(N)}(y)| + |\nabla\varphi_t^{(N)}(y)||\varphi_t^{(N)}(x)|\right)\|a_y\psi\|\, \|a^\sharp(j_{1,x})\psi\|\\ &\le \delta\int \mathrm{d}x\mathrm{d}y|\varphi_t^{(N)}(x)|^2\|\nabla_y a_y\psi\|^2 + C_\delta\int \mathrm{d}x\mathrm{d}y\frac{1}{|x-y|^2}|\varphi_t^{(N)}(y)|^2\|j_{1,x}\|_2^2\|(\mathcal{N}+1)^{1/2}\psi\|^2\\ &\quad + C\int \mathrm{d}x\mathrm{d}y\frac{1}{|x-y|^2}|\varphi_t^{(N)}(y)|^2\|j_{1,x}\|_2^2\|(\mathcal{N}+1)^{1/2}\psi\|^2 + C\int \mathrm{d}x\mathrm{d}y|\nabla\varphi_t^{(N)}(x)|^2\|a_y\psi\|^2\\ &\quad + C\int \mathrm{d}x\mathrm{d}y\frac{1}{|x-y|^2}|\varphi_t^{(N)}(x)|^2\|a_y\psi\|^2 + C\int \mathrm{d}x\mathrm{d}y|\nabla\varphi_t^{(N)}(y)|^2\|j_{1,x}\|_2^2\|(\mathcal{N}+1)^{1/2}\psi\|^2.\end{aligned}$$

Using Hardy's inequality, we conclude that for every $\delta > 0$ there exists $C_\delta > 0$ (depending on $\|j_1\|_2$, δ, $\|\varphi_t^{(N)}\|_{H^1}$) such that

$$\left|\langle\psi, \int \mathrm{d}x\, a^*(\nabla_x k_x) a^\sharp(j_{1,x})\psi\rangle\right| \le \delta\langle\psi, \mathcal{K}\psi\rangle + C_\delta(1+\|j_1\|_2^2)\,\langle\psi, (\mathcal{N}+1)\psi\rangle.$$

To show (2.61), we write

$$\begin{aligned}\int \mathrm{d}x\, a^*(\nabla_x k_x) a(\nabla_x k_x) &= \int \mathrm{d}x\mathrm{d}y_1\mathrm{d}y_2\, \nabla_x k(y_1,x)\nabla_x \overline{k}(y_2,x)\, a_{y_1}^* a_{y_2}\\ &=: \int \mathrm{d}y_1\mathrm{d}y_2\; g(y_1,y_2) a_{y_1}^* a_{y_2}.\end{aligned}$$

We have

$$\begin{aligned}&\Big|\int \mathrm{d}y_1\mathrm{d}y_2\, g(y_1,y_2)\langle\psi, a_{y_1}^* a_{y_2}\psi\rangle\Big|\\ &\qquad\le \int \mathrm{d}y_1\mathrm{d}y_2|g(y_1,y_2)|\|a_{y_1}\psi\|\, \|a_{y_2}\psi\|\\ &\qquad\le \left(\int \mathrm{d}y_1\mathrm{d}y_2|g(y_1,y_2)|^2\right)^{1/2}\left(\int \mathrm{d}y_1\mathrm{d}y_2\, \|a_{y_1}\psi\|^2\, \|a_{y_2}\psi\|^2\right)^{1/2}\\ &\qquad= \|g\|_2\, \|\mathcal{N}^{1/2}\psi\|^2.\end{aligned}$$

Moreover, from the definition (2.31) of the kernel k_t and from the bounds of Lemma 2.3.2, we find

$$\begin{aligned}\|g\|_2^2 \leq C \int \mathrm{d}y_1\mathrm{d}y_2\mathrm{d}x_1\mathrm{d}x_2 \frac{|\varphi_t^{(N)}(x_1)|^2|\varphi_t^{(N)}(x_2)|^2|\varphi_t^{(N)}(y_1)|^2|\varphi_t^{(N)}(y_2)|^2}{|x_1-y_1|^2|x_1-y_2|^2|x_2-y_1|^2|x_2-y_2|^2} \\ + C\int \mathrm{d}y_1\mathrm{d}y_2\mathrm{d}x_1\mathrm{d}x_2 \frac{|\nabla\varphi_t^{(N)}(x_1)|^2|\nabla\varphi_t^{(N)}(x_2)|^2|\varphi_t^{(N)}(y_1)|^2|\varphi_t^{(N)}(y_2)|^2}{|x_1-y_1||x_1-y_2||x_2-y_1||x_2-y_2|} \\ \leq C\int \mathrm{d}y_1\mathrm{d}y_2\mathrm{d}x_1\mathrm{d}x_2 \frac{|\varphi_t^{(N)}(x_1)|^6|\varphi_t^{(N)}(x_2)|^2}{|x_1-y_1|^2|x_1-y_2|^2|x_2-y_1|^2|x_2-y_2|^2} \\ + C\int \mathrm{d}y_1\mathrm{d}y_2\mathrm{d}x_1\mathrm{d}x_2 \frac{|\nabla\varphi_t^{(N)}(x_1)|^2|\nabla\varphi_t^{(N)}(x_2)|^2|\varphi_t^{(N)}(y_1)|^2|\varphi_t^{(N)}(y_2)|^2}{|x_1-y_1|^2|x_2-y_2|^2} \\ \leq C\int \mathrm{d}x_1 dx_2 \frac{1}{|x_1-x_2|^2}|\varphi_t^{(N)}(x_1)|^6|\varphi_t^{(N)}(x_2)|^2 \\ + C\left(\sup_x \int \mathrm{d}y \frac{1}{|x-y|^2}|\varphi_t^{(N)}(y)|^2\right)^2 \|\varphi_t^{(N)}\|_{H^1}^4 \\ \leq C\end{aligned}$$

for a constant C depending only on the H^1-norm of $\varphi_t^{(N)}$. The last two bounds prove (2.61).

The inequalities (2.62), (2.63) can be proven similarly to (2.60) and (2.61); this time, however, the bounds will contain the norm $\|\dot{\varphi}_t^{(N)}\|_{H^1}$, which is bounded by $Ce^{K|t|}$, as proven in Proposition 2.3.1. □

Proof of Proposition 2.6.1. We prove the first bound in (2.57). To this end, we observe that Lemma 2.6.2 can be used to bound all factors on the r. h. s. of (2.55) (using the uniform estimates for $\|\nabla_1 p(k_t)\|_{L^2(\mathbb{R}^3\times\mathbb{R}^3)}, \|\nabla_1 r_{k_t}\|_{L^2(\mathbb{R}^3\times\mathbb{R}^3)}$ from Lemma 2.3.3), with two exceptions, given by the term

$$\int \mathrm{d}x \nabla_x a_x^* a^*(\nabla_x k_x) \tag{2.65}$$

and its hermitian conjugate. To control (2.65), we use that, from (2.31),

$$\nabla_x k_t(y,x) = -N^2\nabla w(N(x-y))\varphi_t^{(N)}(x)\varphi_t^{(N)}(y) - Nw(N(x-y))\nabla\varphi_t^{(N)}(x)\varphi_t^{(N)}(y).$$

Hence

$$\begin{aligned}\int \mathrm{d}x\, \nabla_x a_x^* a^*(\nabla_x k_x) = &- N^2 \int \mathrm{d}x\mathrm{d}y \nabla w(N(x-y))\varphi_t^{(N)}(x)\varphi_t^{(N)}(y)\nabla_x a_x^* a_y^* \\ &- N\int \mathrm{d}x\mathrm{d}y\, w(N(x-y))\nabla\varphi_t^{(N)}(x)\varphi_t^{(N)}(y)\nabla_x a_x^* a_y^*.\end{aligned} \tag{2.66}$$

The last term can be written as

$$\int \mathrm{d}x \nabla_x a_x^* a^*(j_x) \tag{2.67}$$

with $j(y,x) = -Nw(N(x-y))\nabla\varphi_t^{(N)}(x)\varphi_t^{(N)}(y)$. Combining Lemma 2.3.2 and Proposition 2.3.1, we find that $j \in L^2(\mathbb{R}^3\times\mathbb{R}^3)$, with uniformly bounded norm. Hence, Lemma 2.6.2 implies that, for every $\delta > 0$, there exists $C_\delta > 0$ with

$$\left|\int \mathrm{d}x\, \langle\psi, \nabla_x a_x^* a^*(j_x)\psi\rangle\right| \leq \delta\|\mathcal{K}^{1/2}\psi\|^2 + C_\delta\|(\mathcal{N}+1)^{1/2}\psi\|^2. \tag{2.68}$$

The first term on the r. h. s. of (2.66), on the other hand, can be written as

$$\begin{aligned}-N^2 \int \mathrm{d}x\mathrm{d}y \nabla w(N(x-y)) \varphi_t^{(N)}(x)\varphi_t^{(N)}(y)\nabla_x a_x^* a_y^* \\ = N^3 \int \mathrm{d}x\mathrm{d}y (\Delta w)(N(x-y))\varphi_t^{(N)}(x)\varphi_t^{(N)}(y) a_x^* a_y^* \\ + N^2 \int \mathrm{d}x\mathrm{d}y \nabla w(N(x-y))\nabla\varphi_t^{(N)}(x)\varphi_t^{(N)}(y) a_x^* a_y^*.\end{aligned}$$

The first contribution on the r. h. s. of the last equation is large and appears explicitly on the r. h. s. of (2.56) (it will cancel later, when combined with terms arising from $\widehat{\mathcal{L}}_{2,N}^{(0)}$ and $\mathcal{L}_{4,N}^{(0)}$). The second term, on the other hand, is an error; integrating by parts, it can be expressed as

$$\begin{aligned}N^2 \int \mathrm{d}x\mathrm{d}y \nabla w(N(x-y))\nabla\varphi_t^{(N)}(x)\varphi_t^{(N)}(y) a_x^* a_y^* \\ = -N \int \mathrm{d}x\mathrm{d}y w(N(x-y))\nabla\varphi_t^{(N)}(x)\nabla\varphi_t^{(N)}(y) a_x^* a_y^* \\ - N \int \mathrm{d}x\mathrm{d}y w(N(x-y))\nabla\varphi_t^{(N)}(x)\varphi_t^{(N)}(y) a_x^* \nabla_y a_y^* \\ = -\int \mathrm{d}x \nabla\varphi_t^{(N)}(x) a_x^* a^*(N w(N(x-.)\nabla\varphi_t^{(N)}) + \int \mathrm{d}y \nabla_y a_y^* a^*(j_y)\end{aligned}$$

with $j(x,y) = -N w(N(x-y))\nabla\varphi_t^{(N)}(x)\varphi_t^{(N)}(y)$. The second term is bounded as in (2.68). The first term, on the other hand, is estimated by

$$\begin{aligned}\Big| \int \mathrm{d}x \nabla\varphi_t^{(N)}(x) \langle a_x\psi, a^*(N w(N(x-.))\nabla\varphi_t^{(N)})\psi\rangle \Big| \\ \leq C \sup_x \|N w(N(x-.))\nabla\varphi_t^{(N)}\|_2 \|(\mathcal{N}+1)^{1/2}\psi\|^2 \\ \leq C\|\varphi_t^{(N)}\|_{H^2}\|(\mathcal{N}+1)^{1/2}\psi\|^2\end{aligned} \tag{2.69}$$

and (2.27).

Also the second bound in (2.57) follows from Lemma 2.6.2. In fact, when one takes the commutator of $\mathcal{N}$ with the terms on the r. h. s. of (2.55) one either finds zero (for all terms with one creation and one annihilation operators, which therefore preserve the number of particles), or one finds again the same terms (up to a possible change of sign). This follows because by the canonical commutation relations

$$[\mathcal{N}, a(f)] = -a(f) \qquad \text{and} \qquad [\mathcal{N}, a^*(f)] = a^*(f)$$

for every $f \in L^2(\mathbb{R}^3)$. Finally, the third bound in (2.57) is a consequence of Lemma 2.6.2 as well. In fact, the time derivative $\dot{\mathcal{E}}_K(t)$ is a sum of terms very similar to the terms appearing on the r. h. s. of (2.55), with the difference that one of the appearing kernels contains a time-derivative. Combining the estimates from Lemma 2.6.2 (including, in this case, also (2.62), (2.63)) with the bounds for $\|\nabla_1 \dot{p}_{k_t}\|_2$, $\|\nabla_1 \dot{r}_{k_t}\|_2$ from Lemma 2.3.4 and with the bound for $\|\dot{\varphi}_t^{(N)}\|_{H^1}$ from Proposition 2.3.1 (needed to control terms similar to (2.66), (2.69), with a factor of $\varphi_t^{(N)}$ replaced by $\dot{\varphi}_t^{(N)}$), we obtain the last inequality in (2.57). □

Properties of the non-kinetic part $T^*\widehat{\mathcal{L}}^{(0)}_{2,N}(t)T$

We consider now the other quadratic terms, collected in $\widehat{\mathcal{L}}^{(0)}_{2,N}(t)$, defined by $\mathcal{L}^{(0)}_{2,N}(t) = \mathcal{K} + \widehat{\mathcal{L}}^{(0)}_{2,N}(t)$. We have

$$\begin{aligned} T^*\widehat{\mathcal{L}}^{(0)}_{2,N}(t)T = & \int \mathrm{d}x \left(N^3V(N.) * |\varphi_t^{(N)}|^2\right)(x)(a^*(c_x)+a(s_x))(a(c_x)+a^*(s_x)) \\ & + \int \mathrm{d}x\mathrm{d}y\, N^3V(N(x-y))\varphi_t^{(N)}(x)\overline{\varphi}_t^{(N)}(y)(a^*(c_x)+a(s_x))(a(c_y)+a^*(s_y)) \\ & + \frac{1}{2}\int \mathrm{d}x\mathrm{d}y\, N^3V(N(x-y)) \\ & \qquad \times \left[\varphi_t^{(N)}(x)\varphi_t^{(N)}(y)(a^*(c_x)+a(s_x))(a^*(c_y)+a(s_y)) + \text{h.c.}\right]. \end{aligned}$$

Expanding the products, and bringing all terms to normal-order, we find

$$\begin{aligned} & T^*\widehat{\mathcal{L}}^{(0)}_{2,N}(t)T \\ & \quad = \int \mathrm{d}x \left(N^3V(N.) * |\varphi_t^{(N)}|^2\right)(x) \\ & \qquad\qquad \times \left[a^*(c_x)a(c_x) + a^*(s_x)a(s_x) + a^*(c_x)a^*(s_x) + a(s_x)a(c_x) + \langle s_x, s_x\rangle\right] \\ & \qquad + \int \mathrm{d}x\mathrm{d}y N^3V(N(x-y))\varphi_t^{(N)}(x)\overline{\varphi}_t^{(N)}(y) \\ & \qquad\qquad \times \left[a^*(c_x)a(c_y) + a^*(s_y)a(s_x) + a^*(c_x)a^*(s_y) + a(s_x)a(c_y) + \langle s_x, s_y\rangle\right] \\ & \qquad + \frac{1}{2}\int \mathrm{d}x\mathrm{d}y N^3V(N(x-y))\varphi_t^{(N)}(x)\varphi_t^{(N)}(y) \\ & \qquad\qquad \times \left[a^*(c_x)a^*(c_y) + a^*(c_x)a(s_y) + a^*(c_y)a(s_x) + a(s_x)a(s_y) + \langle s_x, c_y\rangle\right] \\ & \qquad + \frac{1}{2}\int \mathrm{d}x\mathrm{d}y N^3V(N(x-y))\overline{\varphi}_t^{(N)}(x)\overline{\varphi}_t^{(N)}(y) \\ & \qquad\qquad \times \left[a(c_x)a(c_y) + a^*(s_y)a(c_x) + a^*(s_x)a(c_y) + a^*(s_x)a^*(s_y) + \langle c_y, s_x\rangle\right]. \end{aligned} \tag{2.70}$$

The properties of $T^*\widehat{\mathcal{L}}^{(0)}_{2,N}(t)T$ are summarized in the following proposition.

Proposition 2.6.3. *We have*

$$\begin{aligned} & T^*\widehat{\mathcal{L}}^{(0)}_{2,N}(t)T \\ & \quad = \int dx (N^3V(N.) * |\varphi_t^{(N)}|^2)(x)\langle s_x, s_x\rangle \\ & \qquad + \int dx\,dy N^3V(N(x-y))\varphi_t^{(N)}(x)\overline{\varphi}_t^{(N)}(y)\langle s_x, s_y\rangle \, + \\ & \qquad + Re \int dx\,dy N^3V(N(x-y))\varphi_t^{(N)}(x)\varphi_t^{(N)}(y)\langle s_x, c_y\rangle \\ & \qquad + \frac{1}{2}\int dx\,dy N^3V(N(x-y))\left[\varphi_t^{(N)}(x)\varphi_t^{(N)}(y)\, a_x^*a_y^* + \overline{\varphi}_t^{(N)}(x)\overline{\varphi}_t^{(N)}(y)\, a_xa_y\right] \\ & \qquad + \mathcal{E}_2(t) \end{aligned}$$

where the error $\mathcal{E}_2(t)$ is such that, for appropriate constants $C, K > 0$,

$$\begin{aligned} \pm\mathcal{E}_2(t) &\leq Ce^{K|t|}\,(\mathcal{N}+1), \\ \pm\,[\mathcal{N},\mathcal{E}_2(t)] &\leq Ce^{K|t|}\,(\mathcal{N}+1), \\ \pm\dot{\mathcal{E}}_2(t) &\leq C\,e^{K|t|}\,(\mathcal{N}+1). \end{aligned} \tag{2.71}$$

To show Proposition 2.6.3, we will make use of the next lemma.

Lemma 2.6.4. *Let $j_1, j_2 \in L^2(\mathbb{R}^3 \times \mathbb{R}^3)$. Let $j_{i,x}(z) := j_i(z,x)$ for $i = 1,2$. Then there exists a constant C such that*

$$\begin{aligned} \int dx\,dy N^3V(N(x-y))|\varphi_t^{(N)}(x)||\varphi_t^{(N)}(y)|\|a^\sharp(j_{1,x})\psi\|\,\|a^\sharp(j_{2,y})\psi\| \\ \leq C\|\varphi_t^{(N)}\|_{H^2}^2\,\|j_1\|_2\,\|j_2\|_2\,\|(\mathcal{N}+1)^{1/2}\psi\|^2. \end{aligned} \tag{2.72}$$

Moreover,

$$\begin{aligned} \int dx\,dy N^3V(N(x-y))|\varphi_t^{(N)}(x)||\varphi_t^{(N)}(y)|\|a^\sharp(j_{1,x})\psi\|\|a_y\psi\| \\ \leq C\|\varphi_t^{(N)}\|_{H^2}^2\,\|j_1\|_2\|(\mathcal{N}+1)^{1/2}\psi\|^2 \end{aligned} \tag{2.73}$$

and

$$\int dx\,dy N^3V(N(x-y))|\varphi_t^{(N)}(x)||\varphi_t^{(N)}(y)|\,\|a_x\psi\|\,\|a_y\psi\| \leq C\|\varphi_t^{(N)}\|_{H^2}^2\,\|(\mathcal{N}+1)^{1/2}\psi\|^2. \tag{2.74}$$

The bounds remain true if both creation and/or annihilation operators act on the same variable, in the sense that

$$\begin{aligned} &\int dx\,dy N^3V(N(x-y))|\varphi_t^{(N)}(x)|^2\|a^\sharp(j_{1,y})\psi\|\,\|a^\sharp(j_{2,y})\psi\| \\ &\qquad\qquad \leq C\|\varphi_t^{(N)}\|_{H^2}^2\|j_1\|_2\|j_2\|_2\,\|(\mathcal{N}+1)^{1/2}\psi\|^2, \\ &\int dx\,dy N^3V(N(x-y))|\varphi_t^{(N)}(x)|^2\|a^\sharp(j_{1,y})\psi\|\,\|a_y\psi\| \leq C\|\varphi_t^{(N)}\|_{H^2}^2\|j_1\|_2\|(\mathcal{N}+1)^{1/2}\psi\|^2, \\ &\int dx\,dy N^3V(N(x-y))|\varphi_t^{(N)}(x)|^2\|a_y\psi\|^2 \leq C\|\varphi_t^{(N)}\|_{H^2}^2\|\mathcal{N}^{1/2}\psi\|^2. \end{aligned} \tag{2.75}$$

Proof. To prove (2.72), we notice that for any $\alpha > 0$

$$\begin{aligned} &\int \mathrm{d}x\mathrm{d}y N^3V(N(x-y))|\varphi_t^{(N)}(x)||\varphi_t^{(N)}(y)|\|a^\sharp(j_{1,x})\psi\|\,\|a^\sharp(j_{2,y})\psi\| \\ &\quad\leq \alpha\int \mathrm{d}x\mathrm{d}y N^3V(N(x-y))|\varphi_t^{(N)}(x)|^2\|j_{2,y}\|_2^2\|(\mathcal{N}+1)^{1/2}\psi\|^2 \\ &\qquad + \alpha^{-1}\int \mathrm{d}x\mathrm{d}y N^3V(N(x-y))|\varphi_t^{(N)}(y)|^2\|j_{1,x}\|_2^2\|(\mathcal{N}+1)^{1/2}\psi\|^2 \\ &\quad\leq \|N^3V(N.)*|\varphi_t^{(N)}|^2\|_\infty\left(\alpha\|j_1\|_2^2+\alpha^{-1}\|j_2\|_2^2\right)\,\|(\mathcal{N}+1)^{1/2}\psi\|^2. \end{aligned}$$

Using $\|N^3V(N.) * |\varphi_t^{(N)}|^2\|_\infty \leq C\|\varphi_t^{(N)}\|_{H^2}^2$, and optimizing over $\alpha > 0$, we obtain (2.72). Analogously, (2.73) follows from

$$\begin{aligned}\int \mathrm{d}x\mathrm{d}y N^3V(N(x-y))|\varphi_t^{(N)}(x)||\varphi_t^{(N)}(y)|\|a^\sharp(j_{1,x})\psi\|\|a_y\psi\| \\ \leq \alpha \int \mathrm{d}x\mathrm{d}y N^3V(N(x-y))|\varphi_t^{(N)}(x)|^2\|a_y\psi\|^2 \\ + \alpha^{-1}\int \mathrm{d}x\mathrm{d}y N^3V(N(x-y))|\varphi_t^{(N)}(y)|^2\|j_{1,x}\|_2^2\|(\mathcal{N}+1)^{1/2}\psi\|^2 \\ \leq \|N^3V(N.) * |\varphi_t^{(N)}|^2\|_\infty(\alpha+\alpha^{-1}\|j_1\|_2^2)\|(\mathcal{N}+1)^{1/2}\psi\|^2\end{aligned}$$

for any $\alpha > 0$. Optimizing over α gives (2.73). Eq. (2.74) follows from Cauchy-Schwarz. The bounds in (2.75) can be shown similarly. □

Proof of Proposition 2.6.3. To prove the first bound in (2.71), we notice that the quadratic terms on the r. h. s. of (2.70) can be controlled with Lemma 2.6.4, decomposing, if needed, $a(c_x) = a_x + a(p_x)$ and then applying (2.72), (2.73), or (2.74). There are two exceptions, given by the terms proportional to $a^*(c_x)a^*(c_y)$ and its hermitian conjugate, proportional to $a(c_x)a(c_y)$. For these two terms the bounds from Lemma 2.6.4 do not apply. Instead, using $a^*(c_x) = a_x^* + a^*(p_x)$, we write

$$\begin{aligned}\int \mathrm{d}x\mathrm{d}y N^3V(N(x-y))\varphi_t^{(N)}(x)\varphi_t^{(N)}(y)a^*(c_x)a^*(c_y) \\ = \int \mathrm{d}x\mathrm{d}y N^3V(N(x-y))\varphi_t^{(N)}(x)\varphi_t^{(N)}(y)a_x^*a_y^* \\ + \int \mathrm{d}x\mathrm{d}y N^3V(N(x-y))\varphi_t^{(N)}(x)\varphi_t^{(N)}(y)a^*(p_x)a_y^* \\ + \int \mathrm{d}x\mathrm{d}y N^3V(N(x-y))\varphi_t^{(N)}(x)\varphi_t^{(N)}(y)a^*(c_x)a^*(p_y).\end{aligned} \tag{2.76}$$

The contribution of the last two terms can be bounded by Lemma 2.6.4, because one of the arguments of the creation operators is square integrable. In fact

$$\begin{aligned}\Big|\int \mathrm{d}x\mathrm{d}y N^3V(N(x-y))\varphi_t^{(N)}(x)\varphi_t^{(N)}(y)\langle\psi, a^*(p_x)a_y^*\psi\rangle\Big| \\ \leq \int \mathrm{d}x\mathrm{d}y N^3V(N(x-y))|\varphi_t^{(N)}(x)||\varphi_t^{(N)}(y)|\|a_y\psi\|\,\|a^*(p_x)\psi\| \\ \leq C\|\varphi_t^{(N)}\|_{H^2}^2\,\|(\mathcal{N}+1)^{1/2}\psi\|^2 \leq Ce^{K|t|}\|(\mathcal{N}+1)^{1/2}\psi\|^2\end{aligned}$$

by (2.73) and (2.27), and similarly for the last term on the r. h. s. of (2.76). The hermitian conjugate of (2.76), proportional to $a(c_x)a(c_y)$, can be handled identically.

The second bound in (2.71) follows similarly, using the fact that the commutator of $\mathcal{N}$ with the terms on the r. h. s. of (2.70) leaves their form unchanged (apart from the constant terms and the quadratic terms with one creation and one annihilation operators, whose contribution to the commutator $[\mathcal{N}, \mathcal{E}_2(t)]$ vanishes).

Also the third bound in (2.71) can be proven analogously, using the bounds for $\|\dot{\mathrm{sh}}_{k_t}\|_2$ and $\|\dot{p}_{k_t}\|_2$, as proven in Lemma 2.3.4 . When the time derivative hits the factor $\varphi_t^{(N)}(x)$ or $\varphi_t^{(N)}(y)$, it generates a contribution which is bounded by $\|\dot{\varphi}_t^{(N)}\|_{H^2} \leq C\|\varphi_t^{(N)}\|_{H^4}^4 \leq Ce^{K|t|}$ (for some K depending only on $\|\varphi\|_{H^1}$; here we used Proposition 2.3.1). □

2.6.3. Analysis of the cubic terms $T^*\mathcal{L}_{3,N}^{(0)}(t)T$

We consider now the contributions arising from the cubic terms in $\mathcal{L}_{3,N}^{(0)}(t)$. We have

$$\begin{aligned}
&T^*\mathcal{L}_{3,N}^{(0)}(t)T \\
&= \frac{1}{\sqrt{N}}\int \mathrm{d}x\mathrm{d}y\, N^3V(N(x-y)) \\
&\qquad \times \Big[\varphi_t^{(N)}(y)\,(a^*(c_x)+a(s_x))(a^*(c_y)+a(s_y))(a(c_x)+a^*(s_x)) + \text{h.c.}\Big] \\
&= \frac{1}{\sqrt{N}}\int \mathrm{d}x\mathrm{d}y N^3V(N(x-y))\varphi_t^{(N)}(y) \\
&\qquad \times [\,a^*(c_x)a^*(c_y)a^*(s_x) + a^*(c_x)a^*(c_y)a(c_x) + a^*(c_x)a(s_y)a^*(s_x) + a^*(c_x)a(s_y)a(c_x) \\
&\qquad\quad + a(s_x)a^*(c_y)a^*(s_x) + a(s_x)a^*(c_y)a(c_x) + a(s_x)a(s_y)a^*(s_x) + a(s_x)a(s_y)a(c_x)] \\
&\quad + \text{h.c.}
\end{aligned}$$

Writing the terms in normal-order, we find

$$\begin{aligned}
&T^*\mathcal{L}_{3,N}^{(0)}(t)T \\
&= \frac{1}{\sqrt{N}}\int \mathrm{d}x\mathrm{d}y N^3V(N(x-y))\varphi_t^{(N)}(y) \\
&\qquad \times [a^*(c_x)a^*(c_y)a^*(s_x) + a^*(c_x)a^*(c_y)a(c_x) + a^*(c_x)a^*(s_x)a(s_y) + a^*(c_x)a(s_y)a(c_x) \\
&\qquad\quad + a^*(c_y)a^*(s_x)a(s_x) + a^*(c_y)a(s_x)a(c_x) + a^*(s_x)a(s_x)a(s_y) + a(s_x)a(s_y)a(c_x)] \\
&\quad + \frac{1}{\sqrt{N}}\int \mathrm{d}x\mathrm{d}y N^3V(N(x-y))\varphi_t^{(N)}(y) \\
&\qquad \times [\langle s_y, s_x\rangle(a^*(c_x)+a(s_x)) + \langle s_x, c_y\rangle\,(a(c_x)+a^*(s_x)) + \langle s_x, s_x\rangle\,(a^*(c_y)+a(s_y))] \\
&\quad + \text{h.c.}
\end{aligned} \tag{2.77}$$

The properties of $T^*\mathcal{L}_{3,N}^{(0)}(t)T$ are summarized in the following proposition.

Proposition 2.6.5. *We have*

$$\begin{aligned}
&T^*\mathcal{L}_{3,N}^{(0)}T \\
&= \frac{1}{\sqrt{N}}\int dx\,dy N^3V(N(x-y)) \\
&\qquad \times \Big[\varphi_t^{(N)}(y)\overline{k}_t(x,y)\,(a(c_x)+a^*(s_x)) + \overline{\varphi}_t^{(N)}(y)k_t(x,y)\,(a^*(c_x)+a(s_x))\Big] \\
&\quad + \mathcal{E}_3(t) \\
&= -\sqrt{N}\int dx\,dy N^3V(N(x-y))w(N(x-y))|\varphi_t^{(N)}(y)|^2\varphi_t^{(N)}(x)(a(c_x)+a^*(s_x)) + h.c. \\
&\quad + \mathcal{E}_3(t)
\end{aligned} \tag{2.78}$$

where we used the definition (2.31) of the kernel k_t and where the error term $\mathcal{E}_3(t)$ is such *that for every $\delta > 0$ there exists a constant $C_\delta > 0$ with*

$$\begin{aligned}
\pm\mathcal{E}_3(t) &\leq \delta \int dx\, dy N^2 V(N(x-y)) a_x^* a_y^* a_x a_y + \delta \frac{\mathcal{N}^2}{N} + C_\delta e^{K|t|} (\mathcal{N}+1)\,, \\
\pm\left[\mathcal{N}, \mathcal{E}_3(t)\right] &\leq \delta \int dx\, dy N^2 V(N(x-y)) a_x^* a_y^* a_x a_y + \delta \frac{\mathcal{N}^2}{N} + C_\delta e^{K|t|} (\mathcal{N}+1)\,, \qquad (2.79)\\
\pm\dot{\mathcal{E}}_3(t) &\leq \delta \int dx\, dy N^2 V(N(x-y)) a_x^* a_y^* a_x a_y + \delta \frac{\mathcal{N}^2}{N} + C_\delta e^{K|t|} (\mathcal{N}+1)\,.
\end{aligned}$$

Notice here that the first term on the r. h. s. of (2.78) cancels exactly with the contribution (2.54); we will make use of this crucial observation in the proof of Theorem 2.3.5 below.

Proof. To bound the cubic terms on the r. h. s. of (2.77), we systematically apply Cauchy-Schwarz. This way, we control cubic terms by quartic and quadratic contributions, which are then estimated making use of Lemma 2.6.4 (the quadratic part) and Lemmas 2.6.7 and 2.6.8 (the quartic part). For example,

$$\begin{aligned}
&\Big| \frac{1}{\sqrt{N}} \int \mathrm{d}x\mathrm{d}y N^3 V(N(x-y)) \varphi_t^{(N)}(y) \langle \psi, a^*(c_x) a^*(c_y) a^*(s_x)\psi\rangle \Big| \\
&\qquad \leq \frac{1}{\sqrt{N}} \int \mathrm{d}x\mathrm{d}y N^3 V(N(x-y)) |\varphi_t^{(N)}(y)| \|a(c_x)a(c_y)\psi\| \, \|a^*(s_x)\psi\| \\
&\qquad \leq \frac{\delta}{N} \int \mathrm{d}x\mathrm{d}y\, N^3 V(N(x-y)) \|a(c_x)a(c_y)\psi\|^2 \\
&\qquad\quad + C_\delta \int \mathrm{d}x\mathrm{d}y N^3 V(N(x-y)) |\varphi_t^{(N)}(y)|^2 \|a^*(s_x)\psi\|^2 \\
&\qquad \leq \frac{C\delta}{N} \int \mathrm{d}x\mathrm{d}y N^3 V(N(x-y)) \|a_y a_x \psi\|^2 + C_\delta \|(\mathcal{N}+1)^{1/2}\psi\|^2
\end{aligned}$$

where, in the last line, we used (2.87) (from Lemma 2.6.8) and (2.75) (from Lemma 2.6.4). All other cubic terms can be bounded similarly. We always separate the three creation and/or annihilation operators putting a small weight δ in front of the quartic term and in such a way that, in the resulting quartic contribution, two operators depend on the x and two on the y variable. The corresponding quadratic term depends on x and can always be bounded by (2.75). It should be noted that the quartic contribution has either the form $\|a(c_x)a(c_y)\psi\|^2$ or $\|a(c_x)a^\sharp(j_y)\psi\|^2$ or $\|a^\sharp(j_{1,x})a^\sharp(j_{2,y})\psi\|^2$, with square-integrable arguments j_1, j_2 (here $a^\sharp$ is either a or a^*). These terms can always be controlled using Lemma 2.6.7 or Lemma 2.6.8. As for the linear contributions on the r. h. s. of (2.77), the first and third can simply be bounded by $N^{-1/2}(\mathcal{N}+1)^{1/2}$, since

$$|\langle s_y, s_x\rangle| \leq C|\varphi_t^{(N)}(x)||\varphi_t^{(N)}(y)|.$$

To bound the second linear term, we write

$$\begin{aligned}
&\frac{1}{\sqrt{N}} \int \mathrm{d}x\mathrm{d}y N^3 V(N(x-y)) \varphi_t^{(N)}(y) \langle s_x, c_y\rangle (a(c_x) + a^*(s_x)) \\
&\qquad = \frac{1}{\sqrt{N}} \int \mathrm{d}x\mathrm{d}y N^3 V(N(x-y)) \varphi_t^{(N)}(y) \overline{k}_t(x,y)\, (a(c_x) + a^*(s_x)) + \widetilde{\mathcal{E}}(t)
\end{aligned}$$

where $\pm\widetilde{\mathcal{E}}(t) \leq N^{-1/2}(\mathcal{N}+1)^{1/2}$ because, using Lemma 2.3.3,

$$|\langle s_x, c_y\rangle - \overline{k}_t(x,y)| \leq C|\varphi_t^{(N)}(x)||\varphi_t^{(N)}(y)|.$$

From (2.27), this concludes the proof of the first estimate in (2.79). The other two estimates are proven analogously, using the fact that the commutators of $\mathcal{N}$ with the terms on the r. h. s. of (2.77) have the same form as the terms on the r. h. s. of (2.77) (with possibly just a different sign), and using the bounds for $\|\dot{\mathrm{sh}}_{k_t}\|_2$ and $\|\dot{p}_{k_t}\|_2$ from Lemma 2.3.4, and the bound for $\|\dot{\varphi}_t^{(N)}\|_{H^2}$ from Proposition 2.3.1. □

2.6.4. Analysis of the quartic terms $T^*\mathcal{L}_{4,N}^{(0)}T$

We consider next the contributions arising from the quartic part $\mathcal{L}_{4,N}^{(0)}$ of $\mathcal{L}_N^{(0)}(t)$. We have

$$\begin{aligned} T^*\mathcal{L}_{4,N}^{(0)}(t)T =& \frac{1}{2N}\int \mathrm{d}x\mathrm{d}y\, N^3V(N(x-y)) \\ & \times (a^*(c_x)+a(s_x))(a^*(c_y)+a(s_y))(a(c_y)+a^*(s_y))(a(c_x)+a^*(s_x)). \end{aligned}$$

Expanding the products, we find

$$\begin{aligned} &2T^*\mathcal{L}_{4,N}^{(0)}(t)T \\ &= \int \mathrm{d}x\mathrm{d}y\, N^2V(N(x-y))\Big[a^*(c_x)a^*(c_y)a^*(s_y)a^*(s_x) + a^*(c_x)a^*(c_y)a^*(s_y)a(c_x) \\ &\quad + a^*(c_x)a^*(c_y)a(c_y)a^*(s_x) + a^*(c_x)a^*(c_y)a(c_y)a(c_x) + a^*(c_x)a(s_y)a^*(s_y)a^*(s_x) \\ &\quad + a^*(c_x)a(s_y)a^*(s_y)a(c_x) + a^*(c_x)a(s_y)a(c_y)a^*(s_x) + a^*(c_x)a(s_y)a(c_y)a(c_x) \\ &\quad + a(s_x)a^*(c_y)a^*(s_y)a^*(s_x) + a(s_x)a^*(c_y)a^*(s_y)a(c_x) + a(s_x)a^*(c_y)a(c_y)a^*(s_x) \\ &\quad + a(s_x)a^*(c_y)a(c_y)a(c_x) + a(s_x)a(s_y)a^*(s_y)a^*(s_x) + a(s_x)a(s_y)a^*(s_y)a(c_x) \\ &\quad + a(s_x)a(s_y)a(c_y)a^*(s_x) + a(s_x)a(s_y)a(c_y)a(c_x)\Big]. \end{aligned}$$

Writing all terms in normal-order, we obtain

$$\begin{aligned} &2T^*\mathcal{L}_{4,N}^{(0)}(t)T \\ &= \int \mathrm{d}x\mathrm{d}y\, N^2V(N(x-y))\Big[a^*(c_x)a^*(c_y)a^*(s_y)a^*(s_x) + a^*(c_x)a^*(c_y)a^*(s_y)a(c_x) \\ &\quad + a^*(c_x)a^*(c_y)a^*(s_x)a(c_y) + a^*(c_x)a^*(c_y)a(c_y)a(c_x) + a^*(c_x)a^*(s_y)a^*(s_x)a(s_y) \\ &\quad + a^*(c_x)a^*(s_y)a(s_y)a(c_x) + a^*(c_x)a^*(s_x)a(s_y)a(c_y) + a^*(c_x)a(s_y)a(c_y)a(c_x) \\ &\quad + a^*(c_y)a^*(s_y)a^*(s_x)a(s_x) + a^*(c_y)a^*(s_y)a(s_x)a(c_x) + a^*(c_y)a^*(s_x)a(s_x)a(c_y) \\ &\quad + a^*(c_y)a(s_x)a(c_y)a(c_x) + a^*(s_y)a^*(s_x)a(s_x)a(s_y) + a^*(s_y)a(s_x)a(s_y)a(c_x) \\ &\quad + a^*(s_x)a(s_x)a(s_y)a(c_y) + a(s_x)a(s_y)a(c_y)a(c_x)\Big] \\ &\quad + \int \mathrm{d}x\mathrm{d}y\, N^2V(N(x-y))\Big[\langle c_y,s_x\rangle a^*(c_x)a^*(c_y) + \langle s_x,c_y\rangle a(c_y)a(c_x) \\ &\quad + 2\langle s_y,s_y\rangle a^*(c_x)a^*(s_x) + 2\langle s_y,s_y\rangle a(s_x)a(c_x) + 2\langle s_y,s_x\rangle a^*(c_x)a^*(s_y) \\ &\quad + 2\langle s_x,s_y\rangle a(s_y)a(c_x) + 2\langle s_y,s_y\rangle a^*(c_x)a(c_x) + 2\langle s_y,s_x\rangle a^*(c_x)a(c_y) \\ &\quad + 2\langle s_x,s_y\rangle a^*(s_x)a(s_y) + 2\langle s_y,s_y\rangle a^*(s_x)a(s_x) + \langle c_y,s_x\rangle a^*(c_x)a(s_y) \\ &\quad + \langle s_x,c_y\rangle a^*(s_y)a(c_x) + \langle s_x,c_y\rangle a^*(s_y)a^*(s_x) + \langle c_y,s_x\rangle a(s_x)a(s_y) \\ &\quad + \langle s_x,c_y\rangle a^*(s_x)a(c_y) + \langle c_y,s_x\rangle a^*(c_y)a(s_x)\Big] + \end{aligned} \tag{2.80}$$

$$+\int \mathrm{d}x\mathrm{d}y\, N^2 V(N(x-y)) \left[|\langle s_x, c_y\rangle|^2 + |\langle s_x, s_y\rangle|^2 + \langle s_y, s_y\rangle\langle s_x, s_x\rangle \right].$$

The properties of $T^*\mathcal{L}_{4,N}^{(0)}T$ are summarized in the next proposition.

Proposition 2.6.6. *We have*

$$\begin{aligned} 2T^*\mathcal{L}_{4,N}^{(0)}(t)T = &\int dx\,dy N^2 V(N(x-y)) \left[|\langle s_x, c_y\rangle|^2 + |\langle s_x, s_y\rangle|^2 + \langle s_y, s_y\rangle\langle s_x, s_x\rangle \right] \\ &+ \int dx\,dy N^2 V(N(x-y)) a_x^* a_y^* a_y a_x \\ &+ \int dx\,dy\, N^2 V(N(x-y)) \left(k(x,y) a_x^* a_y^* + \overline{k}(x,y) a_x a_y \right) + \mathcal{E}_4(t) \end{aligned} \tag{2.81}$$

where the error $\mathcal{E}_4(t)$ is such that, for every $\delta > 0$, there exists a constant $C_\delta > 0$ with

$$\begin{aligned} \pm\, \mathcal{E}_4(t) &\leq \delta \int dx\,dy N^2 V(N(x-y)) a_x^* a_y^* a_y a_x + C_\delta \frac{\mathcal{N}^2}{N} + C_\delta e^{K|t|}(\mathcal{N}+1), \\ \pm\, [\mathcal{N}, \mathcal{E}_4(t)] &\leq \delta \int dx\,dy N^2 V(N(x-y)) a_x^* a_y^* a_y a_x + C_\delta \frac{\mathcal{N}^2}{N} + C_\delta e^{K|t|}(\mathcal{N}+1), \\ \pm \dot{\mathcal{E}}_4(t) &\leq \delta \int dx\,dy N^2 V(N(x-y)) a_x^* a_y^* a_y a_x + C_\delta e^{K|t|} \left(\frac{\mathcal{N}^2}{N} + \mathcal{N} + 1 \right). \end{aligned} \tag{2.82}$$

To prove Proposition 2.6.6, we will make use of the following two lemmas.

Lemma 2.6.7. *Suppose $j_1, j_2 \in L^2(\mathbb{R}^3 \times \mathbb{R}^3)$ are kernels with the property that*

$$M_i := \max\left(\sup_x \int dy\, |j_i(x,y)|^2, \sup_y \int dx\, |j_i(x,y)|^2 \right) < \infty$$

for $i = 1, 2$. Let $j_{i,x}(z) := j_i(z,x)$ and recall the definition $c_x(z) = ch_{k_t}(z,x)$ from (2.53). Then there exists a constant C depending only on M_1, M_2 and on the L^2-norms $\|j_1\|_2$, $\|j_2\|_2$ such that

$$\int dx\,dy N^3 V(N(x-y)) \|a^\sharp(j_{1,x}) a_y \psi\|^2 \leq C M_1 \|(\mathcal{N}+1)\psi\|^2 \tag{2.83}$$

and

$$\int dx\,dy N^3 V(N(x-y)) \|a^\sharp(j_{1,x}) a^\sharp(j_{2,y})\psi\|^2 \leq C \min\left(M_1 \|j_2\|_2^2, M_2 \|j_1\|_2^2 \right) \|(\mathcal{N}+1)\psi\|^2. \tag{2.84}$$

As a consequence

$$\int dx\,dy N^3 V(N(x-y)) \|a^\sharp(j_{1,x}) a(c_y)\psi\|^2 \leq C M_1 \|(\mathcal{N}+1)\psi\|^2. \tag{2.85}$$

The inequalities remain true (and are easier to prove) if both operators act on the same variable. In other words

$$\begin{aligned} &\int dx\,dy N^3 V(N(x-y)) \|a^\sharp(j_{1,x}) a_x \psi\|^2 \leq C M_1 \|(\mathcal{N}+1)\psi\|^2, \\ &\int dx\,dy N^3 V(N(x-y)) \|a^\sharp(j_{1,x}) a^\sharp(j_{2,x})\psi\|^2 \leq C \min(M_1 \|j_2\|_2^2, M_2 \|j_1\|_2^2) \|(\mathcal{N}+1)\psi\|^2, \\ &\int dx\,dy N^3 V(N(x-y)) \|a^\sharp(j_{1,x}) a(c_y)\psi\|^2 \leq C M_1 \|(\mathcal{N}+1)\psi\|^2. \end{aligned} \tag{2.86}$$

Here $a^\sharp$ is either the annihilation operator a or the creation operator a^*.

Proof. To prove (2.83), we observe that

$$\begin{aligned}
&\int \mathrm{d}x\mathrm{d}y N^3 V(N(x-y))\|a^\sharp(j_{1,x})a_y\psi\|^2 \\
&\qquad\qquad \leq \int \mathrm{d}x\mathrm{d}y N^3 V(N(x-y))\|j_{1,x}\|_2^2\|(\mathcal{N}+1)^{1/2}a_y\psi\|^2 \\
&\qquad\qquad \leq M_1 \int \mathrm{d}x\mathrm{d}y N^3 V(N(x-y))\|a_y\mathcal{N}^{1/2}\psi\|^2 \\
&\qquad\qquad = CM_1\|\mathcal{N}\psi\|^2.
\end{aligned}$$

As for (2.84), we notice that (considering for example the case $a^\sharp(j_{2,y}) = a^*(j_{2,y})$)

$$\begin{aligned}
&\int \mathrm{d}x\mathrm{d}y N^3 V(N(x-y))\|a^\sharp(j_{1,x})a^*(j_{2,y})\psi\|^2 \\
&\qquad \leq \int \mathrm{d}x\mathrm{d}y N^3 V(N(x-y))\|j_{1,x}\|_2\|(\mathcal{N}+1)^{1/2}a^*(j_{2,y})\psi\|^2 \\
&\qquad \leq \int \mathrm{d}x\mathrm{d}y N^3 V(N(x-y))\|j_{1,x}\|_2^2\|a^*(j_{2,y})(\mathcal{N}+2)^{1/2}\psi\|^2 \\
&\qquad \leq \int \mathrm{d}x\mathrm{d}y N^3 V(N(x-y))\|j_{1,x}\|_2^2\|j_{2,y}\|_2^2\|(\mathcal{N}+1)^{1/2}(\mathcal{N}+2)^{1/2}\psi\|^2 \\
&\qquad \leq CM_1\|j_2\|_2^2\|(\mathcal{N}+1)\psi\|^2.
\end{aligned}$$

Eq. (2.85) follows from the first two, by writing $a(c_y) = a_y + a(p_y)$ (recall here that we are using the notation $p_y(z) = p(k_t)(z,y)$ with the kernel $p(k_t) \in L^2(\mathbb{R}^3 \times \mathbb{R}^3)$ defined in Lemma 2.3.3). Eq. (2.86) follows similarly; in this case, however, one can immediately integrate over the variable y, simplifying the proof. □

Terms of the form (2.85), but with $j_{1,x}$ replaced by c_x (which is not in L^2) are treated differently.

Lemma 2.6.8. *Recall the definition $c_x(z) = ch_{k_t}(z,x)$ from (2.53). Then there exists a constant $C > 0$ with*

$$\begin{aligned}
\int dxdy N^3 V(N(x-y))\|a(c_x)a(c_y)\psi\|^2 \leq C \int dxdy N^3 V(N(x-y))\|a_x a_y\psi\|^2 \\
+ C\,\|(\mathcal{N}+1)\psi\|^2.
\end{aligned} \tag{2.87}$$

More precisely, we have

$$\int dxdy N^3 V(N(x-y))\|a(c_x)a(c_y)\psi\|^2 = \int dxdy N^3 V(N(x-y))\|a_x a_y\psi\|^2 + \widetilde{\mathcal{E}}(t) \tag{2.88}$$

where the error $\widetilde{\mathcal{E}}(t)$ is such that, for every $\delta > 0$, there exists a constant C_δ with

$$\pm\widetilde{\mathcal{E}}(t) \leq \delta \int dxdy N^3 V(N(x-y))\|a_x a_y\psi\|^2 + C_\delta\|(\mathcal{N}+1)\psi\|^2.$$

Proof. We write $a(c_x) = a_x + a(p_x)$, using the notation $p_x(z) = p(k_t)(z,x)$ introduced in (2.53). We have

$$\|a(c_x)a(c_y)\psi\| \leq \|a_x a_y\psi\| + \|a_x a(p_y)\psi\| + \|a(p_x)a(c_y)\psi\|.$$

Therefore, using (2.83) and (2.85), we immediately find (using Lemma 2.3.3 to bound $\|p\|_2$ and $\sup_x \|p_x\|_2$)

$$\int \mathrm{d}x\mathrm{d}y N^3 V(N(x-y))\|a(c_x)a(c_y)\psi\|^2 \leq C\int \mathrm{d}x\mathrm{d}y N^3 V(N(x-y))\|a_x a_y\psi\|^2 + C\|(\mathcal{N}+1)\psi\|^2.$$

To prove (2.88), we notice that

$$\begin{aligned}
&\int \mathrm{d}x\mathrm{d}y N^3 V(N(x-y))\|a(c_x)a(c_y)\psi\|^2 \\
&\quad= \int \mathrm{d}x\mathrm{d}y N^3 V(N(x-y))\langle\psi, a^*(c_x)a^*(c_y)a(c_y)a(c_x)\psi\rangle \\
&\quad= \int \mathrm{d}x\mathrm{d}y N^3 V(N(x-y))\langle\psi, a_x^* a_y^* a_y a_x\psi\rangle \\
&\qquad+ \int \mathrm{d}x\mathrm{d}y N^3 V(N(x-y))\Big\langle\psi, \big[a^*(p_x)a_y^* a_y a_x + a^*(c_x)a^*(p_y)a_y a_x \\
&\qquad\qquad + a^*(c_x)a^*(c_y)a(p_y)a_x + a^*(c_x)a^*(c_y)a(c_y)a(p_x)\big]\psi\Big\rangle \\
&\quad=: \int \mathrm{d}x\mathrm{d}y N^3 V(N(x-y))\|a_x a_y\psi\|^2 + \widetilde{\mathcal{E}}(t)
\end{aligned}$$

where

$$\begin{aligned}
|\widetilde{\mathcal{E}}(t)| \leq &\int \mathrm{d}x\mathrm{d}y N^3 V(N(x-y))\Big[\|a(p_x)a_y\psi\|\|a_y a_x\psi\| + \|a(c_x)a(p_y)\psi\|\|a_y a_x\psi\| \\
&\qquad + \|a(c_x)a(c_y)\psi\|\|a(p_y)a_x\psi\| + \|a(c_x)a(c_y)\psi\|\|a(c_y)a(p_x)\psi\|\Big] \\
&\leq \delta\int \mathrm{d}x\mathrm{d}y N^3 V(N(x-y))\left[\|a_x a_y\psi\|^2 + \|a(c_x)a(c_y)\psi\|^2\right] \\
&\quad + C_\delta\int \mathrm{d}x\mathrm{d}y N^3 V(N(x-y))\left[\|a(p_x)a_y\psi\|^2 + \|a(c_x)a(p_y)\psi\|^2\right] \\
&\leq \delta\int \mathrm{d}x\mathrm{d}y N^3 V(N(x-y))\|a_x a_y\psi\|^2 + C_\delta\|(\mathcal{N}+1)\psi\|^2.
\end{aligned}$$

Here, in the last inequality, we used (2.83), (2.85) from Lemma 2.6.7 and (2.87). □

Proof of Proposition 2.6.6. To prove the first bound in (2.82) we observe that all quartic terms on the r. h. s. of (2.80) can be bounded using Lemmas 2.6.7 and 2.6.8. For example, the contribution arising from the first term on the r. h. s. of (2.80) is bounded by

$$\begin{aligned}
&\Big|\int \mathrm{d}x\mathrm{d}y\, N^2 V(N(x-y))\langle\psi, a^*(c_x)a^*(c_y)a^*(s_y)a^*(s_x)\psi\rangle\Big| \\
&\qquad\leq \int \mathrm{d}x\mathrm{d}y N^2 V(N(x-y))\|a(c_x)a(c_y)\psi\|\|a^*(s_y)a^*(s_x)\psi\| \\
&\qquad\leq \delta\int \mathrm{d}x\mathrm{d}y N^2 V(N(x-y))\|a(c_x)a(c_y)\psi\|^2 \\
&\qquad\quad + C_\delta\int \mathrm{d}x\mathrm{d}y N^2 V(N(x-y))\|a^*(s_y)a^*(s_x)\psi\|^2 \\
&\qquad\leq C\delta\int \mathrm{d}x\mathrm{d}y N^2 V(N(x-y))\|a_x a_y\psi\|^2 + \frac{C_\delta}{N}\|(\mathcal{N}+1)\psi\|^2
\end{aligned}$$

where, in the last inequality, we used (2.87) and (2.84). All the other quartic terms on the r. h. s. of (2.80), with the exception of the fourth term (the one containing only c_x or c_y as arguments of the creation and annihilation operators), can be bounded similarly; the key observation here is that all these terms have at least one creation or annihilation operator with square integrable argument (this allow us to apply Lemma 2.6.7). Moreover, in all these terms, the quartic expression does not contain the annihilation operators $a(c_x)$ and $a(c_y)$ in the two factors on the left, nor the creation operators $a^*(c_x)$ and $a^*(c_y)$ in the two factors on the right (in Lemma 2.6.7, in particular in (2.85) it is of course important that the factor $a(c_y)$ in the norm appears as an annihilation and not as a creation operator). To bound the fourth term on the r. h. s. of (2.80), where all the arguments of the creation and annihilation operators are not integrable, we cannot apply Lemma 2.6.7. Instead, we use (2.88) from Lemma 2.6.8. We obtain

$$\begin{aligned}\int \mathrm{d}x\mathrm{d}y N^2 V(N(x-y)) \langle \psi, a^*(c_x) a^*(c_y) a(c_y) a(c_x) \psi \rangle \\ = \int \mathrm{d}x\mathrm{d}y N^2 V(N(x-y)) \langle \psi, a_x^* a_y^* a_y a_x \psi \rangle + \widetilde{\mathcal{E}}(t)\end{aligned}$$

where the error $\widetilde{\mathcal{E}}(t)$ is such that, for every $\delta > 0$, there exists $C_\delta > 0$ with

$$|\widetilde{\mathcal{E}}(t)| \leq \delta \int \mathrm{d}x\mathrm{d}y N^2 V(N(x-y)) \|a_x a_y \psi\|^2 + \frac{C_\delta}{N} \|(\mathcal{N}+1)\psi\|^2.$$

The quadratic terms on the r. h. s. of (2.80) can be bounded using Lemma 2.6.4. To this end, we observe that

$$|\langle s_x, s_y \rangle|, |\langle s_x, c_y \rangle| \leq CN |\varphi_t^{(N)}(x)| |\varphi_t^{(N)}(y)|.$$

It is therefore easy to check that all the quadratic terms, with the exception of the first two (the quadratic terms appearing on the eighth line of (2.80)), have a form suitable to apply one of the bounds in Lemma 2.6.4. More precisely, we apply (2.72), if the arguments of the two creation and/or annihilation operators are either s_x or s_y. If, on the other hand, one of the two arguments is c_x or c_y and the other one is s_x or s_y, we write $a^\sharp(c_x) = a_x^\sharp + a^\sharp(p_x)$ and then we apply (2.72) (to bound the contribution proportional to $a^\sharp(p_x)$) and (2.73) (to bound the contribution proportional to $a_x^\sharp$). Finally, if both arguments are either c_x or c_y (and we have exactly one creation and one annihilation operators), we write $a^\sharp(c_x) = a_x^\sharp + a^\sharp(p_x)$ and we apply (2.72), (2.73) and (2.74). To control the two remaining quadratic contributions, we observe that, writing $a^*(c_x) = a_x^* + a^*(p_x)$,

$$\begin{aligned}\int \mathrm{d}x\mathrm{d}y N^2 V(N(x-y)) \langle c_y, s_x \rangle \langle \psi, a^*(c_x) a^*(c_y) \psi \rangle \\ = \int \mathrm{d}x\mathrm{d}y N^2 V(N(x-y)) \langle c_y, s_x \rangle \langle \psi, a_x^* a_y^* \psi \rangle \\ + \int \mathrm{d}x\mathrm{d}y N^2 V(N(x-y)) \langle c_y, s_x \rangle \langle \psi, a^*(p_x) a_y^* \psi \rangle \\ + \int \mathrm{d}x\mathrm{d}y N^2 V(N(x-y)) \langle c_y, s_x \rangle \langle \psi, a^*(c_x) a^*(p_y) \psi \rangle.\end{aligned} \tag{2.89}$$

Since $|\langle c_y, s_x \rangle| \leq CN |\varphi_t^{(N)}(x)| |\varphi_t^{(N)}(y)|$, the last two terms can be bounded (in absolute value) using (2.73) and (2.74), respectively. We find

$$\Big|\int \mathrm{d}x\mathrm{d}y N^2 V(N(x-y))\langle c_y, s_x\rangle \langle \psi, a^*(p_x) a^*_y \psi\rangle\Big| \leq C\|\varphi_t^{(N)}\|^2_{H^2}\, \|(\mathcal{N}+1)^{1/2}\psi\|^2,$$
$$\Big|\int \mathrm{d}x\mathrm{d}y N^2 V(N(x-y))\langle c_y, s_x\rangle \langle \psi, a^*(c_x) a^*(p_y) \psi\rangle\Big| \leq C\|\varphi_t^{(N)}\|^2_{H^2}\, \|(\mathcal{N}+1)^{1/2}\psi\|^2.$$

As for the first term on the r. h. s. of (2.89), we notice that

$$\langle c_y, s_x\rangle = k(x,y) + g(x,y)$$

where $g(x,y) = r(x,y) + \langle p_y, s_x\rangle$ is such that

$$|g(x,y)| \leq C|\varphi_t^{(N)}(x)|\,|\varphi_t^{(N)}(y)|.$$

Therefore,

$$\begin{aligned}\int \mathrm{d}x\mathrm{d}y N^2 V(N(x-y))\langle c_y, s_x\rangle\langle \psi, a^*_x a^*_y \psi\rangle = &\int \mathrm{d}x\mathrm{d}y N^2 V(N(x-y)) k(x,y)\langle \psi, a^*_x a^*_y\psi\rangle \\ &+ \int \mathrm{d}x\mathrm{d}y N^2 V(N(x-y)) g(x,y)\langle\psi, a^*_x a^*_y \psi\rangle.\end{aligned}$$

The second term can be bounded by

$$\begin{aligned}&\Big|\int \mathrm{d}x dy\, N^2 V(N(x-y)) g(x,y)\langle \psi, a^*_x a^*_y\psi\rangle\Big| \\ &\quad\leq C\int \mathrm{d}x\mathrm{d}y N^2 V(N(x-y))|\varphi_t^{(N)}(x)||\varphi_t^{(N)}(y)|\|a_x a_y\psi\|\,\|\psi\| \\ &\quad\leq \delta\int \mathrm{d}x\mathrm{d}y N^2 V(N(x-y))\|a_x a_y \psi\|^2 + C_\delta \int \mathrm{d}x\mathrm{d}y N^2 V(N(x-y))|\varphi_t^{(N)}(x)|^2|\varphi_t^{(N)}(y)|^2 \\ &\quad\leq \delta\int \mathrm{d}x\mathrm{d}y N^2 V(N(x-y))\|a_x a_y\psi\|^2 + C_\delta\|\varphi_t^{(N)}\|^2_{H^2}.\end{aligned}$$

Proceeding analogously to control the second quadratic term on the r. h. s. of (2.80), we conclude that

$$\begin{aligned}\int \mathrm{d}x\mathrm{d}y\, N^2 V(N(x-y))\,&[\langle c_y, s_x\rangle\, a^*(c_x) a^*(c_y) + \langle s_x, c_y\rangle\, a(c_y) a(c_x)] \\ &= \int \mathrm{d}x\mathrm{d}y\, N^2 V(N(x-y))\,\big[k(x,y) a^*_x a^*_y + \overline{k}(x,y) a_x a_y\big] \\ &\quad + \widetilde{\mathcal{E}}(t)\end{aligned}$$

where the error $\widetilde{\mathcal{E}}(t)$ is such that, for every $\delta > 0$ there exists C_δ with

$$\pm\,\widetilde{\mathcal{E}}(t) \leq \delta\int \mathrm{d}x\mathrm{d}y N^2 V(N(x-y)) a^*_x a^*_y a_y a_x + C_\delta\|\varphi_t^{(N)}\|^2_{H^2}\,(\mathcal{N}+1).$$

We then use (2.27) to conclude the proof of the first bound in (2.82).

The proof of the second inequality in (2.82) is analogous, because commuting the terms contributing to $\mathcal{E}_4(t)$ with the number of particles operator $\mathcal{N}$ either gives zero or leaves the terms essentially invariant (up to a constant and a possible sign change). Finally, also the third estimate in (2.82) can be proven similarly, because the time derivative of the terms contributing to $\mathcal{E}_4(t)$ can be expressed as linear combination of terms having the same form, just with one argument c_x, c_y, s_x or s_y replaced by its time derivative. These terms can then be handled as above, using however the bounds for $\|\dot{\mathrm{sh}}_{k_t}\|_2$ and $\|\dot{p}_{k_t}\|_2$ from Lemma 2.3.4 and the bound for $\|\dot{\varphi}_t^{(N)}\|_{H^2}$ from Proposition 2.3.1. □

2.6.5. Analysis of $[i\partial_t T^*]T$

In this subsection we will show that the term $[i\partial_t T^*]T$ is only an error term, in the sense that it can be controlled with the number operator $\mathcal{N}$, without any need for employing cancellations. We set

$$B := \frac{1}{2}\int \mathrm{d}x\mathrm{d}y\, \left(k_t(x,y)a_x^* a_y^* - \overline{k_t(x,y)}a_x a_y\right)$$

and

$$\dot{B} := \frac{1}{2}\int \mathrm{d}x\mathrm{d}y\, \left(\dot{k}_t(x,y)a_x^* a_y^* - \overline{\dot{k}_t(x,y)}a_x a_y\right)$$

with

$$k_t(x,y) = -Nw(N(x-y))\varphi_t^{(N)}(x)\varphi_t^{(N)}(y)$$

and

$$\dot{k}_t(x,y) = -Nw(N(x-y))\left(\dot{\varphi}_t^{(N)}(x)\varphi_t^{(N)}(y) + \varphi_t^{(N)}(x)\dot{\varphi}_t^{(N)}(y)\right).$$

Then $T = \exp(B)$. Using the BCH formula (2.22), we find

$$(\partial_t T^*)\, T = -\int_0^1 \mathrm{d}\lambda\, e^{-\lambda B(t)}\dot{B}(t)e^{\lambda B(t)} = \sum_{n\geq 0}\frac{(-1)^{n+1}}{(n+1)!}\,\mathrm{ad}_B^n(\dot{B}). \tag{2.90}$$

More precisely, the integral can first be expanded as a finite sum and an error term; the error term however converges to zero in expectation values on the domain $D(\mathcal{N})$ of the number operator (this can be shown as in Lemma 2.2.1). By the estimates in Prop. 2.6.10, the series is absolutely convergent in expectation values. Since $D(\mathcal{N})$ is invariant w. r. t. the fluctuation dynamics $\mathcal{U}(t,s)$ (this is proven similarly to Prop. 2.4.2), we can use (2.90) to compute the expectation of $(\partial_t T^*)T$ in the vector $\mathcal{U}(t,0)\psi$ for any $\psi \in D(\mathcal{N})$.

Next, we compute the terms on the r. h. s. of (2.90).

Lemma 2.6.9. *For each $n \in \mathbb{N}$ there exist $f_{n,1}, f_{n,2} \in L^2(\mathbb{R}^3 \times \mathbb{R}^3)$ such that*

$$\begin{aligned}\mathrm{ad}_B^n(\dot{B}) &= \frac{1}{2}\int dx\,dy\,\left(f_{n,1}(x,y)a_y^* a_x^* + f_{n,2}(x,y)a_x a_y\right) \quad \textit{for all even } n \textit{ and}\\ \mathrm{ad}_B^n(\dot{B}) &= \frac{1}{2}\int dx\,dy\,\left(f_{n,1}(x,y)a_x^* a_y + f_{n,2}(x,y)a_x a_y^*\right) \quad \textit{for all odd } n\end{aligned} \tag{2.91}$$

where

$$\|f_{n,i}\|_2 \leq 2^n \|k_t\|_2^n \|\dot{k}_t\|_2, \tag{2.92}$$

for all $n \geq 0$ and $i = 1,2$,

$$\|\dot{f}_{n,i}\|_2 \leq \begin{cases} \|\ddot{k}_t\|_2 & \textit{if } n = 0\\ 4^n \|k_t\|_2^{n-1}\left(\|\ddot{k}_t\|_2\|k_t\|_2 + \|\dot{k}_t\|_2^2\right) & \textit{if } n \geq 1\end{cases} \tag{2.93}$$

and

$$\int dx\,|f_{n,i}(x,x)| \leq 2^n\|k_t\|_2^n\|\dot{k}_t\|_2, \qquad \int dx\,|\dot{f}_{n,i}(x,x)| \leq 4^n\|k_t\|_2^{n-1}\left(\|\dot{k}_t\|_2^2 + \|\ddot{k}_t\|_2\|k_t\|_2\right) \tag{2.94}$$

for all $n \geq 1$.

Proof. The proof is by induction in n. For $n = 0$,

$$\mathrm{ad}_B^0(\dot{B}) = \dot{B} = \frac{1}{2}\int \mathrm{d}x\mathrm{d}y \left(\dot{k}_t(x,y)a_x^* a_y^* - \overline{\dot{k}_t(x,y)}a_x a_y\right).$$

Hence $f_{0,1}(x,y) = \dot{k}_t(x,y)$ and $f_{0,2}(x,y) = \overline{\dot{k}_t(x,y)}$, and the estimates (2.92) and (2.93) are clearly satisfied. Suppose now the statement holds for some $n \in \mathbb{N}$. We prove the step to $(n+1)$. We start with the case that n is even: Using the canonical commutation relations (1.32), we find

$$\begin{aligned}
&\mathrm{ad}_B^{n+1}(\dot{B}) \\
&= [B, \mathrm{ad}_B^n(\dot{B})] \\
&= \left[\frac{1}{2}\int \mathrm{d}x\mathrm{d}y \left(k_t(x,y)a_x^* a_y^* - \overline{k_t(x,y)}a_x a_y\right), \frac{1}{2}\int \mathrm{d}x\mathrm{d}y \left(f_{n,1}(x,y)a_x^* a_y^* + f_{n,2}(x,y)a_x a_y\right)\right] \\
&= \frac{1}{2}\int \mathrm{d}x\mathrm{d}z \left(f_{n+1,1}(x,z)a_x^* a_z + f_{n+1,2}(x,z)a_x a_z^*\right),
\end{aligned}$$

where

$$\begin{aligned}
f_{n+1,1}(x,z) &= -\frac{1}{2}\int \mathrm{d}y \left(k_t(x,y)\left(f_{n,2}(z,y) + f_{n,2}(y,z)\right) + \overline{k_t(y,z)}\left(f_{n,2}(x,y) + f_{n,2}(y,x)\right)\right), \\
f_{n+1,2}(x,z) &= -\frac{1}{2}\int \mathrm{d}y \left(k_t(y,z)\left(f_{n,1}(x,y) + f_{n,1}(y,x)\right) + \overline{k_t(x,y)}\left(f_{n,1}(z,y) + f_{n,1}(y,z)\right)\right).
\end{aligned} \tag{2.95}$$

By Cauchy-Schwarz (similarly to (2.24)), we have

$$\begin{aligned}
\|f_{n+1,1}\|_2 &\leq 2\|k_t\|_2\|f_{n,2}\|_2 \leq 2^{n+1}\|k_t\|_2^{n+1}\|\dot{k}_t\|_2, \\
\|f_{n+1,2}\|_2 &\leq 2\|k_t\|_2\|f_{n,1}\|_2 \leq 2^{n+1}\|k_t\|_2^{n+1}\|\dot{k}_t\|_2,
\end{aligned} \tag{2.96}$$

where we used the induction assumption. Moreover, again by Cauchy-Schwarz,

$$\int \mathrm{d}x\, |f_{n+1,1}(x,x)| \leq 2\|k_t\|_2\|f_{n,2}\|_2 \leq 2^{n+1}\|k_t\|_2^{n+1}\|\dot{k}_t\|_2.$$

As for the time-derivative of $f_{n+1,i}$, we find

$$\begin{aligned}
\dot{f}_{n+1,1}(x,z) = -\frac{1}{2}\int \mathrm{d}y\Big(&\dot{k}_t(x,y)\left(f_{n,2}(z,y) + f_{n,2}(y,z)\right) + k_t(x,y)\left(\dot{f}_{n,2}(z,y) + \dot{f}_{n,2}(y,z)\right) \\
&+ \overline{\dot{k}_t(y,z)}\left(f_{n,2}(x,y) + f_{n,2}(y,x)\right) + \overline{k_t(y,z)}\left(\dot{f}_{n,2}(x,y) + \dot{f}_{n,2}(y,x)\right)\Big)
\end{aligned}$$

and similarly for $\dot{f}_{n+1,2}$. Hence, we find

$$\begin{aligned}
\|\dot{f}_{n+1,1}\|_2 &\leq 2\left(\|\dot{k}_t\|_2\|f_{n,2}\|_2 + \|k_t\|_2\|\dot{f}_{n,2}\|_2\right) \\
&\leq 2\left(2^n\|k_t\|_2^n\|\dot{k}_t\|_2^2 + 4^n\|k_t\|_2^n\left(\|\ddot{k}_t\|_2\|k_t\|_2 + \|\dot{k}_t\|_2^2\right)\right) \\
&\leq (2^{n+1} + 4^n)\|k_t\|_2^n\|\dot{k}_t\|_2^2 + 2\cdot 4^n\|k_t\|_2^{n+1}\|\ddot{k}_t\|_2 \\
&\leq 4^{n+1}\|k_t\|_2^n\left(\|\ddot{k}_t\|_2\|k_t\|_2 + \|\dot{k}_t\|_2^2\right),
\end{aligned}$$

proving (2.93) for $i = 1$. The same bound for $i = 2$ and the second bound in (2.94) for $i = 1, 2$ can be proven similarly.

We now prove the case where n is odd: using again the canonical commutation relations

$$\begin{aligned}
&\mathrm{ad}_B^{n+1}(\dot{B}) \\
&= \left[\frac{1}{2}\int \mathrm{d}x\mathrm{d}y \left(k_t(x,y)a_x^* a_y^* - \overline{k_t(x,y)}a_x a_y\right), \frac{1}{2}\int \mathrm{d}x\mathrm{d}y \left(f_{n,1}(x,y)a_x^* a_y + f_{n,2}(x,y)a_x a_y^*\right)\right] \\
&= \frac{1}{2}\int \mathrm{d}x\mathrm{d}z \big(a_x^* a_z^* f_{n+1,1}(x,z) + a_x a_z f_{n+1,2}(x,z)\big)
\end{aligned}$$

where

$$\begin{aligned}
f_{n+1,1}(x,z) &= -\int \mathrm{d}y\, k_t(x,y)\left(f_{n,1}(z,y) + f_{n,2}(y,z)\right), \\
f_{n+1,2}(x,z) &= -\int \mathrm{d}y\, \overline{k_t(x,y)}\left(f_{n,1}(y,z) + f_{n,2}(z,y)\right).
\end{aligned} \tag{2.97}$$

The bounds (2.92), (2.93), (2.94) follow as above. □

Using Lemma 2.6.9, we obtain the following properties of $(\partial_t T^*)T$.

Proposition 2.6.10. *There exists a constant $C > 0$ with*

$$\begin{aligned}
\pm\,(i\partial_t T^*)T &\leq Ce^{K|t|}\,(\mathcal{N}+1), \\
\pm\,[\mathcal{N}, (i\partial_t T^*)T] &\leq Ce^{K|t|}\,(\mathcal{N}+1), \\
\pm\partial_t\left[(i\partial_t T^*)T\right] &\leq Ce^{K|t|}\,(\mathcal{N}+1).
\end{aligned} \tag{2.98}$$

Proof. We observe first of all that, for all $f_1, f_2 \in L^2(\mathbb{R}^3 \times \mathbb{R}^3)$ with $\int \mathrm{d}x\,|f_2(x,x)| < \infty$, we have

$$\left|\left\langle \psi, \int \mathrm{d}x\mathrm{d}y \left(f_1(x,y)a_x^* a_y^* + f_2(x,y)a_x a_y\right)\psi\right\rangle\right| \leq (\|f_1\|_2 + \|f_2\|_2)\,\langle\psi, (\mathcal{N}+1)\psi\rangle \tag{2.99}$$

and

$$\begin{aligned}
&\left|\langle\psi, \int \mathrm{d}x\mathrm{d}y\,(f_1(x,y)a_x^* a_y + f_2(x,y)a_x a_y^*)\psi\rangle\right| \\
&\qquad\leq (\|f_1\|_2 + \|f_2\|_2)\langle\psi, \mathcal{N}\psi\rangle + \int |f_2(x,x)|\mathrm{d}x\,\|\psi\|^2.
\end{aligned} \tag{2.100}$$

In fact, (2.99) follows because

$$\begin{aligned}
&\left|\langle\psi, \int \mathrm{d}x\mathrm{d}y\,(f_1(x,y)a_x^* a_y^* + f_2(x,y)a_x a_y)\psi\rangle\right| \\
&\qquad\leq \int \mathrm{d}x\,\left(\|a_x\psi\|\|a^*(f_1(x,.))\psi\| + \|a^*(f_2(x,.))\psi\|\|a_x\psi\|\right) \\
&\qquad\leq \|(\mathcal{N}+1)^{1/2}\psi\| \int \mathrm{d}x\,(\|f_1(x,.)\|_2 + \|f_2(x,.)\|_2)\,\|a_x\psi\| \\
&\qquad\leq (\|f_1\|_2 + \|f_2\|_2)\|(\mathcal{N}+1)^{1/2}\psi\|^2.
\end{aligned}$$

Eq. (2.100) can be proven similarly. Combining the last estimates with Lemma 2.6.9 and with (2.90), we find

$$\begin{aligned}
|\langle\psi,(\partial_t T^*)T\psi\rangle| &\leq \sum_{n\geq 0}\frac{1}{(n+1)!}\left|\langle\psi,\mathrm{ad}^n_B(\dot{B})\psi\rangle\right| \\
&\leq \sum_{n\geq 0}\frac{1}{(n+1)!}\left(\|f_{n,1}\|_2+\|f_{n,2}\|_2\right)\|(\mathcal{N}+1)^{1/2}\psi\|^2 \\
&\quad+\sum_{n\geq 1}\frac{1}{(2n)!}\left(\int \mathrm{d}x\,|f_{2n-1,2}(x,x)|dx\right)\|\psi\|^2 \\
&\leq C\sum_{n\geq 0}\frac{(2\|k_t\|_2)^n}{(n+1)!}\|\dot{k}_t\|_2\,\|(\mathcal{N}+1)^{1/2}\psi\|^2+\sum_{n\geq 1}\frac{(2\|k_t\|_2)^n}{(2n)!}\|\dot{k}_t\|_2\|\psi\|^2 \\
&\leq Ce^{2\|k_t\|_2}\|\dot{k}_t\|_2\,\|(\mathcal{N}+1)^{1/2}\psi\|^2 \\
&\leq Ce^{K|t|}\,\|(\mathcal{N}+1)^{1/2}\psi\|^2
\end{aligned}$$

using also Lemma 2.3.4. The second inequality in (2.98) follows similarly because, essentially, the only consequence of taking the commutator with $\mathcal{N}$ is to eliminate the terms $\mathrm{ad}^n_B(\dot{B})$ for all odd n. Also the third bound in (2.98) can be proven analogously, taking the time derivative of the expressions for $\mathrm{ad}^n_B(\dot{B})$ given in (2.91), using the bounds for $\|\dot{f}_{n,i}\|_2$ in (2.93) and (2.94) and, finally, using the estimate for $\|\ddot{k}_t\|_2$ proven in Lemma 2.3.4. □

2.6.6. Cancellations in the generator (proof of Theorem 2.3.5)

Proof of Theorem 2.3.5. In this subsection, we combine the results of the previous subsections to obtain a proof of Theorem 2.3.5. From (2.54) and Propositions 2.6.1, 2.6.3, 2.6.5, 2.6.6 it follows that

$$\begin{aligned}
\mathcal{L}_N(t) = C_N(t)+\mathcal{K}+\frac{1}{2N}\int \mathrm{d}x\mathrm{d}y\,N^3V(N(x-y))a^*_x a^*_y a_y a_x \\
+\Big[N^3\int \mathrm{d}x\mathrm{d}y\,(\Delta w)(N(x-y))\varphi^{(N)}_t(x)\varphi^{(N)}_t(y)a^*_x a^*_y \\
+\frac{1}{2}\int \mathrm{d}x\mathrm{d}y\,N^3V(N(x-y))\big(1-w(N(x-y))\big)\varphi^{(N)}_t(x)\varphi^{(N)}_t(y)\,a^*_x a^*_y+\mathrm{h.c.}\Big] \\
+\mathcal{E}(t)
\end{aligned} \tag{2.101}$$

where the constant $C_N(t)$ is defined in (2.34) and the error $\mathcal{E}(t)$ is such that, for every $\delta>0$ there exists $C_\delta>0$ with

$$\begin{aligned}
\pm\mathcal{E}(t) &\leq \delta\left(\mathcal{K}+\int \mathrm{d}x\mathrm{d}yN^2V(N(x-y))a^*_x a^*_y a_y a_x\right)+C_\delta\frac{\mathcal{N}^2}{N}+C_\delta e^{K|t|}\,(\mathcal{N}+1)\,, \\
\pm[\mathcal{N},\mathcal{E}(t)] &\leq \delta\left(\mathcal{K}+\int \mathrm{d}x\mathrm{d}yN^2V(N(x-y))a^*_x a^*_y a_y a_x\right)+C_\delta\frac{\mathcal{N}^2}{N}+C_\delta e^{K|t|}\,(\mathcal{N}+1)\,, \\
\pm\dot{\mathcal{E}}(t) &\leq \delta\left(\mathcal{K}+\int \mathrm{d}x\mathrm{d}yN^2V(N(x-y))a^*_x a^*_y a_y a_x\right)+C_\delta e^{K|t|}\left(\frac{\mathcal{N}^2}{N}+\mathcal{N}+1\right).
\end{aligned} \tag{2.102}$$

In deriving (2.101), we made use of the crucial cancellation between the linear contributions in (2.54) and the linear terms in (2.78). Next, we notice another crucial cancellation. The terms on the second and third line in (2.101) can be written as

$$N^3 \int \mathrm{d}x\mathrm{d}y\, a_x^* a_y^* \left[\left(-\Delta + \frac{1}{2} V \right) (1-w) \right] (N(x-y)) \varphi_t^{(N)}(x) \varphi_t^{(N)}(y) = 0$$

since $f = 1 - w$ is a solution of the zero-energy scattering equation $(-\Delta + (1/2)V)f = 0$.

We conclude that

$$\mathcal{L}_N(t) = C_N(t) + \mathcal{K} + \frac{1}{2N} \int \mathrm{d}x\mathrm{d}y N^3 V(N(x-y)) a_x^* a_y^* a_y a_x + \mathcal{E}(t) \tag{2.103}$$

where the error $\mathcal{E}(t)$ satisfies (2.102). Then (2.36) follows from the first bound in (2.102), taking $\delta = 1/2$. Also (2.38) and (2.39) follow from the second and third bounds in (2.102), since both $\mathcal{K}$ and the quartic term on the r. h. s. of (2.103) commute with $\mathcal{N}$ and are time-independent.

This concludes the proof of Theorem 2.3.5. □

2.A. Properties of the solution of the Gross-Pitaevskii equation

Proof of Proposition 2.3.1. (i) This part of the proposition is standard. One proves first local well-posedness of the two equations in $H^1(\mathbb{R}^3)$. The time of existence depends only on the H^1-norm of the initial data. Since $V, f \geq 0$, the H^1-norm is bounded by the energy, which is conserved. Hence one obtains global existence and a uniform bound on the H^1-norm.

(ii) Also this part is rather standard, but since the non-linearity in (2.25) depends on N, and we need bounds uniform in N, we sketch the proof of the bound (2.27) for $\|\varphi_t^{(N)}\|_{H^n}$ (the bound for $\|\varphi_t\|_{H^n}$ can be proven analogously). We present the proof for the case $t > 0$. We claim, first of all, that there exists $T > 0$ depending only on $\|\varphi\|_{H^1}$ and $n \in \mathbb{N}$ such that

$$\sup_{t \in [0,T]} \|\varphi_t^{(N)}\|_{H^n} \leq 2\|\varphi\|_{H^n} + \sup_{t \in [0,T]} \|\varphi_t^{(N)}\|_{H^{n-1}}^3. \tag{2.104}$$

Introducing the short-hand notation $U_N(x) = N^3 V(Nx) f(Nx)$, we write the solution $\varphi_t^{(N)}$ of (2.25) as

$$\varphi_t^{(N)} = e^{it\Delta}\varphi - i \int_0^t \mathrm{d}s\, e^{i(t-s)\Delta} (U_N * |\varphi_s^{(N)}|^2) \varphi_s^{(N)}.$$

Differentiating this equation w. r. t. the spatial variables we find that

$$\partial^\alpha \varphi_t^{(N)} = e^{it\Delta}\partial^\alpha\varphi - i \int_0^t \mathrm{d}s\, e^{i(t-s)\Delta} \sum_{\beta \leq \alpha} \sum_{\nu \leq \beta} \binom{\alpha}{\beta} \binom{\beta}{\nu} \big(U_N * (\partial^\nu \overline{\varphi}_s^{(N)} \partial^{\beta-\nu} \varphi_s^{(N)}) \big) \partial^{\alpha-\beta} \varphi_s^{(N)}.$$

Here α is a three-dimensional multi-index of non-negative integers, with $|\alpha| \leq n$.

The $L_t^\infty([0,T], L_x^2)$-norm of the above expression can be controlled using Strichartz estimates for the free Schrödinger evolution $e^{it\Delta}$ (see [KT98, Theorem 1.2]). We find

$$\begin{aligned}
&\|\partial^\alpha \varphi_{(.)}^{(N)}\|_{L_t^\infty L_x^2} \\
&\leq \|\partial^\alpha\varphi\|_{L^2} + \sum_{\beta \leq \alpha} \sum_{\nu \leq \beta} \binom{\alpha}{\beta} \binom{\beta}{\nu} \big\| \big(U_N * (\partial^\nu \overline{\varphi}_{(.)}^{(N)} \partial^{\beta-\nu} \varphi_{(.)}^{(N)}) \big) \partial^{\alpha-\beta} \varphi_{(.)}^{(N)} \big\|_{L_t^2 L_x^{6/5}} \\
&\leq \|\partial^\alpha\varphi\|_{L^2} + T^{1/2} \sum_{\beta \leq \alpha} \sum_{\nu \leq \beta} \binom{\alpha}{\beta} \binom{\beta}{\nu} \sup_{t \in [0,T]} \big\| \big(U_N * (\partial^\nu \overline{\varphi}_t^{(N)} \partial^{\beta-\nu} \varphi_t^{(N)}) \big) \partial^{\alpha-\beta} \varphi_t^{(N)} \big\|_{L_x^{6/5}}.
\end{aligned}$$

By Hölder and Young inequality, we find

$$\begin{aligned}&\|\partial^\alpha \varphi^{(N)}_{(.)}\|_{L^\infty_t L^2_x}\\ &\leq \|\partial^\alpha \varphi\|_{L^2} + CT^{1/2} \sum_{\beta\leq\alpha}\sum_{\nu\leq\beta} \binom{\alpha}{\beta}\binom{\beta}{\nu} \sup_{t\in[0,T]} \|\partial^\nu \varphi_t^{(N)}\|_{L^{p_1}} \|\partial^{\beta-\nu}\varphi_t^{(N)}\|_{L^{p_2}} \, \|\partial^{\alpha-\beta}\varphi_t^{(N)}\|_{L^{p_3}}\end{aligned}$$

for $p_1, p_2, p_3 \geq 1$ with $p_1^{-1} + p_2^{-1} + p_3^{-1} = 5/6$. It is important to note that the indices (p_1, p_2, p_3) can be chosen differently for each term in the summation. In some of the terms with $|\alpha| = n$, all n derivatives hit the same $\varphi_t^{(N)}$. Since $1/6 + 1/6 + 1/2 = 5/6$, these terms can be bounded by

$$\|\varphi_t^{(N)}\|_{L^6}^2 \, \|\partial^\alpha \varphi_t^{(N)}\|_{L^2} \leq C\|\varphi_t^{(N)}\|_{H^n} \tag{2.105}$$

for C depending only on $\|\varphi\|_{H^1}$ (recall here that the H^1-norm is bounded uniformly in t, by part (i)). In some of the other terms, one $\varphi_t^{(N)}$ has $n-1$ derivatives, one has at most one derivative and the last one has no derivatives. Since $\|\partial^\gamma \varphi_t^{(N)}\|_{L^6} \leq \|\varphi_t^{(N)}\|_{H^n}$, if $|\gamma| \leq n-1$, these terms are bounded by the r. h. s. of (2.105). In all other terms, the three copies of $\varphi_t^{(N)}$ have at most $n-2$ derivatives. These terms are bounded by

$$\|\partial^{\gamma_1}\varphi_t^{(N)}\|_{L^6}\|\partial^{\gamma_2}\varphi_t^{(N)}\|_{L^6}\|\partial^{\gamma_3}\varphi_t^{(N)}\|_{L^2} \leq C\|\varphi_t^{(N)}\|_{H^{n-1}}^3$$

for all multi-indices $\gamma_1, \gamma_2, \gamma_3$ with $|\gamma_i| \leq n-2$, for $i = 1, 2, 3$. We conclude that

$$\|\partial^\alpha \varphi^{(N)}_{(.)}\|_{L^\infty_t L^2_x} \leq \|\partial^\alpha\varphi\|_{L^2} + CT^{1/2} \sup_{t\in[0,T]} \|\varphi_t^{(N)}\|_{H^n} + CT^{1/2} \sup_{t\in[0,T]} \|\varphi_t^{(N)}\|_{H^{n-1}}^3.$$

Summing over all α with $|\alpha| \leq n$, we find

$$\sup_{t\in[0,T]} \|\varphi_t^{(N)}\|_{H^n} \leq \|\varphi\|_{H^n} + CT^{1/2} \sup_{t\in[0,T]} \|\varphi_t^{(N)}\|_{H^n} + CT^{1/2} \sup_{t\in[0,T]} \|\varphi_t^{(N)}\|_{H^{n-1}}^3.$$

Choosing $T > 0$ so small that $CT^{1/2} \leq 1/2$, we find (2.104).

To show (2.27), we iterate now (2.104). We proceed by induction over n. For $n = 1$, the claim follows from part (i). Suppose now that $\|\varphi_t^{(N)}\|_{H^{(n-1)}} \leq C_{n-1}\exp(K_{n-1}|t|)$, for constants C_{n-1}, K_{n-1} depending on $\|\varphi\|_{H^{(n-1)}}$ and, respectively, on $\|\varphi\|_{H^1}$. Let T be as in (2.104). For an arbitrary $t > 0$, there exists an integer $j \in \mathbb{N}$ such that $(j-1)T < t \leq jT$. Then

$$\begin{aligned}\|\varphi_t^{(N)}\|_{H^n} &\leq \sup_{s\in[(j-1)T,jT]} \|\varphi_s^{(N)}\|_{H^n}\\ &\leq 2\|\varphi^{(N)}_{(j-1)T}\|_{H^n} + 2 \sup_{s\in[(j-1)T,jT]} \|\varphi_s^{(N)}\|_{H^{n-1}}^3\\ &\leq 2\|\varphi^{(N)}_{(j-1)T}\|_{H^n} + 2C_{n-1}^3 e^{3K_{n-1}jT}.\end{aligned}$$

Similarly we have

$$\|\varphi^{(N)}_{(j-1)T}\|_{H^n} \leq 2\|\varphi^{(N)}_{(j-2)T}\|_{H^n} + 2C_{n-1}^3 e^{3K_{n-1}(j-1)T}.$$

Iterating j-times, we obtain

$$\|\varphi_t^{(N)}\|_{H^n} \leq 2^j\|\varphi\|_{H^n} + 2C_{n-1}^3 \sum_{\ell=0}^{j} 2^\ell e^{3K_{n-1}(j-\ell)T} \leq C_n e^{K_n t},$$

for some constant C_n depending on $\|\varphi\|_{H^n}$ and K_n depending only on $\|\varphi\|_{H^1}$.

(iii)[6] From the modified Gross-Pitaevskii equation (2.25), letting $U_N(x) = N^3V(Nx)f(Nx)$, we find

$$\begin{aligned}
\|\dot{\varphi}_t^{(N)}\|_2 &\le \|\varphi_t^{(N)}\|_{H^2} + \left\|\left(U_N * |\varphi_t^{(N)}|^2\right)\varphi_t^{(N)}\right\|_2 \\
&\le \|\varphi_t^{(N)}\|_{H^2} + \left\|U_N * |\varphi_t^{(N)}|^2\right\|_2 \|\varphi_t^{(N)}\|_\infty \\
&\le \|\varphi_t^{(N)}\|_{H^2} + C\|U_N\|_1\|\varphi_t^{(N)}\|_4^2\,\|\varphi_t^{(N)}\|_\infty \\
&\le C\|\varphi_t^{(N)}\|_{H^2}^3 \le Ce^{K|t|}
\end{aligned}$$

for a constant C depending only on $\|\varphi\|_{H^2}$ and $\|U_N\|_1$, and for $K > 0$ depending only on $\|\varphi\|_{H^1}$. Here we used part (ii). Applying the gradient to (2.25), we find

$$\begin{aligned}
i\nabla\dot{\varphi}_t^{(N)} &= -\nabla\Delta\varphi_t^{(N)} + \left(U_N * |\varphi_t^{(N)}|^2\right)\nabla\varphi_t^{(N)} \\
&\quad + \left(U_N * \overline{\varphi}_t^{(N)}\nabla\varphi_t^{(N)}\right)\varphi_t^{(N)} + \left(U_N * \nabla\overline{\varphi}_t^{(N)}\varphi_t^{(N)}\right)\varphi_t^{(N)}.
\end{aligned} \tag{2.106}$$

Clearly, $\|\nabla\Delta\varphi_t^{(N)}\|_2 \le \|\varphi_t^{(N)}\|_{H^3}$. The second term on the first line is bounded in norm by

$$\begin{aligned}
\left\|(U_N * |\varphi_t^{(N)}|^2)\nabla\varphi_t^{(N)}\right\|_2 &\le \|(U_N * |\varphi_t^{(N)}|^2)\|_\infty \|\nabla\varphi_t^{(N)}\|_2 \\
&\le \|U_N\|_1\|\varphi_t^{(N)}\|_\infty^2\|\nabla\varphi_t^{(N)}\|_2 \le C\|\varphi_t^{(N)}\|_{H^2}^3.
\end{aligned}$$

The terms on the second line of (2.106) can be bounded similarly. From part (ii), we conclude that $\|\nabla\dot{\varphi}_t^{(N)}\|_2 \le C\exp(K|t|)$. Analogously, we can also show that $\|\nabla^2\dot{\varphi}_t^{(N)}\|_2 \le Ce^{K|t|}$. We conclude that $\|\dot{\varphi}_t^{(N)}\|_{H^2} \le Ce^{K|t|}$. Finally, (2.25) implies

$$\begin{aligned}
-\ddot{\varphi}_t^{(N)} = &- \Delta i\dot{\varphi}_t^{(N)} + \left(U_N * (\overline{\varphi}_t^{(N)} i\dot{\varphi}_t^{(N)})\right)\varphi_t^{(N)} \\
&+ \left(U_N * (i\dot{\overline{\varphi}}_t^{(N)}\varphi_t^{(N)})\right)\varphi_t^{(N)} + \left(U_N * |\varphi_t^{(N)}|^2\right) i\dot{\varphi}_t^{(N)}.
\end{aligned}$$

Plugging in the r. h. s. of (2.25) for $i\dot{\varphi}_t^{(N)}$, we arrive at

$$\begin{aligned}
-\ddot{\varphi}_t^{(N)} &= \Delta^2\varphi_t^{(N)} - \Delta\left((U_N * |\varphi_t^{(N)}|^2)\varphi_t^{(N)}\right) + \left(U_N * |\varphi_t^{(N)}|^2\right)^2\varphi_t^{(N)} \\
&\quad + (U_N * \overline{\varphi}_t^{(N)}(-\Delta\varphi_t^{(N)}))\varphi_t^{(N)} + 2\left[U_N * \left(|\varphi_t^{(N)}|^2(U_N * |\varphi_t^{(N)}|^2)\right)\right]\varphi_t^{(N)} \\
&\quad + (U_N * (-\Delta\overline{\varphi}_t^{(N)})\varphi_t^{(N)})\varphi_t^{(N)} + \left(U_N * |\varphi_t^{(N)}|^2\right)(-\Delta\varphi_t^{(N)}).
\end{aligned}$$

Proceeding similarly as above, we find that $\|\ddot{\varphi}_t^{(N)}\|_2 \le C\|\varphi_t^{(N)}\|_{H^4} \le C\exp(K|t|)$.

(iv) Using (2.16) and (2.25), we find

$$\begin{aligned}
\partial_t\|\varphi_t - \varphi_t^{(N)}\|_2^2 &= -2\,\mathrm{Im}\left\langle\varphi_t, (U_N * |\varphi_t^{(N)}|^2 - 8\pi a_0|\varphi_t|^2)\varphi_t^{(N)}\right\rangle \\
&= -2\,\mathrm{Im}\left\langle\varphi_t, (U_N * |\varphi_t|^2 - 8\pi a_0|\varphi_t|^2)\varphi_t^{(N)}\right\rangle \\
&\quad - 2\,\mathrm{Im}\left\langle\varphi_t, \left(U_N * (|\varphi_t^{(N)}|^2 - |\varphi_t|^2)\right)\varphi_t^{(N)}\right\rangle.
\end{aligned} \tag{2.107}$$

[6]Some typos in [BdS12] in this part were corrected here.

The second term on the r. h. s. can be written as

$$\operatorname{Im}\left\langle \varphi_t, \left(U_N * \left(|\varphi_t^{(N)}|^2 - |\varphi_t|^2\right)\right) \varphi_t^{(N)} \right\rangle = \operatorname{Im}\left\langle \varphi_t, \left(U_N * \left(|\varphi_t^{(N)}|^2 - |\varphi_t|^2\right)\right) (\varphi_t - \varphi_t^{(N)}) \right\rangle .$$

Hence, by Hölder's and triangle's inequality,

$$\begin{aligned}
&\left| \operatorname{Im}\left\langle \varphi_t, \left(U_N * \left(|\varphi_t^{(N)}|^2 - |\varphi_t|^2\right)\right) \varphi_t^{(N)} \right\rangle \right| \\
&\qquad \leq \|\varphi_t\|_\infty \left\| \left(U_N * \left(|\varphi_t^{(N)}|^2 - |\varphi_t|^2\right)\right) (\varphi_t - \varphi_t^{(N)}) \right\|_1 \\
&\qquad \leq \|\varphi_t\|_\infty \left\| U_N * (|\varphi_t^{(N)}|^2 - |\varphi_t|^2) \right\|_2 \|\varphi_t - \varphi_t^{(N)}\|_2 \\
&\qquad \leq \|U_N\|_1 \|\varphi_t\|_\infty \|\varphi_t - \varphi_t^{(N)}\|_2 \left\| |\varphi_t^{(N)}|^2 - |\varphi_t|^2 \right\|_2 \\
&\qquad \leq \|U_N\|_1 \|\varphi_t\|_\infty \left(\|\varphi_t\|_\infty + \|\varphi_t^{(N)}\|_\infty \right) \|\varphi_t - \varphi_t^{(N)}\|_2^2 \\
&\qquad \leq C \left(\|\varphi_t\|_{H^2}^2 + \|\varphi_t^{(N)}\|_{H^2}^2 \right) \|\varphi_t - \varphi_t^{(N)}\|_2^2.
\end{aligned} \tag{2.108}$$

As for the first term on the r. h. s. of (2.107), we find (since $\int U_N(y)dy = 8\pi a_0$)

$$\begin{aligned}
&\left| \left\langle \varphi_t, \left(U_N * |\varphi_t|^2 - 8\pi a_0 |\varphi_t|^2\right) \varphi_t^{(N)} \right\rangle \right| \\
&\qquad = \left| \int \mathrm{d}x\, \overline{\varphi}_t(x) \varphi_t^{(N)}(x) \int \mathrm{d}y\, U_N(y) \left(|\varphi_t(x-y)|^2 - |\varphi_t(x)|^2 \right) \right| \\
&\qquad \leq \int \mathrm{d}x \mathrm{d}y\, U_N(y)\, |\varphi_t(x)| |\varphi_t^{(N)}(x)| \left| |\varphi_t(x-y)|^2 - |\varphi_t(x)|^2 \right| .
\end{aligned}$$

Writing $U_N(x) = N^3 U(Nx)$, with $U(x) = V(x) f(x)$ and changing integration variables, we find

$$\begin{aligned}
&\left| \left\langle \varphi_t, \left(U_N * |\varphi_t|^2 - 8\pi a_0 |\varphi_t|^2\right) \varphi_t^{(N)} \right\rangle \right| \\
&\qquad \leq \int \mathrm{d}x \mathrm{d}y U(y) |\varphi_t(x)| |\varphi_t^{(N)}(x)| \left| |\varphi_t(x - y/N)|^2 - |\varphi_t(x)|^2 \right| .
\end{aligned}$$

Using

$$\begin{aligned}
\left| |\varphi_t(x-y/N)|^2 - |\varphi_t(x)|^2 \right| &= \left| \int_0^1 \mathrm{d}s \frac{\mathrm{d}}{\mathrm{d}s} |\varphi_t(x - sy/N)|^2 \right| \\
&\leq 2|y| N^{-1} \int_0^1 \mathrm{d}s\, |\nabla \varphi_t(x - sy/N)| |\varphi_t(x - sy/N)|
\end{aligned}$$

we conclude that

$$\begin{aligned}
&\left| \left\langle \varphi_t, \left(U_N * |\varphi_t|^2 - 8\pi a_0 |\varphi_t|^2\right) \varphi_t^{(N)} \right\rangle \right| \\
&\leq 2N^{-1} \int \mathrm{d}x \mathrm{d}y \int_0^1 \mathrm{d}s\, U(y) |y| |\varphi_t(x)| |\varphi_t^{(N)}(x)| |\nabla \varphi_t(x - sy/N)| |\varphi_t(x - sy/N)| \\
&\leq 2N^{-1} \|\varphi_t\|_\infty^2 \int \mathrm{d}x \mathrm{d}y \int_0^1 \mathrm{d}s\, U(y) |y| \left(|\varphi_t^{(N)}(x)|^2 + |\nabla \varphi_t(x - sy/N)|^2 \right) \\
&\leq C N^{-1} \|\varphi_t\|_\infty^2 \left(\|\varphi_t^{(N)}\|_2^2 + \|\nabla \varphi_t\|_2^2 \right) \\
&\leq C N^{-1} \|\varphi_t\|_{H^2}^2
\end{aligned} \tag{2.109}$$

where the constant C depends on $\int \mathrm{d}y U(y)|y|$ and on $\|\varphi\|_{H^1}$. Inserting (2.109) and (2.108) into (2.107), and using the estimate from part (ii) for $\|\varphi_t\|_{H^2}$, we find

$$\partial_t \|\varphi_t^{(N)} - \varphi_t\|_2^2 \leq C e^{K|t|} \|\varphi_t^{(N)} - \varphi_t\|_2^2 + \frac{C}{N} e^{K|t|}.$$

The claim now follows from Grönwall's inequality, since $\varphi_{t=0} = \varphi_{t=0}^{(N)}$. □

2.B. Properties of the kernel k_t

This section is devoted to the proof of Lemma 2.3.3 and Lemma 2.3.4.

Proof of Lemma 2.3.3. Recall that the constant C here can depend on $\|\varphi\|_{H^1}$.

(i) We will make use of the bounds (2.30). The first bound implies immediately that

$$|k(x,y)| \leq \min\left(N|\varphi(x)||\varphi(y)|, \frac{1}{|x-y|}|\varphi(x)||\varphi(y)|\right) \tag{2.110}$$

and therefore, by Hardy's inequality

$$\|k\|_2^2 \leq C \int \mathrm{d}x\mathrm{d}y \frac{1}{|x-y|^2} |\varphi(x)|^2 |\varphi(y)|^2 \leq C\|\varphi\|_{H^1}^2 \|\varphi\|_2^2 \leq C\,.$$

As for the gradient of k, we have

$$\nabla_1 k(x,y) = -N^2 \nabla w(N(x-y))\varphi(x)\varphi(y) - N w(N(x-y))\nabla\varphi(x)\varphi(y)$$

and thus, from the second bound in (2.30),

$$\begin{aligned}\|\nabla_1 k\|_2^2 &\leq C \int \mathrm{d}x\mathrm{d}y \, \frac{N^4}{(N^2|x-y|^2+1)^2} |\varphi(x)|^2 |\varphi(y)|^2 \\ &\leq CN \int \mathrm{d}x \frac{N^3}{(N^2|x|^2+1)^2} \|\varphi\|_{H^1}^4 \leq CN\end{aligned}$$

where we used Young and then Sobolev inequalities, and for the very last inequality the substitution $Nx \mapsto y$. Next we compute

$$\begin{aligned}\nabla_1(k\overline{k})(x,y) &= \nabla_x \int \mathrm{d}z \, k(x,z)\overline{k}(z,y) \\ &= \nabla_x \left[\varphi(x)\varphi(y) \int \mathrm{d}z N^2 w(N(x-z)) w(N(z-y)) |\varphi(z)|^2 \right] \\ &= \nabla\varphi(x)\varphi(y) \int \mathrm{d}z N^2 w(N(x-z)) w(N(z-y)) |\varphi(z)|^2 \\ &\quad + \varphi(x)\varphi(y) \int \mathrm{d}z N^3 \nabla w(N(x-z)) w(N(z-y)) |\varphi(z)|^2.\end{aligned}$$

Using (2.30), we find

$$\begin{aligned}\|\nabla_1(k\overline{k})\|_2^2 &\leq C\int \mathrm{d}x\mathrm{d}y\mathrm{d}z_1\mathrm{d}z_2\, \frac{|\nabla\varphi(x)|^2|\varphi(y)|^2|\varphi(z_1)|^2|\varphi(z_2)|^2}{|x-z_1||z_1-y||x-z_2||z_2-y|} \\ &\quad + C\int \mathrm{d}x\mathrm{d}y\mathrm{d}z_1\mathrm{d}z_2\, \frac{|\varphi(x)|^2|\varphi(y)|^2|\varphi(z_1)|^2|\varphi(z_2)|^2}{|x-z_1|^2|z_1-y||x-z_2|^2|z_2-y|} \\ &\leq C\int \mathrm{d}x\mathrm{d}y\mathrm{d}z_1\mathrm{d}z_2\, \frac{|\nabla\varphi(x)|^2|\varphi(y)|^2|\varphi(z_1)|^2|\varphi(z_2)|^2}{|x-z_1|^2|z_2-y|^2} \\ &\quad + C\int \mathrm{d}x\mathrm{d}y\mathrm{d}z_1\mathrm{d}z_2\, \frac{|\varphi(x)|^2|\varphi(y)|^2|\varphi(z_1)|^2|\varphi(z_2)|^2}{|x-z_1|^2|z_1-y|^2|x-z_2|^2} \\ &\leq C\|\varphi\|_{H^1}^3\|\varphi\|_2^2.\end{aligned}$$

(ii) The pointwise bound for $k(x,y)$ follows directly from (2.30), as noticed in (2.110). To bound $|r(k)(x,y)|$, we observe that, by Hölder's inequality, (2.30) and part (i),

$$\begin{aligned}&|(k\overline{k})^n k(x,y)| \\ &\quad = |k\overline{k}(k\overline{k})^{n-1}k(x,y)| \\ &\quad = |\varphi(x)||\varphi(y)| \\ &\quad\quad \times \left|\int \mathrm{d}z_1\mathrm{d}z_2\, N^2 w(N(x-z_1))w(N(z_2-y))\varphi(z_1)\varphi(z_2)\overline{k}(k\overline{k})^{n-1}(z_1,z_2)\right| \\ &\quad \leq |\varphi(x)||\varphi(y)|\, \|\overline{k}(k\overline{k})^{n-1}\|_2 \\ &\quad\quad \times \left(\int \mathrm{d}z_1 N^2 w(N(x-z_1))^2|\varphi(z_1)|^2 \int \mathrm{d}z_2\, N^2 w(N(z_2-y))^2|\varphi(z_2)|^2\right)^{1/2} \\ &\quad \leq C|\varphi(x)||\varphi(y)|\|\nabla\varphi\|_2^2\|k\|_2^{2n-1}.\end{aligned}$$

Thus

$$|r(k)(x,y)| \leq \sum_{n=1}^{\infty}\frac{1}{(2n+1)!}|(k\overline{k})^n k(x,y)| \leq C|\varphi(x)||\varphi(y)|e^{\|k\|_2}.$$

The pointwise estimate for $p(k)(x,y)$ can be proven similarly. This completes the proof of part (ii). Part (iii) follows easily from the pointwise bounds in part (ii). □

Proof of Lemma 2.3.4. In the following proof we will use the bounds $\|\dot{\varphi}_t^{(N)}\|_{H^2}, \|\ddot{\varphi}_t^{(N)}\|_2 \leq Ce^{K|t|}$ from Proposition 2.3.1.

(i) From (2.32), we find

$$\|\dot{k}_t\|^2 \leq 4\int \mathrm{d}x\mathrm{d}y\, \frac{1}{|x-y|^2}|\dot{\varphi}_t^{(N)}(x)|^2|\varphi_t^{(N)}(y)|^2 \leq C\|\dot{\varphi}_t^{(N)}\|_2^2\|\varphi_t^{(N)}\|_{H^1}^2 \leq Ce^{K|t|} \tag{2.111}$$

by Hardy's inequality, and from Proposition 2.3.1, part (iii). Similarly,

$$\|\ddot{k}_t\|_2 \leq C\|\ddot{\varphi}_t^{(N)}\|_2 + C\|\dot{\varphi}_t^{(N)}\|_2\|\nabla\dot{\varphi}_t^{(N)}\|_2 \leq Ce^{K|t|}$$

by Proposition 2.3.1. Writing $p(k_t) = \sum_{n\geq 0}(k_t\overline{k}_t)^n/(2n!)$, we find immediately

$$\|\dot{p}(k_t)\|_2 \leq \sum_{n\geq 0}\frac{1}{(2n)!}n\|\dot{k}_t\|_2\|k_t\|_2^{2n-1} \leq \|\dot{k}_t\|_2\, e^{\|k_t\|_2} \leq Ce^{K|t|}$$

applying (2.111). The bound for $\dot{r}(k_t)$ can be proven analogously.

(ii) From 2.2.1, part (v), we have

$$\|\nabla_1 \dot{p}(k_t)\|_2 \leq Ce^{\|k_t\|_2}\left(\|\dot{k}_t\|_2\,\|\nabla_1(k_t\overline{k}_t)\|_2 + C\|\nabla_1(k_t\dot{\overline{k}}_t)\|_2 + C\|\nabla_1(\dot{k}_t\overline{k}_t)\|_2\right).$$

We are left with the task of estimating $\|\nabla_1(k_t\dot{\overline{k}}_t)\|_2$ and $\|\nabla_1(\dot{k}_t\overline{k}_t)\|_2$. We start by applying the product rule:

$$\begin{aligned}
&\|\nabla_1(k_t\dot{\overline{k}}_t)\|_2^2 \\
&= \int \mathrm{d}x\mathrm{d}y \left|\nabla_x \int \mathrm{d}z \left(Nw(N(x-z))\dot{\overline{\varphi}}_t^{(N)}(x)\overline{\varphi}_t^{(N)}(z) + Nw(N(x-z))\ \overline{\varphi}_t^{(N)}(x)\dot{\overline{\varphi}}_t^{(N)}(z)\right)\right. \\
&\qquad\qquad \left. \times\, Nw(N(z-y))\varphi_t^{(N)}(z)\varphi_t^{(N)}(y)\right|^2 \\
&\leq 4\int \mathrm{d}x\mathrm{d}y \left|\int \mathrm{d}z N^2\nabla w(N(z-x))\dot{\overline{\varphi}}_t^{(N)}(x)|\varphi_t^{(N)}(z)|^2\varphi_t^{(N)}(y)Nw(N(y-z))\right|^2 \qquad (2.112)\\
&\quad + 4\int \mathrm{d}x\mathrm{d}y \left|\int \mathrm{d}z\, Nw(N(z-x))\nabla\dot{\overline{\varphi}}_t^{(N)}(x)|\varphi_t^{(N)}(z)|^2\varphi_t^{(N)}(y)Nw(N(y-z))\right|^2 \qquad (2.113)\\
&\quad + 4\int \mathrm{d}x\mathrm{d}y \left|\int \mathrm{d}z\, N^2\nabla w(N(z-x))\overline{\varphi}_t^{(N)}(x)\dot{\overline{\varphi}}_t^{(N)}(z)\right. \\
&\qquad\qquad\qquad \left.\times\varphi_t^{(N)}(z)\varphi_t^{(N)}(y)\, Nw(N(y-z))\right|^2 \qquad (2.114)\\
&\quad + 4\int \mathrm{d}x\mathrm{d}y \left|\int \mathrm{d}z\, Nw(N(z-y))\nabla\overline{\varphi}_t^{(N)}(x)\dot{\overline{\varphi}}_t^{(N)}(z)\varphi_t^{(N)}(z)\varphi_t^{(N)}(y)Nw(N(y-z))\right|^2. \qquad (2.115)
\end{aligned}$$

Next, we estimate the four terms on the r. h. s. of the last equation. For the summands (2.113) and (2.115) we use that, from (2.30), $Nw(Nx) \leq C|x|^{-1}$. Applying Hardy's inequality, both terms are bounded by $C\|\nabla\dot{\varphi}_t^{(N)}\|_2^2 \leq C\exp(K|t|)$, using Proposition 2.3.1. Since, again by (2.30), $N^2\nabla w(Nx) \leq C|x|^{-2}$, the contribution (2.112) is bounded by

$$\begin{aligned}
&C\int \mathrm{d}x\mathrm{d}y \left(\int \mathrm{d}z \frac{1}{|x-z|^2|z-y|}|\dot{\varphi}_t^{(N)}(x)||\varphi_t^{(N)}(z)|^2|\varphi_t^{(N)}(y)|\right)^2 \\
&\qquad = C\int \mathrm{d}x\mathrm{d}y\mathrm{d}z_1\mathrm{d}z_2 \frac{|\dot{\varphi}_t^{(N)}(x)|^2|\varphi_t^{(N)}(y)|^2|\varphi_t^{(N)}(z_1)|^2|\varphi_t^{(N)}(z_2)|^2}{|z_1-y||z_2-y||x-z_1|^2|x-z_2|^2} \\
&\qquad = C\int \mathrm{d}x\,|\dot{\varphi}_t^{(N)}(x)|^2 \int \mathrm{d}z_1\mathrm{d}z_2 \frac{|\varphi_t^{(N)}(z_1)|^2|\varphi_t^{(N)}(z_2)|^2}{|x-z_1|^2|x-z_2|^2}\int \mathrm{d}y\,\frac{|\varphi_t^{(N)}(y)|^2}{|z_1-y||z_2-y|} \\
&\qquad \leq C\|\dot{\varphi}_t^{(N)}\|_2^2\|\varphi_t^{(N)}\|_{H^1}^6 \leq Ce^{K|t|}
\end{aligned}$$

by Proposition 2.3.1. Analogously, we can also bound the contribution (2.114). This shows the bound for $\|\nabla_1\dot{p}(k_t)\|_2$. The bounds for $\|\nabla_2\dot{p}(k_t)\|_2, \|\nabla_2\dot{p}(k_t)\|_2, \|\nabla_2\dot{p}(k_t)\|_2$ are proven similarly.

(iii) From (2.32), using $Nw(Nx) \leq C|x|^{-1}$, we find immediately that

$$\sup_x \|\dot{k}_t(.,x)\|_2 \leq C\left(\|\nabla\dot{\varphi}_t^{(N)}\|_2\|\varphi_t^{(N)}\|_\infty + \|\nabla\varphi_t^{(N)}\|_2\|\dot{\varphi}_t^{(N)}\|_\infty\right) \leq Ce^{K|t|}$$

by Proposition 2.3.1. To show the bound for $\dot{p}(k_t)$, we observe that

$$\begin{aligned} \dot{p}(k_t)(x,y) &= \partial_t \sum_{n\geq 0} \frac{1}{(2n)!} \int \mathrm{d}z_1 \mathrm{d}z_2\, k_t(x,z_1)(\overline{k}_t k_t)^{(n-1)}(z_1,z_2)\overline{k}_t(z_2,y) \\ &= \sum_{n\geq 0} \frac{1}{(2n)!} \Big[\int \mathrm{d}z_1 \mathrm{d}z_2\, \dot{k}_t(x,z_1)(\overline{k}_t k_t)^{(n-1)}(z_1,z_2)\overline{k}_t(z_2,y) \\ &\qquad + \int \mathrm{d}z_1 \mathrm{d}z_2\, k_t(x,z_1)(\partial_t(\overline{k}_t k_t)^{(n-1)})(z_1,z_2)\overline{k}_t(z_2,y) \\ &\qquad + \int \mathrm{d}z_1 \mathrm{d}z_2\, k_t(x,z_1)(\overline{k}_t k_t)^{(n-1)}(z_1,z_2)\dot{\overline{k}}_t(z_2,y) \Big]. \end{aligned} \tag{2.116}$$

The first term in the parenthesis can be bounded in absolute value by

$$\begin{aligned} &\Big| \int dz_1 dz_2\, \dot{k}_t(x,z_1)(\overline{k}_t k_t)^{(n-1)}(z_1,z_2)\overline{k}_t(z_2,y) \Big| \\ &\leq C \int \mathrm{d}z_1 \mathrm{d}z_2\, \frac{1}{|x-z_1|} \left(|\dot{\varphi}_t^{(N)}(x)||\varphi_t^{(N)}(z_1)| + |\varphi_t^{(N)}(x)||\dot{\varphi}_t^{(N)}(z_1)| \right) \\ &\qquad\qquad \times |(\overline{k}_t k_t)^{(n-1)}(z_1,z_2)|\, \frac{1}{|y-z_2|} |\varphi_t^{(N)}(z_2)||\varphi_t^{(N)}(y)| \\ &\leq C|\varphi_t^{(N)}(x)||\varphi_t^{(N)}(y)| \int \mathrm{d}z_1 \mathrm{d}z_2\, \frac{1}{|x-z_1||y-z_2|} |\dot{\varphi}_t^{(N)}(z_1)||\varphi_t^{(N)}(z_2)|\, |(\overline{k}_t k_t)^{(n-1)}(z_1,z_2)| \\ &\quad + C|\dot{\varphi}_t^{(N)}(x)||\varphi_t^{(N)}(y)| \int \mathrm{d}z_1 \mathrm{d}z_2\, \frac{1}{|x-z_1||y-z_2|} |\varphi_t^{(N)}(z_1)||\varphi_t^{(N)}(z_2)|\, |(\overline{k}_t k_t)^{(n-1)}(z_1,z_2)| \\ &\leq C\|(\overline{k}_t k_t)^{n-1}\|_2 \left(|\varphi_t^{(N)}(x)||\varphi_t^{(N)}(y)|\|\nabla \dot{\varphi}_t^{(N)}\|\|\nabla \varphi_t^{(N)}\| + |\dot{\varphi}_t^{(N)}(x)||\varphi_t^{(N)}(y)|\|\nabla \varphi_t^{(N)}\|^2 \right). \\ &\leq C\|k_t\|_2^{2(n-1)} (|\dot{\varphi}_t^{(N)}(x)| + |\varphi_t^{(N)}(x)|)|\varphi_t^{(N)}(y)|. \end{aligned}$$

The last term in the parenthesis on the r. h. s. of (2.116) can be bounded analogously. The middle term, on the other hand is bounded in absolute value by

$$\begin{aligned} &\Big| \int \mathrm{d}z_1 \mathrm{d}z_2\, k_t(x,z_1)(\partial_t(\overline{k}_t k_t)^{(n-1)})(z_1,z_2)\overline{k}_t(z_2,y) \Big| \\ &\qquad \leq C|\varphi_t^{(N)}(x)||\varphi_t^{(N)}(y)| \int \mathrm{d}z_1 \mathrm{d}z_2\, \frac{|\varphi_t^{(N)}(z_1)||\varphi_t^{(N)}(z_2)|}{|x-z_1||y-z_2|} |\partial_t(\overline{k}_t k_t)^{n-1}(z_1,z_2)| \\ &\qquad \leq C\|\partial_t(\overline{k}_t k_t)^{n-1}\|_2\, \|\nabla \varphi_t^{(N)}\|_2^2\, |\varphi_t^{(N)}(x)||\varphi_t^{(N)}(y)| \\ &\qquad \leq C\|\dot{k}_t\|_2\, \|k_t\|_2^{2n-3} |\varphi_t^{(N)}(x)||\varphi_t^{(N)}(y)|. \end{aligned}$$

Inserting the last bounds in (2.116), we find

$$|\dot{p}(k_t)(x,y)| \leq C e^{K|t|} e^{\|k_t\|_2} \, (|\varphi_t^{(N)}(x)| + |\dot{\varphi}_t^{(N)}(x)|)(|\varphi_t^{(N)}(y)| + |\dot{\varphi}_t^{(N)}(y)|).$$

Integrating over x and taking the supremum over y gives, as before using (2.27),

$$\sup_y \|\dot{p}(k_t)(.,y)\|_2 \leq C e^{K|t|}.$$

The bound for $\dot{r}(k_t)$ can be proven analogously. Combining the bound for $\dot{r}(k_t)$ with the one for $\dot{k}_t$, we also obtain the bound for $\dot{\mathrm{sh}}(k_t)$. □

2.C. Convergence for N-particle wave functions

In this section, we show how the result of Theorem 2.1.1, stated there for initial data of the form $W(\sqrt{N}\varphi)T(k_0)\psi$ can be extended to a certain class of data with number of particles fixed to N.

Theorem 2.C.1. *Let $\varphi \in H^4(\mathbb{R}^3)$ and suppose $\psi \in \mathcal{F}$ with $\|\psi\|_{\mathcal{F}} = 1$ is such that*

$$\left\langle \psi, \left(\frac{\mathcal{N}^2}{N} + \mathcal{N} + \mathcal{H}_N \right) \psi \right\rangle \leq C \tag{2.117}$$

for a constant $C > 0$. Let P_N denote the projection onto the N-particle sector of the Fock space and assume that

$$\|P_N W(\sqrt{N}\varphi)T(k_0)\psi\| \geq CN^{-1/4} \tag{2.118}$$

for all $N \in \mathbb{N}$ large enough. We consider the time evolution

$$\psi_{N,t} = e^{-i\mathcal{H}_N t} \frac{P_N W(\sqrt{N}\varphi)T(k_0)\psi}{\|P_N W(\sqrt{N}\varphi)T(k_0)\psi\|}$$

and we denote by $\gamma^{(1)}_{N,t}$ the one-particle reduced density associated with the N-particle vector $\psi_{N,t}$. Then there exist constants $C, c_1, c_2 > 0$ with

$$\operatorname{tr} \left| \gamma^{(1)}_{N,t} - |\varphi_t\rangle\langle\varphi_t| \right| \leq \frac{C \exp\left(c_1 \exp(c_2|t|)\right)}{N^{1/4}}$$

for all $t \in \mathbb{R}$ and all N large enough. Here φ_t denotes the solution of the time-dependent Gross-Pitaevskii equation (2.16), with initial data $\varphi_{t=0} = \varphi$.

Remarks.

(i) If we relax (2.118) to the weaker condition $\|P_N W(\sqrt{N}\varphi)T(k_0)\psi\| \geq CN^{-\alpha}$, for some $1/4 \leq \alpha < 1/2$, the proof below still implies the convergence $\gamma^{(1)}_{N,t} \to |\varphi_t\rangle\langle\varphi_t|$ but only with the slower rate $N^{-1/2+\alpha}$.

(ii) The assumption (2.118) and its weaker versions mentioned in the previous remark are very reasonable; let us explain why. The expected number of particles in the Fock space vector $W(\sqrt{N}\varphi)T(k_0)\psi$ is given by

$$\begin{aligned} &\left\langle W(\sqrt{N}\varphi)T(k_0)\psi, \mathcal{N}\, W(\sqrt{N}\varphi)T(k_0)\psi \right\rangle \\ &\qquad = N + \sqrt{N}\langle T(k_0)\psi, \phi(\varphi)T(k_0)\psi\rangle + \langle T(k_0)\psi, \mathcal{N}T(k_0)\psi\rangle \end{aligned} \tag{2.119}$$

with the notation $\phi(\varphi) = a(\varphi) + a^*(\varphi)$. Let us introduce the shorthand notation

$$\langle\mathcal{N}\rangle := \left\langle W(\sqrt{N}\varphi)T(k_0)\psi, \mathcal{N}\, W(\sqrt{N}\varphi)T(k_0)\psi \right\rangle.$$

From Lemma 1.4.2, Lemma 2.4.3 and the assumption (2.117) we then conclude that there exists a constant $C > 0$ with

$$N - CN^{1/2} \leq \langle\mathcal{N}\rangle \leq N + CN^{1/2}. \tag{2.120}$$

The expectation of $\mathcal{N}^2$, on the other hand, is given by

$$\begin{aligned}
&\langle W(\sqrt{N}\varphi)T(k_0)\psi, \mathcal{N}^2\, W(\sqrt{N}\varphi)T(k_0)\psi\rangle \\
&\qquad = \langle T(k_0)\psi, (\mathcal{N} + \sqrt{N}\phi(\varphi) + N)^2 T(k_0)\psi\rangle \\
&\qquad = N^2 + 2N^{3/2}\langle T(k_0)\psi, \phi(\varphi)T(k_0)\psi\rangle + 2N\langle T(k_0)\psi, \mathcal{N}T(k_0)\psi\rangle \\
&\qquad\quad + N\langle T(k_0)\psi, \phi(\varphi)^2 T(k_0)\psi\rangle + \sqrt{N}\langle T(k_0)\psi, (\mathcal{N}\phi(\varphi) + \phi(\varphi)\mathcal{N})\, T(k_0)\psi\rangle \\
&\qquad\quad + \langle T(k_0)\psi, \mathcal{N}^2 T(k_0)\psi\rangle.
\end{aligned}$$

Subtracting the square of (2.119), and applying again Lemma 1.4.2, Lemma 2.4.3 and the assumption (2.117), we estimate the variance of the number of particles in the vector $W(\sqrt{N}\varphi)T(k_0)\psi$ by

$$\left\langle W(\sqrt{N}\varphi)T(k_0)\psi, (\mathcal{N} - \langle\mathcal{N}\rangle)^2 W(\sqrt{N}\varphi)T(k_0)\psi \right\rangle \leq CN$$

for an appropriate constant $C > 0$. We conclude that

$$\left\langle W(\sqrt{N}\varphi)T(k_0)\psi, \mathbf{1}\left(|\mathcal{N} - \langle\mathcal{N}\rangle| \geq K\sqrt{N}\right) W(\sqrt{N}\varphi)T(k_0)\psi \right\rangle \leq CK^{-2}.$$

(Here $\mathbf{1}\big(|\mathcal{N} - \langle\mathcal{N}\rangle| \geq K\sqrt{N}\big)$ denotes the spectral projection defined by applying the functional calculus of the number operator $\mathcal{N}$ to the characteristic function of the set $\big\{x \in \mathbb{N} : |x - \langle\mathcal{N}\rangle| \geq K\sqrt{N}\big\}$.)

Choosing $K > 0$ sufficiently large, we find

$$\left\langle W(\sqrt{N}\varphi)T(k_0)\psi, \mathbf{1}\left(|\mathcal{N} - \langle\mathcal{N}\rangle| \leq K\sqrt{N}\right) W(\sqrt{N}\varphi)T(k_0)\psi \right\rangle \geq 1/2.$$

From (2.120), adjusting the value of K, we obtain

$$\left\langle W(\sqrt{N}\varphi)T(k_0)\psi, \mathbf{1}\left(|\mathcal{N} - N| \leq K\sqrt{N}\right) W(\sqrt{N}\varphi)T(k_0)\psi \right\rangle \geq 1/2.$$

This means that

$$\sum_{j=N-K\sqrt{N}}^{N+K\sqrt{N}} \left\| P_j\, W(\sqrt{N}\varphi)T(k_0)\psi \right\|^2 \geq 1/2.$$

The average value of $\|P_j W(\sqrt{N}\varphi)T(k_0)\psi\|^2$ for j between $N - K\sqrt{N}$ and $N + K\sqrt{N}$ is therefore larger or equal to $N^{-1/2}$, in accordance with the assumption (2.118). In fact, this argument shows that for every N there exists an $M \in [N - K\sqrt{N}, N + K\sqrt{N}]$ with $\|P_M\, W(\sqrt{N}\varphi)T(k_0)\psi\| \geq N^{-1/4}$. Letting

$$\psi_{N,M,t} = e^{-i\mathcal{H}_N t} \frac{P_M\, W(\sqrt{N}\varphi)T(k_0)\psi}{\|P_M\, W(\sqrt{N}\varphi)T(k_0)\psi\|}$$

and denoting by $\gamma^{(1)}_{N,M,t}$ the one-particle reduced density associated with $\psi_{N,M,t}$, one can show, similarly to Theorem 2.C.1, that

$$\operatorname{tr}\left|\gamma^{(1)}_{N,M,t} - |\varphi_t\rangle\langle\varphi_t|\right| \leq \frac{C\, \exp\left(c_1 \exp(c_2|t|)\right)}{N^{1/4}}$$

The fact that the number of particles M does not exactly match the parameter N entering the Hamiltonian and the Weyl operator $W(\sqrt{N}\varphi)$ does not affect the analysis in any substantial way, since $|M - N| \leq CN^{1/2} \ll N$.

Proof of Theorem 2.C.1. We write the integral kernel of $\gamma^{(1)}_{N,t}$ as

$$\begin{aligned}
&\gamma^{(1)}_{N,t}(x,y) \\
&= \frac{1}{N\|P_N W(\sqrt{N}\varphi)T(k_0)\psi\|^2} \\
&\qquad \times \left\langle e^{-i\mathcal{H}_N t} P_N W(\sqrt{N}\varphi)T(k_0)\psi,\ a^*_y a_x e^{-i\mathcal{H}_N t} P_N W(\sqrt{N}\varphi)T(k_0)\psi \right\rangle \\
&= \frac{1}{N\|P_N W(\sqrt{N}\varphi)T(k_0)\psi\|^2} \\
&\qquad \times \left\langle e^{-i\mathcal{H}_N t} P_N W(\sqrt{N}\varphi)T(k_0)\psi,\ W(\sqrt{N}\varphi^{(N)}_t)\left(a^*_y + \sqrt{N}\overline{\varphi}^{(N)}_t(y)\right)\right. \\
&\qquad\qquad \left. \times \left(a_x + \sqrt{N}\varphi^{(N)}_t(x)\right) W^*(\sqrt{N}\varphi^{(N)}_t) e^{-i\mathcal{H}_N t} W(\sqrt{N}\varphi)T(k_0)\psi \right\rangle .
\end{aligned}$$

Hence, we find

$$\begin{aligned}
&\gamma^{(1)}_{N,t}(x,y) - \overline{\varphi}^{(N)}_t(y)\varphi^{(N)}_t(x) \\
&= \frac{\varphi^{(N)}_t(x)}{\sqrt{N}\|P_N W(\sqrt{N}\varphi)T(k_0)\psi\|^2} \\
&\quad \times \left\langle e^{-i\mathcal{H}_N t} P_N W(\sqrt{N}\varphi)T(k_0)\psi,\ W(\sqrt{N}\varphi^{(N)}_t) a^*_y W^*(\sqrt{N}\varphi^{(N)}_t) e^{-i\mathcal{H}_N t} W(\sqrt{N}\varphi)T(k_0)\psi \right\rangle \\
&\quad + \frac{\overline{\varphi}^{(N)}_t(y)}{\sqrt{N}\|P_N W(\sqrt{N}\varphi)T(k_0)\psi\|^2} \\
&\quad \times \left\langle e^{-i\mathcal{H}_N t} P_N W(\sqrt{N}\varphi)T(k_0)\psi,\ W(\sqrt{N}\varphi^{(N)}_t) a_x W^*(\sqrt{N}\varphi^{(N)}_t) e^{-i\mathcal{H}_N t} W(\sqrt{N}\varphi)T(k_0)\psi \right\rangle \\
&\quad + \frac{1}{N\|P_N W(\sqrt{N}\varphi)T(k_0)\psi\|^2} \left\langle e^{-i\mathcal{H}_N t} P_N W(\sqrt{N}\varphi)T(k_0)\psi,\ W(\sqrt{N}\varphi^{(N)}_t)\right. \\
&\qquad\qquad \left. \times a^*_y a_x W^*(\sqrt{N}\varphi^{(N)}_t) e^{-i\mathcal{H}_N t} W(\sqrt{N}\varphi)T(k_0)\psi \right\rangle .
\end{aligned}$$

Therefore, for any compact operator J on $L^2(\mathbb{R}^3)$ we find

$$\begin{aligned}
&\text{tr } J\left(\gamma^{(1)}_{N,t} - |\varphi^{(N)}_t\rangle\langle\varphi^{(N)}_t|\right) \\
&= \frac{1}{\sqrt{N}\|P_N W(\sqrt{N}\varphi)T(k_0)\psi\|^2} \left\langle e^{-i\mathcal{H}_N t} P_N W(\sqrt{N}\varphi)T(k_0)\psi,\ W(\sqrt{N}\varphi^{(N)}_t)\right. \\
&\qquad\qquad \left. \times \left(a(J\varphi^{(N)}_t) + a^*(J\varphi^{(N)}_t)\right) W^*(\sqrt{N}\varphi^{(N)}_t) e^{-i\mathcal{H}_N t} W(\sqrt{N}\varphi)T(k_0)\psi \right\rangle \\
&\quad + \frac{1}{N\|P_N W(\sqrt{N}\varphi)T(k_0)\psi\|^2} \left\langle e^{-i\mathcal{H}_N t} P_N W(\sqrt{N}\varphi)T(k_0)\psi,\ W(\sqrt{N}\varphi^{(N)}_t)\right. \\
&\qquad\qquad \left. \times d\Gamma(J)\, W^*(\sqrt{N}\varphi^{(N)}_t) e^{-i\mathcal{H}_N t} W(\sqrt{N}\varphi)T(k_0)\psi \right\rangle .
\end{aligned}$$

Since $\|d\Gamma(J)\psi\| \leq \|J\|\,\|\mathcal{N}\psi\|$, we find, applying Lemma 1.4.2,

$$\begin{aligned}
&\left| \text{tr } J\left(\gamma^{(1)}_{N,t} - |\varphi^{(N)}_t\rangle\langle\varphi^{(N)}_t|\right) \right| \\
&\quad \leq \frac{\|J\|}{\sqrt{N}\|P_N W(\sqrt{N}\varphi)T(k_0)\psi\|} \|(\mathcal{N}+1)^{1/2}\, W^*(\sqrt{N}\varphi^{(N)}_t) e^{-i\mathcal{H}_N t} W(\sqrt{N}\varphi)T(k_0)\psi\| \\
&\qquad + \frac{\|J\|}{N\|P_N W(\sqrt{N}\varphi)T(k_0)\psi\|} \|\mathcal{N}\, W^*(\sqrt{N}\varphi^{(N)}_t) e^{-i\mathcal{H}_N t} W(\sqrt{N}\varphi)T(k_0)\psi\|
\end{aligned}$$

where $\|J\|$ denotes the operator norm of J. From Lemma 2.4.3, recalling the definition (2.33) of the fluctuation dynamics, we find

$$\begin{aligned}
&\left| \text{tr } J \left(\gamma^{(1)}_{N,t} - |\varphi_t^{(N)}\rangle\langle\varphi_t^{(N)}| \right) \right| \\
&\quad \leq \frac{\|J\|}{\sqrt{N}\|P_N W(\sqrt{N}\varphi)T(k_0)\psi\|} \|\mathcal{N}^{1/2}\, T^*(k_t)\, W^*(\sqrt{N}\varphi_t^{(N)}) e^{-i\mathcal{H}_N t} W(\sqrt{N}\varphi)T(k_0)\psi\| \\
&\qquad + \frac{1}{N\|P_N W(\sqrt{N}\varphi)T(k_0)\psi\|} \|\mathcal{N}\, T^*(k_t)\, W^*(\sqrt{N}\varphi_t^{(N)}) e^{-i\mathcal{H}_N t} W(\sqrt{N}\varphi)T(k_0)\psi\| \\
&\quad \leq \frac{\|(\mathcal{N}+1)^{1/2}\,\mathcal{U}(t,0)\psi\|}{\sqrt{N}\|P_N W(\sqrt{N}\varphi)T(k_0)\psi\|} + \frac{\|\mathcal{N}\,\mathcal{U}(t,0)\psi\|}{N\|P_N W(\sqrt{N}\varphi)T(k_0)\psi\|}.
\end{aligned}$$

Using Proposition 2.4.2, we conclude that

$$\begin{aligned}
\left| \text{tr } J \left(\gamma^{(1)}_{N,t} - |\varphi_t^{(N)}\rangle\langle\varphi_t^{(N)}| \right) \right| \leq\; & \frac{C\|J\|\, \|(\mathcal{N}+1)^{1/2}\,\mathcal{U}(t,0)\psi\|}{\sqrt{N}\|P_N W(\sqrt{N}\varphi)T(k_0)\psi\|} + \frac{C\|(\mathcal{N}+1)^{1/2}\,\psi\|}{\sqrt{N}\|P_N W(\sqrt{N}\varphi)T(k_0)\psi\|} \\
& + \frac{C\|(\mathcal{N}+1)\psi\|}{N\|P_N W(\sqrt{N}\varphi)T(k_0)\psi\|}.
\end{aligned}$$

From the assumptions (2.117) and (2.118), we obtain

$$\left| \text{tr } J \left(\gamma^{(1)}_{N,t} - |\varphi_t^{(N)}\rangle\langle\varphi_t^{(N)}| \right) \right| \leq \frac{C\|J\|}{N^{1/4}} \|(\mathcal{N}+1)^{1/2}\,\mathcal{U}(t,0)\psi\| + \frac{C}{N^{1/4}}.$$

Finally, Theorem 2.4.1 implies that

$$\left| \text{tr } J \left(\gamma^{(1)}_{N,t} - |\varphi_t^{(N)}\rangle\langle\varphi_t^{(N)}| \right) \right| \leq \frac{C\|J\| \exp\left(c_1 \exp(c_2|t|)\right)}{N^{1/4}}. \tag{2.121}$$

Since the Banach space $\mathcal{L}^1(L^2(\mathbb{R}^3))$ is the dual space to the space of compact operators, equipped with the operator norm, (2.121) (followed by Proposition 2.3.1(iv)) implies the claim. □

3. Mean-Field Evolution of Fermionic Systems

In this chapter, we prove that the evolution of a fermionic many-body system in the mean-field regime can be approximated with the Hartree-Fock equation. This chapter is based on the article [BPS13a].

We use the fermionic convention $\operatorname{tr} \gamma_N^{(k)} = \frac{N!}{(N-k)!}$ for the normalization of density matrices, see Section 1.A.

3.1. Introduction

As explained in Section 1.2.3, the fermionic mean-field regime is naturally linked to the semiclassical regime. Recall the Schrödinger equation (1.18) on the semiclassical time scale (for readability, from now on we use t for the semiclassical time that was called τ in Chapter 1; the physical time does not appear anymore)

$$i\varepsilon\partial_t\psi_{N,t} = \left[-\sum_{j=1}^{N} \varepsilon^2\Delta_j + \frac{1}{N}\sum_{i<j}^{N} V(x_i - x_j) \right] \psi_{N,t} \,. \tag{3.1}$$

The mean-field scaling, characterized by the $1/N$ coupling constant in front of the potential energy, is combined with the semiclassical regime characterized by $\varepsilon = N^{-1/3} \ll 1$.

Similarly to the bosonic case, typical initial data can be prepared by confining the N fermions to a volume of order one and cooling them to very low temperatures. In other words, interesting initial data for (3.1) are ground states of Hamilton operators of the form

$$H_N^{\text{trap}} = \sum_{j=1}^{N} \left(-\varepsilon^2\Delta_{x_j} + V_{\text{ext}}(x_j) \right) + \frac{1}{N}\sum_{i<j}^{N} V(x_i - x_j) \tag{3.2}$$

where V_{ext} is an external trapping potential, confining the N particles to a volume of order one. Such initial data are well approximated by Slater determinants

$$\psi_{\text{slater}}(x_1, \dots, x_N) = \frac{1}{\sqrt{N!}} \sum_{\pi\in S_N} \operatorname{sgn}(\pi) f_1(x_{\pi(1)}) f_2(x_{\pi(2)}) \dots f_N(x_{\pi(N)})$$

with a family of N orthonormal orbitals $(f_j)_{j=1}^N$ in $L^2(\mathbb{R}^3)$ ($\operatorname{sgn}(\pi)$ denotes the sign of the permutation $\pi \in S_N$). Slater determinants are quasifree states, so they are completely characterized by their one-particle reduced density matrix, given by the orthogonal projection

$$\omega = \sum_{j=1}^{N} |f_j\rangle\langle f_j| \,.$$

In fact, a simple computation shows that $\langle \psi_{\text{slater}}, H_N^{\text{trap}} \psi_{\text{slater}} \rangle$ is given by the Hartree-Fock energy[1]

$$\begin{aligned}\mathcal{E}_{\text{HF}}(\omega) = \text{tr}\,\left(-\varepsilon^2\Delta + V_{\text{ext}}\right)\omega + \frac{1}{2N}\int \mathrm{d}x\mathrm{d}y V(x-y)\omega(x,x)\omega(y,y) \\ - \frac{1}{2N}\int \mathrm{d}x\mathrm{d}y V(x-y)|\omega(x,y)|^2.\end{aligned} \tag{3.3}$$

We expect that the evolution determined by the Schrödinger equation (3.1) of an initial Slater determinant approximating the ground state of H_N^{trap} remains close to a Slater determinant with an evolved reduced one-particle density, given by the solution of the time-dependent Hartree-Fock equation

$$i\varepsilon\partial_t\omega_t = \left[-\varepsilon^2\Delta + (V * \rho_t) - X_t, \omega_t\right] \tag{3.4}$$

canonically associated with the energy functional (3.3). Here $\rho_t(x) = N^{-1}\omega_t(x,x)$ is the normalized density associated with the one-particle density ω_t, while X_t is the exchange operator, having the kernel

$$X_t(x,y) = N^{-1}V(x-y)\omega_t(x,y)\,.$$

Of course, we cannot expect this last statement to be correct for any initial state close to a Slater determinant. We expect minimizers of the Hartree-Fock energy functional (3.3) to be characterized by a semiclassical structure which is essential to understand the evolution. In fact, as we will argue next, we expect the kernel $\omega(x,y)$ of the reduced density minimizing (or approximately minimizing) the functional (3.3) to be concentrated close to the diagonal and to decay at distances $|x-y| \gg \varepsilon$. To understand the emergence of this semiclassical structure, and to find good characterizations, let us consider a system of N free fermions in a box of volume one, for example with periodic boundary conditions. The ground state of the system is given by the Slater determinant constructed with the N plane waves $f_p(x) = e^{ipx}$ with $p \in (2\pi)\mathbb{Z}^3$ and $|p| \leq cN^{1/3}$, for a suitable constant c (guaranteeing that the total number of orbitals equals exactly N). The corresponding one-particle reduced density has the kernel

$$\omega(x,y) = \sum_{|p|\leq cN^{1/3}} e^{ip\cdot(x-y)}$$

where the sum extends over all $p \in (2\pi)\mathbb{Z}^3$ with $|p| \leq cN^{1/3}$. Letting $q = \varepsilon p$ (with $\varepsilon = N^{-1/3}$), we can write

$$\omega(x,y) = \sum_{|q|\leq c} e^{iq(x-y)/\varepsilon} \simeq \frac{1}{\varepsilon^3}\int_{|q|\leq c} \mathrm{d}q\, e^{iq\cdot(x-y)/\varepsilon} = \frac{1}{\varepsilon^3}\varphi\left(\frac{x-y}{\varepsilon}\right) \tag{3.5}$$

with

$$\varphi(\xi) = \frac{4\pi}{|\xi|^2}\left(\frac{\sin(c|\xi|)}{|\xi|} - c\cos(c|\xi|)\right), \quad \xi \in \mathbb{R}^3. \tag{3.6}$$

Hence, at fixed N and ε, $\omega(x,y)$ decays to zero for $|x-y| \gg \varepsilon$. Moreover, the fact that ω depends only on the difference $x-y$ (for x,y in the box) implies that the density $\omega(x,x)$ is constant inside the box (and zero outside). This is of course a consequence of the fact that we consider a system with external potential vanishing inside, and being infinite outside the

[1] In this formula in [BPS13a], the factors 1/2 are missing; the typo is corrected here.

box. More generically, if particles are trapped by a regular potential V_{ext} with $V_{\text{ext}}(x) \to \infty$ for $|x| \to \infty$, we expect the resulting reduced one-particle density to have approximately the form

$$\omega(x,y) \simeq \frac{1}{\varepsilon^3}\varphi\left(\frac{x-y}{\varepsilon}\right)\chi\left(\frac{x+y}{2}\right) \tag{3.7}$$

for appropriate functions φ and χ, or to be a linear combination of such kernels. While χ determines the density of the particles in space (because $\varphi(0) = 1$, to ensure that $\operatorname{tr}\omega = N$), φ fixes the momentum distribution.

Next we look for suitable bounds, characterizing Slater determinants like (3.7) which have the correct semiclassical structure. To this end, we observe that, if we differentiate the r. h. s. of (3.7) with respect to x or y, a factor ε^{-1} will emerge from the derivative of φ (this produces a kinetic energy of order $N^{5/3}$, as expected). However, if we take the commutator $[\nabla, \omega]$, its kernel will be given by

$$[\nabla,\omega](x,y) = (\nabla_x + \nabla_y)\,\omega(x,y) = \frac{1}{\varepsilon^3}\varphi\left(\frac{x-y}{\varepsilon}\right)\nabla\chi\left(\frac{x+y}{2}\right). \tag{3.8}$$

In this case the derivative only hits the density profile χ; it does not affect φ, and therefore it remains of order one (of course, in the example with plane waves in a box, there is the additional problem that χ is the characteristic function of the box, and therefore that it is not differentiable; this is however a consequence of the pathological choice of the external potential). We express the fact that the derivative in (3.8) does not produce additional ε^{-1} factors through the bound

$$\operatorname{tr}|[\nabla,\omega]| \leq CN. \tag{3.9}$$

Similarly, the fact that $\omega(x,y)$ decays to zero as $|x-y| \gg \varepsilon$, suggests that the commutator $[x,\omega]$, whose kernel is given by

$$[x,\omega](x,y) = (x-y)\omega(x,y), \tag{3.10}$$

is smaller than ω by order ε. In fact, one has to be a bit careful here. Going back to the plane wave example, we observe that the function φ computed in (3.6) does not decay particularly fast at infinity. For this reason, it is not immediately clear that one can extract an ε factor from the difference $(x-y)$ on the r. h. s. of (3.10). Keeping in mind the plane wave example, let us compute the commutator of the reduced density ω with the multiplication operator $e^{ir\cdot x}$, for a fixed $r \in (2\pi)\mathbb{Z}^3$. We find

$$\left[e^{ir\cdot x},\omega\right] = \sum_{|p|\leq cN^{1/3}}\left[|e^{i(r+p)\cdot x}\rangle\langle e^{ip\cdot x}| - |e^{ip\cdot x}\rangle\langle e^{i(p-r)\cdot x}|\right].$$

A straightforward computation shows that

$$\left|\left[e^{ir\cdot x},\omega\right]\right|^2 = \sum_{p\in I_r}|e^{ip\cdot x}\rangle\langle e^{ip\cdot x}| \tag{3.11}$$

where

$$I_r = (2\pi)\mathbb{Z}^3 \cap \left\{p\in\mathbb{R}^3 : |p-r| \leq cN^{1/3}, |p| \geq cN^{1/3} \text{ or } |p-r| \geq cN^{1/3}, |p| \leq cN^{1/3}\right\}.$$

It follows that $|[e^{ir\cdot x},\omega]| = |[e^{ir\cdot x},\omega]|^2$ is a projection, and therefore that

$$\operatorname{tr}\left|\left[e^{ir\cdot x},\omega\right]\right| \leq CN\varepsilon|r|. \tag{3.12}$$

Hence, the trace norm of the commutator is smaller, by a factor ε, compared with the norm of the operators $e^{ip\cdot x}\omega$ and $\omega e^{ip\cdot x}$. The fact that the kernel $\omega(x,y)$ is supported close to the diagonal allows us to extract an additional ε factor from the trace norm of the commutator $[e^{ip\cdot x},\omega]$. Notice, however, that if we considered the Hilbert-Schmidt norm of $[e^{ip\cdot x},\omega]$, we would find from (3.11) that

$$\|\left[e^{ir\cdot x},\omega\right]\|_{HS} = \left(\operatorname{tr}\left|\left[e^{ir\cdot x},\omega\right]\right|^2\right)^{1/2} \leq (CN\varepsilon|r|)^{1/2}.$$

In other words, the Hilbert-Schmidt norm of the commutator $[e^{ip\cdot x},\omega]$ is only smaller than the Hilbert-Schmidt norm of the two operators $e^{ip\cdot x}\omega$ and $\omega e^{ip\cdot x}$ by a factor $\varepsilon^{1/2}$. This is consistent with the fact that, in (3.7), the function φ does not decay fast at infinity (which follows from the fact that ω is a projection corresponding to a characteristic function in momentum space).

So far, we verified the bounds (3.9) and (3.12) for the ground state of a system of confined non-interacting electrons. It is natural to ask whether these bounds also hold in systems with mean-field interaction. Can we still expect the minimizer of the Hamiltonian (3.2) to satisfy (3.9) and (3.12)? We claim that the answer to this question is affirmative, and we propose a heuristic explanation[2]. Semiclassical analysis suggests that the reduced density of the minimizer of (3.2) can be approximated by the Weyl quantization $\omega = \mathrm{Op}^w_M$ of the phase space density $M(p,x) = \chi(|p| \leq (6\pi^2\rho(x))^{1/3})$, where ρ is the minimizer of the Thomas-Fermi type functional

$$\varepsilon_{\mathrm{TF}}(\rho) = \frac{3}{5}(3\pi^2)^{2/3}\int \mathrm{d}x\rho^{5/3}(x) + \int \mathrm{d}x\, V_{\mathrm{ext}}(x)\rho(x) + \frac{1}{2}\int \mathrm{d}x\mathrm{d}y V(x-y)\rho(x)\rho(y)$$

over all non-negative densities $\rho \in L^1(\mathbb{R}^3)\cap L^{5/3}(\mathbb{R}^3)$ normalized so that $\|\rho\|_1 = 1$. Here, the Weyl quantization Op^w_M of M is defined by the kernel

$$\omega(x,y) = \mathrm{Op}^w_M(x,y) = \frac{1}{(2\pi\varepsilon)^3}\int \mathrm{d}p\, M\left(p, \frac{x+y}{2}\right) e^{ip\cdot\frac{x-y}{\varepsilon}}$$

It turns out that the commutators of ω with the position operator x and with the momentum operator ∇ are again Weyl quantizations. In fact, a straightforward computation shows that

$$[x,\omega] = -i\varepsilon\mathrm{Op}^w_{\nabla_p M}, \quad [\nabla,\omega] = \mathrm{Op}^w_{\nabla_q M}.$$

Hence, semiclassical analysis predicts that

$$\operatorname{tr}\,|[x,\omega]| \simeq \frac{\varepsilon}{(2\pi\varepsilon)^3}\int \mathrm{d}p\mathrm{d}q|\nabla_p M(p,q)| = CN\varepsilon\int \rho^{2/3}(q)\mathrm{d}q$$

and that

$$\operatorname{tr}\,|[\nabla,\omega]| \simeq \frac{1}{(2\pi\varepsilon)^3}\int \mathrm{d}p\mathrm{d}q|\nabla_q M(p,q)| = N\int |\nabla\rho(q)|\,\mathrm{d}q$$

[2]We would like to thank Rupert Frank for pointing out this argument to us.

Under general assumptions on V_{ext} and V, we can expect the integrals on the r. h. s. of the last two equations to be finite, and therefore, we can expect the bounds (3.9) and (3.12) to hold true ((3.12) easily follows from the estimate $\operatorname{tr}|[x,\omega]| \leq CN\varepsilon$). Although one could probably turn the heuristic argument that we just presented into a rigorous proof, we do not pursue this question in the present work. Instead, we will just assume our initial data to satisfy (3.9) and (3.12). We consider these bounds as an expression of the semiclassical structure that emerges naturally when one considers states with energy close to the ground state of a trapped Hamiltonian of the form (3.2).

For initial data ψ_N close to Slater determinants and having the correct semiclassical structure characterized by (3.9) and (3.12), we consider the time evolution $\psi_{N,t} = e^{-itH_N/\varepsilon}\psi_N$, generated by the Hamiltonian

$$H_N = -\sum_{j=1}^{N} \varepsilon^2 \Delta_j + \frac{1}{N}\sum_{i<j}^{N} V(x_i - x_j) \tag{3.13}$$

and we denote by $\gamma^{(1)}_{N,t}$ the one-particle reduced density associated with $\psi_{N,t}$. Our main result, Theorem 3.3.1, shows that, under suitable assumptions on the potential V, there exist constants $K, c_1, c_2 > 0$ such that

$$\|\gamma^{(1)}_{N,t} - \omega_{N,t}\|_{\text{HS}} \leq K \exp(c_1 \exp(c_2|t|)) \tag{3.14}$$

and

$$\operatorname{tr}\left|\gamma^{(1)}_{N,t} - \omega_{N,t}\right| \leq KN^{1/6} \exp(c_1 \exp(c_2|t|)) \tag{3.15}$$

where $\omega_{N,t}$ denotes the solution of the time-dependent Hartree-Fock equation (3.4) with the initial data $\omega_{N,t=0} = \gamma^{(1)}_{N,0}$. The bounds (3.14) and (3.15) show that the difference $\gamma^{(1)}_{N,t} - \omega_{N,t}$ is much smaller (both in the Hilbert-Schmidt norm and in the trace class norm) than $\gamma^{(1)}_{N,t}$ and $\omega_{N,t}$ (recall that $\|\omega^{(1)}_{N,t}\|_{\text{HS}}, \|\gamma^{(1)}_{N,t}\|_{\text{HS}} \simeq N^{1/2}$ while $\operatorname{tr}\omega_{N,t}, \operatorname{tr}\gamma^{(1)}_{N,t} \simeq N$).

It turns out that the exchange term is small compared to the other terms in the Hartree-Fock equation (3.4); in fact, for the class of regular potential that we consider in this paper, it is of the relative size $1/N$. As a consequence, the bounds (3.14), (3.15) and also all other bounds that we prove in Theorem 3.3.1 for the difference between $\gamma^{(1)}_{N,t}$ and the solution of the Hartree-Fock equation remain true if we replace the solution of the Hartree-Fock equation $\omega_{N,t}$ by the solution $\widetilde{\omega}_{N,t}$ of the Hartree equation

$$i\varepsilon\partial_t \widetilde{\omega}_{N,t} = \left[-\varepsilon^2\Delta + (V * \widetilde{\rho}_t), \widetilde{\omega}_{N,t}\right] \tag{3.16}$$

with the same initial data $\widetilde{\omega}_{N,t=0} = \gamma^{(1)}_{N,0}$ (here $\widetilde{\rho}_t(x) = N^{-1}\widetilde{\omega}(x,x)$ is the normalized density associated to $\widetilde{\omega}_{N,t}$). For more details, see the last remark after Theorem 3.3.1, and Proposition 3.A.1 in Appendix 3.A.

Observe that both the Hartree-Fock equation (3.4) and the Hartree equation (3.16) still depend on N, through the initial data and through the semiclassical parameter $\varepsilon = N^{-1/3}$. In the semiclassical limit $\varepsilon \to 0$, the Hartree (and the Hartree-Fock) dynamics can be approximated by the solution of the Vlasov equation, as we will explain now. We define the Wigner transform $W_{N,t}$ associated with the solution $\omega_{N,t}$ of the Hartree-Fock equation by

$$W_{N,t}(x,p) = \frac{1}{(2\pi)^3}\int \mathrm{d}y\, \omega_{N,t}\left(x + \varepsilon\frac{y}{2}; x - \varepsilon\frac{y}{2}\right) e^{-ipy}.$$

In the limit $\varepsilon \to 0$, the Wigner transform $W_{N,t}$ of the solution of the Hartree-Fock equation (3.4) (or the Wigner transform of the solution $\widetilde{\omega}_{N,t}$ of the Hartree equation) converges [GIMS98] towards the solution of the Vlasov equation

$$\partial_t W_t^{\rm vl}(x,p) + p \cdot \nabla_x W_t^{\rm vl}(x,p) = \nabla_x \left(V * \rho_t^{\rm vl} \right)(x) \cdot \nabla_p W_t^{\rm vl}(x,p) \,. \tag{3.17}$$

where $\rho_t^{\rm vl}(x) = \int {\rm d}p\, W^{\rm vl}(x,p)$. The difference between the Wigner transform $W_{N,t}$ of $\omega_{N,t}$ and the solution of the Vlasov equation $W_t^{\rm vl}$ is of the order $\varepsilon N = N^{2/3}$, and therefore much larger than the difference between the reduced one-particle density $\gamma_{N,t}^{(1)}$ associated with the solution of the many-body Schrödinger equation and the solution $\omega_{N,t}$ of the Hartree-Fock equation (or the solution $\widetilde{\omega}_{N,t}$ of the Hartree equation). In other words, the Hartree-Fock approximation (or the Hartree approximation) keeps the quantum structure of the problem and gives a much more precise approximation of the many-body evolution compared to the classical Vlasov dynamics. Our result is therefore a dynamical counterpart to [B92, GS94], where the Hartree-Fock theory is shown to give a much better approximation to the ground state energy of a system of atoms or molecules as compared to the Thomas-Fermi energy (although in contrast to [B92, GS94] our analysis does not apply so far to Coulomb interaction).

3.2. Embedding the system in Fock space

We start by embedding the system in Fock space. To define the Hamilton operator $\mathcal{H}_N$ on Fock space $\mathcal{F}$, we set $(\mathcal{H}_N\psi)^{(n)} = \mathcal{H}_N^{(n)}\psi^{(n)}$, with

$$\mathcal{H}_N^{(n)} = \sum_{j=1}^{n} -\varepsilon^2 \Delta_{x_j} + \frac{1}{N}\sum_{i<j}^{n} V(x_i - x_j),$$

where, as discussed before, $\varepsilon = N^{-1/3}$. The Hamiltonian $\mathcal{H}_N$ leaves the n-particle sectors of Fock space invariant. On the N-particle sector, it agrees with (3.13). Notice that in the notation $\mathcal{H}_N$, the index N does not refer to the number of particles, since $\mathcal{H}_N$ acts on the whole Fock space. It reminds instead of the coupling constant $1/N$ in front of the potential energy, and of the semiclassical parameter $\varepsilon = N^{-1/3}$. Of course, in order to recover the mean-field regime, we will consider the time evolution of states in $\mathcal{F}$ having approximately N particles. Observe that, in terms of the operator-valued distributions a_x and a_x^*, we can express the Hamiltonian $\mathcal{H}_N$ as

$$\mathcal{H}_N = \varepsilon^2 \int {\rm d}x\, \nabla_x a_x^* \nabla_x a_x + \frac{1}{2N}\int {\rm d}x{\rm d}y\, V(x-y) a_x^* a_y^* a_y a_x. \tag{3.18}$$

Notice that the kinetic energy $\varepsilon^2 \int {\rm d}x \nabla_x a_x^* \nabla_x a_x$ can also be written as the second quantization $d\Gamma(-\varepsilon^2\Delta)$.

Since it is more convenient in this and the next chapter to use the normalization $\operatorname{tr}\gamma_\psi^{(1)} = N$ for $\psi \in L^2(\mathbb{R}^{3N})$ with $\|\psi\| = 1$, we now give some definitions for fermionic systems again and repeat part of the discussion. Notice also that we simplify the notation by writing γ_ψ for the one-particle reduced density matrix $\gamma_\psi^{(1)}$.

Given a Fock space vector $\psi \in \mathcal{F}$, we define the one-particle reduced density γ_ψ associated with ψ as the non-negative operator with the integral kernel

$$\gamma_\psi(x, y) = \langle \psi, a_y^* a_x \psi \rangle.$$

Notice that γ_ψ is normalized such that $\operatorname{tr} \gamma_\psi = \langle \psi, \mathcal{N} \psi \rangle$. Hence γ_ψ is a trace class operator if the expectation of $\mathcal{N}$ in the vector ψ is finite. A very useful property of one-particle density matrices is that in the sense of operators $0 \leq \gamma_\psi \leq 1$, and especially $\|\gamma_\psi\| \leq 1$ in operator norm on $L^2(\mathbb{R}^3)$. This only holds for fermionic, not for bosonic, one-particle density matrices and allows us to get bounds without loosing factors of N, even if $\operatorname{tr} \gamma_\psi = N$.

In general, if ψ does not have a fixed number of particles, it is also important to track the expectations $\langle \psi, a_y a_x \psi \rangle$ and $\langle \psi, a_x^* a_y^* \psi \rangle$. We define therefore the pairing density α_ψ associated with ψ as the one-particle operator with integral kernel

$$\alpha_\psi(x, y) = \langle \psi, a_y a_x \psi \rangle.$$

Then we also have $\overline{\alpha_\psi}(x, y) = \langle \psi, a_x^* a_y^* \psi \rangle$. The operators γ_ψ and α_ψ can be combined into the generalized one-particle density $\Gamma_\psi : L^2(\mathbb{R}^3) \oplus L^2(\mathbb{R}^3) \to L^2(\mathbb{R}^3) \oplus L^2(\mathbb{R}^3)$ defined in terms of the generalized creation/annihilation operators (1.50) by

$$\langle (f_1, g_1), \Gamma_\psi (f_2, g_2) \rangle = \langle \psi, A^*(f_2, g_2) A(f_1, g_1) \psi \rangle .$$

A simple computation shows that

$$\Gamma_\psi = \begin{pmatrix} \gamma_\psi & \alpha_\psi \\ -\overline{\alpha}_\psi & 1 - \overline{\gamma}_\psi \end{pmatrix}. \tag{3.19}$$

It is simple to check that $0 \leq \Gamma_\psi \leq 1$.

Knowledge of the generalized one-particle density Γ_ψ allows the computation of the expectation of all observables which are quadratic in creation and annihilation operators. To compute expectations of operators involving more than two creation and annihilation operators, one needs higher order correlation functions, having the form

$$\left\langle \psi, a_{x_1}^\sharp \ldots a_{x_k}^\sharp \psi \right\rangle \tag{3.20}$$

where each $a^\sharp$ is either an annihilation or a creation operator. Recall that a quasifree pure state is a vector in $\mathcal{F}$ of the form $\psi = R_\nu \Omega$, where R_ν is the unitary implementor of an implementable Bogoliubov transformation ν. As discussed in Section 1.5 quasifree states are completely described by the one-particle reduced density matrix γ_ψ and the pairing density α_ψ, or in other words by their generalized one-particle reduced density Γ_ψ. If ν is a Bogoliubov transformation of the form (1.60), it is simple to check that the generalized one-particle density associated with $\psi = R_\nu \Omega$ has the form

$$\Gamma_\psi = \begin{pmatrix} v^* v & v^* \overline{u} \\ \overline{u}^* v & \overline{u}^* \overline{u} \end{pmatrix},$$

and we also denote it by $\Gamma_\nu = \Gamma_\psi$. Hence, the reduced density of the quasifree state associated with the Bogoliubov transformation ν is $\gamma_\nu = v^* v$, while the pairing density is $\alpha_\nu = v^* \overline{u}$. As ν is by assumption implementable, v is a Hilbert-Schmidt operator and we conclude that γ_ν is trace class. In particular the expectation value of the number of particles is always finite for quasifree states. Moreover, it follows that $\Gamma_\nu^2 = \Gamma_\nu$, i. e. Γ_ν is a projection. Conversely, for every linear projection $\Gamma : L^2(\mathbb{R}^3) \oplus L^2(\mathbb{R}^3) \to L^2(\mathbb{R}^3) \oplus L^2(\mathbb{R}^3)$ having the form

$$\Gamma = \begin{pmatrix} \gamma & \alpha \\ -\overline{\alpha} & 1 - \overline{\gamma} \end{pmatrix}$$

for a trace class operator γ, there exists a quasifree state, i. e. an implementable Bogoliubov transformation ν, such that $\Gamma = \Gamma_\nu$, i. e. Γ is the generalized one-particle density associated with the Fock space vector $R_\nu \Omega$. Restricting the Hamiltonian (3.18) to quasifree states of the form $R_\nu \Omega$ one obtains the Bardeen-Cooper-Schrieffer (BCS) energy functional. BCS theory plays a very important role in physics. Originally introduced to describe superconductors, it has been later applied to explain the phenomenon of superfluidity observed in dilute gases of fermionic atoms at low temperature. In the last years, there has been a lot of progress in the mathematical understanding of BCS theory; see, for example, [HS08, HHSS08, FHSS11, HS11] for results concerning equilibrium properties and [HLLS10, HS12] for results about the time-evolution in BCS theory.

In this thesis we are interested in quasifree pure states without pairing, i. e. with $\alpha = 0$. Since Γ must be a projection, the assumption $\alpha = 0$ implies that γ is a projection. We require the number of particles to be N, i. e. $\operatorname{tr} \gamma = N$. Then we know that there exists a Bogoliubov transformation ν such that γ is the reduced density of $R_\nu \Omega$. In fact, it is easy to construct such a Bogoliubov transformation. Since we assumed γ to be an orthogonal projection with $\operatorname{tr} \gamma = N$, there must be an orthonormal system $(f_j)_{j=1}^N$ such that $\gamma = \sum_{j=1}^N |f_j\rangle\langle f_j|$. We define $v := \sum_{j=1}^N |\bar{f}_j\rangle\langle f_j|$. Then we have $v^* = \overline{v} = \sum_{j=1}^N |f_j\rangle\langle \bar{f}_j|$ and $v^* v = \sum_{j=1}^N |f_j\rangle\langle f_j| = \gamma$. We also set $u = u^* := 1 - \sum_{j=1}^N |f_j\rangle\langle f_j| = 1 - \gamma$. Then u is a projection and $u^* u = u^2 = u = 1 - \gamma$. Hence $u^* u + v^* v = 1$, and $v^* \overline{u} = 0$. It follows that

$$\nu = \begin{pmatrix} u & \overline{v} \\ v & \overline{u} \end{pmatrix} = \begin{pmatrix} 1 - \gamma & \sum_{j=1}^N |f_j\rangle\langle \bar{f}_j| \\ \sum_{j=1}^N |\bar{f}_j\rangle\langle f_j| & 1 - \bar{\gamma} \end{pmatrix} \tag{3.21}$$

is an implementable Bogoliubov transformation, with

$$\Gamma_\nu = \begin{pmatrix} \gamma & 0 \\ 0 & 1 - \bar{\gamma} \end{pmatrix}. \tag{3.22}$$

Both the quasifree pure state $R_\nu \Omega$ and the N-particle Slater determinant $\psi_{\text{slater}}(\mathbf{x}) = (N!)^{-1/2} \det \left(f_j(x_i)\right)_{i,j \leq N}$ satisfy the Wick theorem and are therefore fully characterized by their generalized one-particle density (up to a phase, which is equivalent to a unitary transformation in the space spanned by $(f_i)_{i=1}^N$). Since (3.22) coincides with the generalized one-particle density of ψ_{slater}, it follows that $R_\nu \Omega = (0, \dots, 0, \psi_{\text{slater}}, 0, \dots)$ (again, up to a phase). Hence, Slater determinants are the only quasifree pure states with vanishing pairing density.

Although we will not make use of this fact, let us notice that unitary implementors of Bogoliubov transformations of the form (3.21), generating Slater determinants, can be also conveniently constructed as particle-hole transformations. This construction has been demonstrated in Section 1.5.

3.3. Main results

The next theorem is our main result. In it, we study the time evolution of initial data close to Slater determinants, and prove that their dynamics can be described in terms of the

Hartree-Fock (or the Hartree) equation. Of course, we cannot start with an arbitrary Slater determinant. Instead, we need the initial data to have the semiclassical structure discussed in the introduction. We encode this requirement in the assumption (3.24) below. We do not expect the result to be correct if the initial data is not semiclassical, i. e. if (3.24) is not satisfied. Notice however that, as discussed before, we expect the semiclassical structure to naturally emerge when one tries to minimize the energy. Hence, the assumption (3.24) is appropriate to study the dynamics of initially trapped fermionic systems close to the ground state of the trapped Hamiltonian (traps are then released (or changed) to observe the dynamics of the particles, which would otherwise be trivial).

Theorem 3.3.1. *Assume that, in the Hamiltonian (3.18), $V \in L^1(\mathbb{R}^3)$ and*

$$\int dp\,(1+|p|)^2|\widehat{V}(p)| < \infty\,. \tag{3.23}$$

Let ω_N be a sequence of orthogonal projections on $L^2(\mathbb{R}^3)$, with $\operatorname{tr}\omega_N = N$ and such that

$$\begin{aligned} \operatorname{tr}\,|[e^{ip\cdot x},\omega_N]| &\leq CN\varepsilon\,(1+|p|) \quad \text{and} \\ \operatorname{tr}\,|[\varepsilon\nabla,\omega_N]| &\leq CN\varepsilon \end{aligned} \tag{3.24}$$

for all $p \in \mathbb{R}^3$ and for a constant $C > 0$. Let ν_N denote the sequence of Bogoliubov transformations constructed in (3.21) such that $R_{\nu_N}\Omega$ has the generalized one-particle density

$$\Gamma_{\nu_N} = \begin{pmatrix} \omega_N & 0 \\ 0 & 1-\overline{\omega}_N \end{pmatrix}.$$

Let $\xi_N \in \mathcal{F}$ be a sequence with $\langle \xi_N, \mathcal{N}\xi_N\rangle \leq C$ uniformly in N. Let $\gamma^{(1)}_{N,t}$ be the reduced one-particle density associated with the evolved vector

$$\psi_{N,t} = e^{-i\mathcal{H}_N t/\varepsilon} R_{\nu_N}\xi_N \tag{3.25}$$

where the Hamiltonian $\mathcal{H}_N$ has been defined in (3.18). On the other hand, denote by $\omega_{N,t}$ the solution of the Hartree-Fock equation

$$i\varepsilon\partial_t\omega_{N,t} = \left[-\varepsilon^2\Delta + (V*\rho_t) - X_t, \omega_{N,t}\right], \tag{3.26}$$

with the initial data $\omega_{N,t=0} = \omega_N$. Here $\rho_t(x) = N^{-1}\omega_{N,t}(x,x)$ is the normalized density and X_t is the exchange operator associated with $\omega_{N,t}$, having the kernel $X_t(x,y) = N^{-1}V(x-y)\omega_{N,t}(x,y)$. Then there exist constants $K, c_1, c_2 > 0$ such that

$$\left\|\gamma^{(1)}_{N,t} - \omega_{N,t}\right\|_{HS} \leq K\exp(c_2\exp(c_1|t|)) \tag{3.27}$$

and

$$\operatorname{tr}\left|\gamma^{(1)}_{N,t} - \omega_{N,t}\right| \leq KN^{1/2}\exp(c_2\exp(c_1|t|)) \tag{3.28}$$

for all $t \in \mathbb{R}$.

Assume additionally that $d\Gamma(\omega_N)\xi_N = 0$ and $\langle \xi_N, \mathcal{N}^2\xi_N\rangle \leq C$ for all $N \in \mathbb{N}$. Then there exist constants $K, c_1, c_2 > 0$ such that

$$\operatorname{tr}\left|\gamma^{(1)}_{N,t} - \omega_{N,t}\right| \leq KN^{1/6}\exp(c_2\exp(c_1|t|)) \tag{3.29}$$

for all $t \in \mathbb{R}$. Moreover, under this additional assumption, we obtain that

$$\left| \text{tr } e^{ix\cdot q + \varepsilon p \cdot \nabla} \left(\gamma^{(1)}_{N,t} - \omega_{N,t} \right) \right| \leq K (1 + |q| + |p|)^{1/2} \exp(c_2 \exp(c_1 |t|)) \tag{3.30}$$

for every $q, p \in \mathbb{R}^3$, $t \in \mathbb{R}$.

Remarks.

- Using (3.42) below, it is simple to check that $R^*_{\nu_N} \mathcal{N} R_{\nu_N} = \mathcal{N} - 2d\Gamma(\omega_N) + N$. The assumption $\langle \xi_N, \mathcal{N} \xi_N \rangle \leq C$ implies therefore that
$$\left| \text{tr } \gamma^{(1)}_{N,0} - \text{tr } \omega_N \right| = \left| \langle \xi_N, R^*_{\nu_N} \mathcal{N} R_{\nu_N} \xi_N \rangle - N \right| \leq C$$
uniformly in N (this bound is of course preserved by the time-evolution). Following the arguments of Section 3.5 it is also easy to check that
$$\|\gamma^{(1)}_{N,0} - \omega_N\|_{\text{HS}} \leq C, \quad \text{and } \text{tr } |\gamma^{(1)}_{N,0} - \omega_N| \leq C N^{1/2},$$
if $\langle \xi_N, \mathcal{N} \xi_N \rangle \leq C$. Under the additional assumption $d\Gamma(\omega_N)\xi_N = 0$, one can even show that
$$\text{tr } \left| \gamma^{(1)}_{N,0} - \omega_N \right| \leq C,$$
uniformly in N (applying the arguments at the beginning of Step 3 in Section 3.5). This proves that, at time $t = 0$, the bulk of the particles is in the quasifree state generated by R_{ν_N}. The small fluctuations around the quasifree state are described by ξ_N. In particular, it follows that the bounds (3.27), (3.28), (3.29) and (3.30) hold at time $t = 0$. Results similar to (3.27), (3.28), (3.29), (3.30) also hold if $\langle \xi_N, \mathcal{N} \xi_N \rangle \simeq N^\alpha$ and $\langle \xi_N, \mathcal{N}^2 \xi_N \rangle \simeq N^\beta$, for some $\alpha, \beta > 0$, but then, of course, the errors become larger.

- Suppose that the initial data is $\omega_N = \sum_{j=1}^N |f_j\rangle\langle f_j|$ for a family $(f_j)_{j=1}^N$ of orthonormal functions in $L^2(\mathbb{R}^3)$. Then the condition $d\Gamma(\omega_N)\xi_N = 0$, required for (3.29) and (3.30), is satisfied if $a(f_i)\xi_N = 0$ for all $i = 1, \ldots, N$, meaning that particles in ξ_N are orthogonal to all orbitals f_j building the quasifree part of the state.

- All our results and our analysis remain valid if we included an external potential in the Hamiltonian (3.18) generating the time-evolution. This is the case if the external potential is not switched off but changed. The external potential would then, of course, also appear in the Hartree-Fock equation (3.26). (Its contribution would cancel completely already in Proposition 3.4.3 and only trivial changes are necessary in Proposition 3.4.4.)

- Eq. (3.27) is optimal in its N dependence (it is easy to find a sequence $\xi_N \in \mathcal{F}$ with $\langle \xi_N, \mathcal{N} \xi_N \rangle < \infty$ such that, already at time $t = 0$, the difference between $\gamma^{(1)}_{N,0}$ and $\omega_{N,0}$ is of order one). On the other hand, we do not expect (3.28) and (3.29) to be optimal (the optimal bound for the trace norm of the difference should be, like (3.27), of order one in N). Since the Hilbert-Schmidt norm of $\gamma^{(1)}_{N,t}$ and of $\omega_{N,t}$ is of the order $N^{1/2}$ (while their trace-norm is of order N), it is not surprising that in (3.27) we get a better rate than in (3.28) and in (3.29). We point out, however, that we can improve (3.29) and get optimal estimates, if we test the difference $\gamma^{(1)}_{N,t} - \omega_{N,t}$ against observables having the correct semiclassical structure, even if these observables are not Hilbert-Schmidt; see (3.30).

- The bounds (3.27), (3.28), (3.29), (3.30) deteriorate quite fast in time. The emergence of a double exponential is a consequence of the fact that when we propagate (3.24) along the solution $\omega_{N,t}$ of the Hartree-Fock equation (3.26) we get an additional factor which is growing exponentially in time. It is reasonable to expect that in many situations, the exponential growth for the commutators $[e^{ip\cdot x}, \omega_{N,t}]$ and $[\varepsilon\nabla, \omega_{N,t}]$ is too pessimistic. In these situation, it would be possible to get better time-dependence on the r. h. s. of (3.27), (3.28), (3.29) and (3.30).

- Let $\widetilde{\omega}_{N,t}$ denote the solution of the Hartree equation

$$i\varepsilon\partial_t\widetilde{\omega}_{N,t} = \left[-\varepsilon^2\Delta + (V * \widetilde{\rho}_t), \widetilde{\omega}_{N,t}\right] \tag{3.31}$$

  with the initial data ω_N. Under the assumptions of Theorem 3.3.1 on the initial density ω_N and on the interaction potential V, we show in Appendix 3.A that the contribution of the exchange term $[X_t, \omega_{N,t}]$ in the Hartree-Fock equation (3.26) is of smaller order, and that

$$\operatorname{tr}|\omega_{N,t} - \widetilde{\omega}_{N,t}| \leq C\exp(c_1\exp(c_2|t|)).$$

  It follows from this remark that the bounds (3.27), (3.28), (3.29) and (3.30) remain true if we replace the solution $\omega_{N,t}$ of the Hartree-Fock equation with the solution $\widetilde{\omega}_{N,t}$ of the Hartree equation (with the same initial data).

We can also control the convergence of higher order reduced densities. Recall that the k-particle reduced density associated with the evolved Fock space vector $\psi_{N,t}$ defined in (3.25) is defined as the non-negative trace class operator $\gamma^{(k)}_{N,t}$ on $L^2(\mathbb{R}^{3k})$ with integral kernel given by

$$\gamma^{(k)}_{N,t}(x_1,\dots x_k, x'_1,\dots x'_k) = \left\langle \psi_{N,t}, a^*_{x'_1}\dots a^*_{x'_k} a_{x_k}\dots a_{x_1}\psi_{N,t}\right\rangle.$$

The k-particle reduced density associated with the evolved quasifree state with one-particle density $\omega_{N,t}$ (obtained through the solution of the Hartree-Fock equation (3.26)) is given, according to Wick's theorem, by

$$\omega^{(k)}_{N,t}(x_1,\dots x_k, x'_1,\dots x'_k) = \sum_{\pi\in S_k}\operatorname{sgn}(\pi)\prod_{j=1}^{k}\omega_t(x_j, x'_{\pi(j)}). \tag{3.32}$$

Recall also that the normalization is $\operatorname{tr}\,\omega^{(k)}_{N,t} = N!/(N-k)!$.

Theorem 3.3.2. *We use the same notations and assume the same conditions as in Theorem 3.3.1 (the condition $d\Gamma(\omega_N)\xi_N = 0$ is not required here). Let $k \in \mathbb{N}$ and assume, additionally, that the sequence ξ_N is such that $\langle\xi_N, (\mathcal{N}+1)^k\xi_N\rangle \leq C$. Then there exist constants $D, c_1, c_2 > 0$ (with c_1 depending only on V and on the constant on the r. h. s. of (3.24)), and D, c_2 depending on V and on the constants on the r. h. s. of (3.24) and on k) such that*

$$\left\|\gamma^{(k)}_{N,t} - \omega^{(k)}_{N,t}\right\|_{HS} \leq DN^{(k-1)/2}\exp(c_2\exp(c_1|t|)) \tag{3.33}$$

and

$$\operatorname{tr}\left|\gamma^{(k)}_{N,t} - \omega^{(k)}_{N,t}\right| \leq DN^{k-\frac{1}{2}}\exp(c_2\exp(c_1|t|)). \tag{3.34}$$

Remark. The N-dependence of the bound (3.33) is optimal. On the other hand, the N-dependence of (3.34) is not expected to be optimal, the optimal bound for the trace norm of the difference $\gamma^{(k)}_{N,t} - \omega^{(k)}_{N,t}$ should be of the order N^{k-1}.

In order to show Theorem 3.3.1 and Theorem 3.3.2 we are going to compare the fully evolved Fock space vector $\psi_{N,t} = e^{-i\mathcal{H}_N t/\varepsilon} R_{\nu_N} \xi_N$ with the quasifree state on $\mathcal{F}$ with reduced one-particle density given by the solution $\omega_{N,t}$ of the Hartree-Fock equation (3.26). To this end, we write $\omega_{N,t} = \sum_{j=1}^N |f_{j,t}\rangle\langle f_{j,t}|$ for an orthonormal family $(f_{j,t})_{j=1}^N$ in $L^2(\mathbb{R}^3)$. Recall that alternatively, the functions $f_{j,t}$ can be determined by solving the system of N coupled non-linear equations

$$\begin{aligned} i\varepsilon\partial_t f_{j,t}(x) = -\varepsilon^2 \Delta f_{j,t}(x) &+ \frac{1}{N}\sum_{i=1}^N \int \mathrm{d}y V(x-y)|f_{i,t}(y)|^2 f_{j,t}(x) \\ &- \frac{1}{N}\sum_{i=1}^N \int \mathrm{d}y V(x-y) f_{j,t}(y)\overline{f}_{i,t}(y) f_{i,t}(x) \end{aligned}$$

with the initial data $f_{j,t=0} = f_j$ appearing in (3.21). Using this equivalent form of the Hartree-Fock equation, we can avoid any ambiguity between $\omega_{N,t}$ and the decomposition into orbitals. We define then $u_{N,t} = 1 - \omega_{N,t}$ and $v_{N,t} = \sum_{j=1}^N |\overline{f}_{j,t}\rangle\langle f_{j,t}|$. Similarly to (3.21), we define the Bogoliubov transformation

$$\nu_{N,t} = \begin{pmatrix} u_{N,t} & \overline{v}_{N,t} \\ v_{N,t} & \overline{u}_{N,t} \end{pmatrix} = \begin{pmatrix} 1-\omega_{N,t} & \sum_{j=1}^N |f_{j,t}\rangle\langle \overline{f}_{j,t}| \\ \sum_{j=1}^N |\overline{f}_{j,t}\rangle\langle f_{j,t}| & 1-\overline{\omega}_{N,t} \end{pmatrix}. \tag{3.35}$$

The generalized reduced density matrix associated with the quasifree state $R_{\nu_{N,t}}\Omega$ is given by

$$\Gamma_{\nu_{N,t}} = \begin{pmatrix} \omega_{N,t} & 0 \\ 0 & 1-\overline{\omega}_{N,t} \end{pmatrix}.$$

We expect $\psi_{N,t}$ to be close to the quasifree state $R_{\nu_{N,t}}\Omega$. To prove that this is indeed the case, we define $\xi_{N,t} \in \mathcal{F}$ so that

$$\psi_{N,t} = e^{-i\mathcal{H}_N t/\varepsilon} R_{\nu_N} \xi_N = R_{\nu_{N,t}} \xi_{N,t}$$

for every $t \in \mathbb{R}$. Equivalently, $\xi_{N,t} = \mathcal{U}_N(t,0)\xi_N$, where we defined the two-parameter group of unitary transformations

$$\mathcal{U}_N(t,s) = R^*_{\nu_{N,t}} e^{-i\mathcal{H}_N(t-s)/\varepsilon} R_{\nu_{N,s}} \tag{3.36}$$

for any $t, s \in \mathbb{R}$. We refer to $\mathcal{U}_N$ as the fluctuation dynamics; it describes the evolution of particles which are outside the quasifree state.

As we will show in detail in Section 3.5, the problem of proving the convergence of $\gamma^{(1)}_{N,t}$ towards the solution of the Hartree-Fock equation ω_t can be reduced to the problem of controlling the expectation of the number of particles operator (and of its powers) in the vector $\xi_{N,t}$, or, equivalently, of controlling the growth of the number of particles operator with respect to the fluctuation dynamics $\mathcal{U}_N$.

3.4. Bounds on growth of fluctuations

In this section we prove bounds for the growth of the expectation of the number of particles operator and of its powers with respect to the fluctuation dynamics $\mathcal{U}_N(t,s)$. To obtain such estimates, we will make use of the following lemma, where we collect a series of important bounds for operators on the fermionic Fock space.

Lemma 3.4.1. *For every bounded operator O on $L^2(\mathbb{R}^3)$, we have*

$$\|d\Gamma(O)\psi\| \leq \|O\| \, \|\mathcal{N}\psi\|$$

for every $\psi \in \mathcal{F}$. If O is a Hilbert-Schmidt operator, we also have the bounds

$$\begin{aligned} \|d\Gamma(O)\psi\| &\leq \|O\|_{HS} \, \|\mathcal{N}^{1/2}\psi\|, \\ \left\| \int dx\, dx'\, O(x,x') a_x a_{x'} \psi \right\| &\leq \|O\|_{HS} \, \|\mathcal{N}^{1/2}\psi\|, \\ \left\| \int dx\, dx'\, O(x,x') a_x^* a_{x'}^* \psi \right\| &\leq 2\|O\|_{HS} \, \|(\mathcal{N}+1)^{1/2}\psi\|. \end{aligned} \tag{3.37}$$

for every $\psi \in \mathcal{F}$. Finally, if O is a trace class operator, we obtain

$$\begin{aligned} \|d\Gamma(O)\| &\leq 2\,\mathrm{tr}\,|O|\,, \\ \left\| \int dx\, dx'\, O(x,x') a_x a_{x'} \right\| &\leq 2\,\mathrm{tr}\,|O|\,, \\ \left\| \int dx\, dx'\, O(x,x') a_x^* a_{x'}^* \right\| &\leq 2\,\mathrm{tr}\,|O|\,. \end{aligned} \tag{3.38}$$

Proof. For any bounded operator O on $L^2(\mathbb{R}^3)$ we have

$$\|d\Gamma(O)\psi\|^2 = \sum_{n=1}^{\infty} \sum_{i,j=1}^{n} \langle \psi^{(n)}, O^{(i)} O^{(j)} \psi^{(n)} \rangle \leq \|O\|^2 \sum_{n=1}^{\infty} n^2 \|\psi^{(n)}\|^2 = \|O\|^2 \|\mathcal{N}\psi\|^2 \,.$$

For a Hilbert-Schmidt operator O on $L^2(\mathbb{R}^3)$, we have, using (1.34),

$$\begin{aligned} \left\| \int \mathrm{d}x \mathrm{d}x'\, O(x',x)\, a^\sharp_{x'} a_x \psi \right\| &\leq \int \mathrm{d}x\, \|a^\sharp(O(.,x)) a_x \psi\| \\ &\leq \int \mathrm{d}x\, \|O(.,x)\|_2 \, \|a_x\psi\| \\ &\leq \|O\|_{\mathrm{HS}} \left(\int \mathrm{d}x\, \|a_x\psi\|^2 \right)^{1/2} \leq \|O\|_{\mathrm{HS}} \|\mathcal{N}^{1/2}\psi\| \end{aligned} \tag{3.39}$$

where $a^\sharp$ is either an annihilation operator a or a creation operator a^*. This proves the first two bounds in (3.37). The third bound in (3.37) can be reduced to the previous bound as follows:

$$\begin{aligned} \left\| \int \mathrm{d}x \mathrm{d}y\, O(x,y) a_x^* a_y^* \psi \right\| &= \sup_{\varphi \in \mathcal{F},\ \|\varphi\|=1} \left| \left\langle \varphi, \int \mathrm{d}x \mathrm{d}y\, O(x,y) a_x^* a_y^* \psi \right\rangle \right| \\ &= \sup_{\varphi \in \mathcal{F},\ \|\varphi\|=1} \left| \left\langle \int \mathrm{d}x \mathrm{d}y\, \overline{O(x,y)} a_x a_y (\mathcal{N}+1)^{-1/2} \varphi, (\mathcal{N}+3)^{1/2} \psi \right\rangle \right| \\ &\leq \sup_{\varphi \in \mathcal{F},\ \|\varphi\|=1} \|O\|_{\mathrm{HS}} \|\mathcal{N}^{1/2} (\mathcal{N}+1)^{-1/2} \varphi\| \|(\mathcal{N}+3)^{1/2}\psi\| \\ &\leq \|O\|_{\mathrm{HS}} \|(\mathcal{N}+3)^{1/2}\psi\|. \end{aligned}$$

Finally, we prove (3.38). Assume first that O is a selfadjoint trace class operator. Then we have the spectral decomposition

$$O = \sum_j \lambda_j |f_j\rangle\langle f_j|$$

for a real sequence $(\lambda_j)_j$ of eigenvalues with $\sum_j |\lambda_j| = \mathrm{tr}|O|$ and an orthonormal family of eigenvectors $f_j \in L^2(\mathbb{R}^3)$. We find

$$\left\| \int \mathrm{d}x\mathrm{d}x'\, O(x,x')\, a_x^\sharp a_{x'}^\sharp \right\| \leq \sum_j |\lambda_j| \left\| \int \mathrm{d}x\mathrm{d}x'\, f_j(x')\overline{f}_j(x)\, a_x^\sharp a_{x'}^\sharp \right\| = \sum_j |\lambda_j| \left\| a^\sharp(\widetilde{f}_j) a^\sharp(\widetilde{f}_j) \right\|$$

where $\widetilde{f}_j$ is either f_j or its complex conjugate $\overline{f}_j$. We conclude from (1.34) that

$$\left\| \int \mathrm{d}x\mathrm{d}x'\, O(x,x') a_x^\sharp a_{x'}^\sharp \right\| \leq \sum_j |\lambda_j| \|f_j\|^2 = \mathrm{tr}\,|O|\,. \tag{3.40}$$

Now, for an arbitrary, not necessarily selfadjoint, trace class operator O, we write

$$O = \frac{O+O^*}{2} + i\frac{O-O^*}{2i}\,.$$

Therefore, applying (3.40), we find

$$\begin{aligned} &\left\| \int \mathrm{d}x\mathrm{d}x'\, O(x,x')\, a_x^\sharp a_{x'}^\sharp \right\| \\ &\leq \left\| \int \mathrm{d}x\mathrm{d}x' \left(\frac{O+O^*}{2}\right)(x,x')\, a_x^\sharp a_{x'}^\sharp \right\| + \left\| \int \mathrm{d}x\mathrm{d}x' \left(\frac{O-O^*}{2i}\right)(x,x')\, a_x^\sharp a_{x'}^\sharp \right\| \\ &\leq \mathrm{tr} \left| \frac{O+O^*}{2} \right| + \mathrm{tr} \left| \frac{O-O^*}{2i} \right| \leq 2\,\mathrm{tr}\,|O|\,. \qquad \square \end{aligned}$$

We are now ready to state the main result of this section, which is a bound for the growth of the expectation of $(\mathcal{N}+1)^k$ with respect to the fluctuation dynamics.

Theorem 3.4.2. *Assume (3.23) and (3.24). Let* $\mathcal{U}_N(t,s)$ *be the fluctuation dynamics defined in (3.36) and* $k \in \mathbb{N}$. *Then there exist a constant* $c_1 > 0$, *depending only on* V, *and a constant* $c_2 > 0$ *depending on* V *and on* k *such that*

$$\left\langle \xi, \mathcal{U}_N(t,0)^* (\mathcal{N}+1)^k\, \mathcal{U}_N(t,0)\xi \right\rangle \leq \exp(c_2 \exp(c_1|t|))\, \langle \xi, (\mathcal{N}+1)^k \xi \rangle. \tag{3.41}$$

The first step in the proof of Theorem 3.4.2 is an explicit computation of the time derivative of the expectation of the evolved moments of the number of particles operator appearing on the l. h. s. of (3.41). Recall from (3.36) that $\mathcal{U}_N(t,0) = R^*_{\nu_{N,t}} e^{-i\mathcal{H}_N t/\varepsilon} R_{\nu_N}$, where

$$\nu_{N,t} = \begin{pmatrix} u_{N,t} & \overline{v}_{N,t} \\ v_{N,t} & \overline{u}_{N,t} \end{pmatrix}$$

is the Bogoliubov transform defined in (3.35), with $v^*_{N,t} v_{N,t} = \omega_{N,t}$ and $u_{N,t} = 1 - \omega_{N,t}$.

In the rest of this section, we will use the shorthand notation $R_t \equiv R_{\nu_{N,t}}$, $u_t \equiv u_{N,t}$, $v_t \equiv v_{N,t}$ and $\overline{v}_t \equiv \overline{v}_{N,t}$. Moreover, we define the functions $u_{t,x}, v_{t,x}, \overline{v}_{t,x}$ by $u_{t,x}(y) := u_{N,t}(y,x)$,

$v_{t,x}(y) := v_{N,t}(y,x)$ and $\overline{v}_{t,x}(y) := \overline{v}_{N,t}(y,x)$, where $u_{N,t}(y,x)$, $v_{N,t}(y,x)$ and $\overline{v}_{N,t}(y,x)$ denote the integral kernels of the operators $u_{N,t}$, $v_{N,t}$ and $\overline{v}_{N,t}$. Notice that, from (1.63), the action of the Bogoliubov transformation R_t on the operator-valued distributions a_x, a_x^* is given by

$$R_t^* a_x R_t = a(u_{t,x}) + a^*(\overline{v}_{t,x}) \quad \text{and} \quad R_t^* a_x^* R_t = a^*(u_{t,x}) + a(\overline{v}_{t,x}). \tag{3.42}$$

Proposition 3.4.3. *Let $\mathcal{U}_N(t,s)$ be the fluctuation dynamics defined in (3.36), $\xi \in \mathcal{F}$, and $k \in \mathbb{N}$. Then*

$$\begin{aligned}
& i\varepsilon \frac{d}{dt} \left\langle \mathcal{U}_N(t,0)\xi, (\mathcal{N}+1)^k \mathcal{U}_N(t,0)\xi \right\rangle \\
&= -\frac{4i}{N} \operatorname{Im} \sum_{j=1}^{k} \int dxdy\, V(x-y) \\
&\quad \times \Big\{ \left\langle \mathcal{U}_N(t,0)\xi, (\mathcal{N}+1)^{j-1} a^*(u_{t,x}) a(\overline{v}_{t,y}) a(u_{t,y}) a(u_{t,x}) (\mathcal{N}+1)^{k-j} \mathcal{U}_N(t,0)\xi \right\rangle \\
&\quad + \left\langle \mathcal{U}_N(t,0)\xi, (\mathcal{N}+1)^{j-1} a(\overline{v}_{t,x}) a(\overline{v}_{t,y}) a(u_{t,y}) a(u_{t,x}) (\mathcal{N}+1)^{k-j} \mathcal{U}_N(t,0)\xi \right\rangle \\
&\quad + \left\langle \mathcal{U}_N(t,0)\xi, (\mathcal{N}+1)^{j-1} a^*(u_{t,y}) a^*(\overline{v}_{t,y}) a^*(\overline{v}_{t,x}) a(\overline{v}_{t,x}) (\mathcal{N}+1)^{k-j} \mathcal{U}_N(t,0)\xi \right\rangle \Big\}.
\end{aligned} \tag{3.43}$$

Proof. A simple computation using (3.42) shows that

$$R_t \mathcal{N} R_t^* = \mathcal{N} - 2d\Gamma(\omega_{N,t}) + N$$

and therefore that

$$\begin{aligned}
\mathcal{U}_N(t,0)^* \mathcal{N} \mathcal{U}_N(t,0) &= R_0^* e^{i\mathcal{H}_N t/\varepsilon} (\mathcal{N} - 2d\Gamma(\omega_{N,t}) + N) e^{-i\mathcal{H}_N t/\varepsilon} R_0 \\
&= R_0^* \mathcal{N} R_0 - 2R_0^* e^{i\mathcal{H}_N t/\varepsilon} d\Gamma(\omega_{N,t}) e^{-i\mathcal{H}_N t/\varepsilon} R_0 + N.
\end{aligned}$$

Hence

$$\begin{aligned}
i\varepsilon \frac{\mathrm{d}}{\mathrm{d}t} \mathcal{U}_N^*(t,0) \mathcal{N} \mathcal{U}_N(t,0) &= -2\, R_0^* e^{i\mathcal{H}_N t/\varepsilon} \left\{ d\Gamma(i\varepsilon\partial_t \omega_{N,t}) - [\mathcal{H}_N, d\Gamma(\omega_{N,t})] \right\} e^{-i\mathcal{H}_N t/\varepsilon} R_0 \\
&= -2\mathcal{U}_N^*(t,0) R_t^* \left\{ d\Gamma(i\varepsilon\partial_t \omega_{N,t}) - [\mathcal{H}_N, d\Gamma(\omega_{N,t})] \right\} R_t \mathcal{U}_N(t,0).
\end{aligned}$$

On the one hand, from the Hartree-Fock equation (3.26) for $\omega_{N,t}$ we find

$$d\Gamma(i\varepsilon\partial_t \omega_{N,t}) = d\Gamma\left(\left[-\varepsilon^2\Delta, \omega_{N,t}\right]\right) + d\Gamma\left([V * \rho_t - X_t, \omega_{N,t}]\right)$$

where we recall the definitions of the normalized density $\rho_t(x) = (1/N)\omega_{N,t}(x,x)$ and of the exchange operator $X_t(x,y) = (1/N)V(x-y)\omega_{N,t}(x,y)$. On the other hand

$$[\mathcal{H}_N, d\Gamma(\omega_{N,t})] = [d\Gamma(-\varepsilon^2\Delta), d\Gamma(\omega_{N,t})] + [\mathcal{V}_N, d\Gamma(\omega_{N,t})]$$

with the interaction term

$$\mathcal{V}_N = \frac{1}{2N} \int \mathrm{d}x\mathrm{d}y V(x-y) a_x^* a_y^* a_y a_x.$$

We conclude that

$$\begin{aligned}
& i\varepsilon \frac{\mathrm{d}}{\mathrm{d}t} \mathcal{U}_N^*(t,0) \mathcal{N} \mathcal{U}_N(t,0) \\
&\quad = -2\mathcal{U}_N^*(t,0) R_t^* \left\{ d\Gamma\left([V * \rho_t - X_t, \omega_{N,t}]\right) - [\mathcal{V}_N, d\Gamma(\omega_{N,t})] \right\} R_t \mathcal{U}_N(t,0).
\end{aligned} \tag{3.44}$$

Next, we compute the two terms in the brackets. The first term is given by

$$\begin{aligned} &d\Gamma([V * \rho_t - X_t, \omega_{N,t}]) \\ &\quad = \frac{1}{N}\int \mathrm{d}z_1 \mathrm{d}z_2\, a^*_{z_1} a_{z_2} \int \mathrm{d}x\, V(z_1 - x)\big[\omega_{N,t}(z_1,z_2)\omega_{N,t}(x,x) - \omega_{N,t}(z_1,x)\omega_{N,t}(x,z_2)\big] \\ &\qquad - \text{h.c.} \end{aligned} \tag{3.45}$$

Using (3.42), we find

$$\begin{aligned} &R^*_t d\Gamma([V * \rho_t - X_t, \omega_{N,t}])R_t \\ &\quad = \frac{1}{N}\int \mathrm{d}z_1 \mathrm{d}z_2\, \left(a^*(u_{t,z_1}) + a(\overline{v}_{t,z_1})\right)\left(a(u_{t,z_2}) + a^*(\overline{v}_{t,z_2})\right) \\ &\qquad \times \int dx\, V(z_1 - x)\big[\omega_{N,t}(z_1,z_2)\omega_{N,t}(x,x) - \omega_{N,t}(z_1,x)\omega_{N,t}(x,z_2)\big] - \text{h.c.} \end{aligned} \tag{3.46}$$

The integration over z_2 can be done explicitly using the property $\int dz_2\, \overline{u}_t(y_1,z_2)\omega_{N,t}(y_2,z_2) = (\omega_{N,t}u_t)(y_2,y_1) = 0$ and the fact that $\omega_{N,t}\overline{v}_t = \overline{v}_t$. We get

$$\begin{aligned} &R^*_t d\Gamma([V * \rho_t - X_t, \omega_{N,t}])R_t \\ &\quad = \frac{1}{N}\int \mathrm{d}z_1\, \left(a^*(u_{t,z_1}) + a(\overline{v}_{t,z_1})\right) \\ &\qquad \times \int \mathrm{d}x\, V(z_1 - x)\big[a^*(\overline{v}_{t,z_1})\omega_{N,t}(x,x) - a^*(\overline{v}_{t,x})\omega_{N,t}(z_1,x)\big] - \text{h.c.} \\ &\quad = \frac{1}{N}\int \mathrm{d}x\mathrm{d}y\, V(x-y)\Big[\omega_{N,t}(x,x)a^*(u_{t,y})a^*(\overline{v}_{t,y}) - \omega_{N,t}(y,x)a^*(u_{t,y})a^*(\overline{v}_{t,x})\Big] - \text{h.c.} \end{aligned} \tag{3.47}$$

where in the last step the contributions containing $a(\overline{v}_{t,z_1})$ are cancelled by their hermitian conjugates.

We now consider the second contribution in the brackets on the r. h. s. of (3.44). Using the canonical anticommutation relations, we obtain

$$[\mathcal{V}_N, \mathrm{d}\Gamma(\omega_{N,t})] = \frac{1}{N}\int \mathrm{d}x\mathrm{d}y\mathrm{d}z\, V(x-y)\omega_{N,t}(z,y)a^*_z a^*_x a_y a_x - \text{h.c.}$$

Conjugating with the Bogoliubov transformation R_t, we find

$$\begin{aligned} &R^*_t[\mathcal{V}_N, \mathrm{d}\Gamma(\omega_{N,t})]R_t \\ &\quad = \frac{1}{N}\int \mathrm{d}x\mathrm{d}y\mathrm{d}z\, V(x-y)\omega_{N,t}(z,y) \\ &\qquad \times \left(a^*(u_{t,z}) + a(\overline{v}_{t,z})\right)\left(a^*(u_{t,x}) + a(\overline{v}_{t,x})\right)\left(a(u_{t,y}) + a^*(\overline{v}_{t,y})\right)\left(a(u_{t,x}) + a^*(\overline{v}_{t,x})\right) \\ &\quad - \text{h.c.} \end{aligned}$$

Integrating over z, using again $\omega_{N,t}u_t = 0$ and $\omega_{N,t}\overline{v}_t = \overline{v}_t$, we find

$$\begin{aligned} &R^*_t[\mathcal{V}_N, \mathrm{d}\Gamma(\omega_{N,t})]R_t \\ &\quad = \frac{1}{N}\int \mathrm{d}x\mathrm{d}y\, V(x-y)a(\overline{v}_{t,y})\left(a^*(u_{t,x}) + a(\overline{v}_{t,x})\right)\left(a(u_{t,y}) + a^*(\overline{v}_{t,y})\right)\left(a(u_{t,x}) + a^*(\overline{v}_{t,x})\right) \\ &\qquad - \text{h.c.} \end{aligned}$$

Since $\langle \overline{v}_{t,y}, u_{t,x} \rangle = 0$ the operators $a(\overline{v}_{t,y})$ and $a^*(u_{t,x})$ anticommute. Taking into account the fact that many contributions cancel after subtracting the hermitian conjugate, we find

$$\begin{aligned}R_t^*[\mathcal{V}_N, \mathrm{d}\Gamma(\omega_{N,t})]R_t \\ = -\frac{1}{N}\int \mathrm{d}x\mathrm{d}y\, V(x-y)\Big[a^*(u_{t,x})a(\overline{v}_{t,y})a(u_{t,y})a(u_{t,x}) \\ + a(\overline{v}_{t,x})a(\overline{v}_{t,y})a(u_{t,y})a(u_{t,x}) - a(\overline{v}_{t,x})a(\overline{v}_{t,y})a^*(\overline{v}_{t,x})a(u_{t,y})\Big] - \text{h.c.}\end{aligned}$$

Normal ordering the last term in the brackets using $\langle \overline{v}_{t,y}, \overline{v}_{t,x} \rangle = \omega_{N,t}(x,y)$, we conclude that

$$\begin{aligned}R_t^*[\mathcal{V}_N, \mathrm{d}\Gamma(\omega_{N,t})]R_t \\ = -\frac{1}{N}\int \mathrm{d}x\mathrm{d}y\, V(x-y)\Big[a^*(u_{t,x})a(\overline{v}_{t,y})a(u_{t,y})a(u_{t,x}) \\ + a(\overline{v}_{t,x})a(\overline{v}_{t,y})a(u_{t,y})a(u_{t,x}) + a^*(u_{t,y})a^*(\overline{v}_{t,y})a^*(\overline{v}_{t,x})a(\overline{v}_{t,x})\Big] - \text{h.c.} \\ + \frac{1}{N}\int \mathrm{d}x\mathrm{d}y\, V(x-y)\Big[\omega_{N,t}(x,x)a^*(u_{t,y})a^*(\overline{v}_{t,y}) - \omega_{N,t}(y,x)a^*(u_{t,y})a^*(\overline{v}_{t,x})\Big] - \text{h.c.}\end{aligned} \tag{3.48}$$

Combining (3.47) with (3.48), we find

$$\begin{aligned}R_t^*\left\{d\Gamma\left([V*\rho_t - X_t, \omega_{N,t}]\right) - [\mathcal{V}_N, d\Gamma(\omega_{N,t})]\right\}R_t \\ = -\frac{1}{N}\int \mathrm{d}x\mathrm{d}y\, V(x-y)\Big[a^*(u_{t,x})a(\overline{v}_{t,y})a(u_{t,y})a(u_{t,x}) \\ + a(\overline{v}_{t,x})a(\overline{v}_{t,y})a(u_{t,y})a(u_{t,x}) + a^*(u_{t,y})a^*(\overline{v}_{t,y})a^*(\overline{v}_{t,x})a(\overline{v}_{t,x})\Big] - \text{h.c.}\end{aligned}$$

From (3.44), we obtain

$$\begin{aligned}i\varepsilon\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{U}_N^*(t,0)\mathcal{N}\mathcal{U}_N(t,0) \\ = -\frac{4i}{N}\,\mathrm{Im}\int \mathrm{d}x\mathrm{d}y\, V(x-y)\,\mathcal{U}_N^*(t,0)\Big[a^*(u_{t,x})a(\overline{v}_{t,y})a(u_{t,y})a(u_{t,x}) \\ + a(\overline{v}_{t,x})a(\overline{v}_{t,y})a(u_{t,y})a(u_{t,x}) + a^*(u_{t,y})a^*(\overline{v}_{t,y})a^*(\overline{v}_{t,x})a(\overline{v}_{t,x})\Big]\mathcal{U}_N(t,0).\end{aligned}$$

Eq. (3.43) now follows from the observation that

$$\begin{aligned}i\varepsilon\frac{\mathrm{d}}{\mathrm{d}t}\Big\langle \xi, \mathcal{U}_N^*(t,0)(\mathcal{N}+1)^k\mathcal{U}_N(t,0)\xi\Big\rangle \\ = \sum_{j=1}^{k}\Big\langle \xi, \mathcal{U}_N^*(t,0)(\mathcal{N}+1)^{j-1} \\ \times \mathcal{U}_N(t,0)\left[i\varepsilon\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{U}_N^*(t,0)\mathcal{N}\mathcal{U}_N(t,0)\right]\mathcal{U}_N^*(t,0)(\mathcal{N}+1)^{k-j}\mathcal{U}_N(t,0)\xi\Big\rangle.\end{aligned}$$

□

Next, we have to bound the three terms on the r. h. s. of (3.43) by the expectation of $(\mathcal{N}+1)^k$ in the vector $\mathcal{U}_N(t,0)\xi$. A key ingredient to obtain such bounds is an estimate for the trace norm of the commutator $[e^{ip\cdot x}, \omega_{N,t}]$. For $t=0$ such an estimate was assumed in (3.24). In the next proposition, whose proof is deferred to Section 3.6, we show that the bound can be propagated to all $t \in \mathbb{R}$.

Proposition 3.4.4. *Let $V \in L^1(\mathbb{R}^3)$ such that*

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

Let ω_N be a non-negative trace class operator on $L^2(\mathbb{R}^3)$, with $\operatorname{tr}\omega_N = N$, $\|\omega_N\| \leq 1$ and such that

$$\begin{aligned} \sup_{p\in\mathbb{R}^3} \frac{1}{1+|p|} \operatorname{tr}|[\omega_N, e^{ip\cdot x}]| &\leq CN\varepsilon \\ \operatorname{tr}|[\omega_N, \varepsilon\nabla]| &\leq CN\varepsilon\,. \end{aligned} \tag{3.49}$$

for all $p \in \mathbb{R}^3$. Let $\omega_{N,t}$ be the solution of the Hartree-Fock equation (3.26) with initial data ω_N. Then, there exist constants $K, c > 0$ only depending on the potential V such that

$$\begin{aligned} \sup_{p\in\mathbb{R}^3} \frac{1}{1+|p|} \operatorname{tr}|[\omega_{N,t}, e^{ip\cdot x}]| &\leq KN\varepsilon\, \exp(c|t|) \\ \operatorname{tr}|[\omega_{N,t}, \varepsilon\nabla]| &\leq KN\varepsilon\, \exp(c|t|) \end{aligned} \tag{3.50}$$

for all $p \in \mathbb{R}^3$ and $t \in \mathbb{R}$.

We are now ready to estimate the three terms appearing on the r. h. s. of (3.43).

Lemma 3.4.5. *Under the assumptions (3.23) und (3.24) of Theorem 3.3.1, there exists a constant $c_1 > 0$ depending on V and a constant $C > 0$ depending on V and on $k \in \mathbb{N}$, such that*

$$\begin{aligned} \Big| \frac{1}{N} \int dx\,dy\, V(x-y) \Big\langle \mathcal{U}_N(t,0)\xi, (\mathcal{N}+1)^{j-1} \Big\{ & a^*(u_{t,x})a(\overline{v}_{t,y})a(u_{t,y})a(u_{t,x}) \\ + a(\overline{v}_{t,x})a(\overline{v}_{t,y})a(u_{t,y})a(u_{t,x}) + a^*(u_{t,y})a^*(\overline{v}_{t,y})a^*(\overline{v}_{t,x})a(\overline{v}_{t,x}) & \Big\} (\mathcal{N}+1)^{k-j}\mathcal{U}_N(t,0)\xi \Big\rangle \Big| \\ \leq C\varepsilon \exp(c_1|t|) \, \langle \mathcal{U}_N(t,0)\xi, (\mathcal{N}+1)^k \mathcal{U}_N(t,0)\xi \rangle & \end{aligned} \tag{3.51}$$

for all $j = 1, \dots, k$ and $t \in \mathbb{R}$.

Proof. We estimate the contributions arising from the three terms in the parenthesis separately. Let us start with the first term,

$$\begin{aligned} \mathrm{I} := \Big| \frac{1}{N} \int \mathrm{d}x\mathrm{d}y\, V(x-y) \Big\langle \mathcal{U}_N(t,0)\xi, (\mathcal{N}+1)^{j-1} & \\ \times a^*(u_{t,x})a(\overline{v}_{t,y})a(u_{t,y})a(u_{t,x})(\mathcal{N}+1)^{k-j}\mathcal{U}_N(t,0)\xi \Big\rangle \Big|\,. & \end{aligned}$$

Inserting $1 = (\mathcal{N}+3)^{k/2-j}(\mathcal{N}+3)^{-k/2+j}$, pulling $(\mathcal{N}+3)^{-k/2+j}$ through the fermionic operators to the right, and using the Cauchy-Schwarz inequality, we get:

$$\begin{aligned} \mathrm{I} \leq \frac{1}{N}\int \mathrm{d}p|\widehat{V}(p)| &\left\| \int \mathrm{d}x\, a^*(u_{t,x})e^{ip\cdot x}a(u_{t,x})(\mathcal{N}+3)^{k/2-j}(\mathcal{N}+1)^{j-1}\mathcal{U}_N(t,0)\xi \right\| \\ \times &\left\| \int \mathrm{d}y\, a(\overline{v}_{t,y})e^{-ip\cdot y}a(u_{t,y})(\mathcal{N}+1)^{k/2}\mathcal{U}_N(t,0)\xi \right\| . \end{aligned} \tag{3.52}$$

The first norm can be bounded using that, for any $\phi \in \mathcal{F}$:

$$\begin{aligned} \left\| \int \mathrm{d}x\, a^*(u_{t,x})e^{ip\cdot x}a(u_{t,x})\phi \right\| &= \left\| \int \mathrm{d}x\mathrm{d}r_1\mathrm{d}r_2\, u_t(r_1,x)e^{ip\cdot x}u_t(x,r_2)a^*_{r_1}a_{r_2}\phi \right\| \\ &= \left\| d\Gamma(u_t e^{ip\cdot x}u_t)\phi \right\| \\ &\leq \|\mathcal{N}\phi\| \end{aligned} \tag{3.53}$$

where the last line follows from Lemma 3.4.1 together with $\|u_t e^{ip\cdot x}u_t\| \leq 1$ (with a slight abuse of notation, $e^{ip\cdot x}$ denotes a multiplication operator). As for the second norm on the r. h. s. of (3.52), we use that:

$$\begin{aligned} \left\| \int \mathrm{d}y\, a(\overline{v}_{t,y})e^{-ip\cdot y}a(u_{t,y})\phi \right\| &= \left\| \int \mathrm{d}r_1\mathrm{d}r_2 \left(v_t e^{-ip\cdot x}u_t\right)(r_1,r_2)a_{r_1}a_{r_2}\phi \right\| \\ &= \left\| \int \mathrm{d}r_1\mathrm{d}r_2 \left(v_t[e^{-ip\cdot x},\omega_{N,t}]\right)(r_1,r_2)a_{r_1}a_{r_2}\phi \right\| \\ &\leq 2\,\mathrm{tr}\left|v_t[e^{-ip\cdot x},\omega_{N,t}]\right| \|\phi\| \\ &\leq 2K\varepsilon(1+|p|)Ne^{c|t|}\|\phi\| \end{aligned} \tag{3.54}$$

where the second line follows from $v_t u_t = 0$ and $u_t = 1-\omega_{N,t}$, the third from Lemma 3.4.1 and the last from $\|v_t\| \leq 1$ and Proposition 3.4.4. Using the bounds (3.53), (3.54) in (3.52) we get:

$$\begin{aligned} \mathrm{I} &\leq 2K\varepsilon\left(\int \mathrm{d}p|\widehat{V}(p)|(1+|p|)\right)e^{c|t|}\left\|\mathcal{N}(\mathcal{N}+3)^{k/2-j}(\mathcal{N}+1)^{j-1}\mathcal{U}_N(t,0)\xi\right\| \\ &\qquad \times \left\|(\mathcal{N}+1)^{k/2}\mathcal{U}_N(t,0)\xi\right\| \\ &\leq C\varepsilon e^{c|t|}\|(\mathcal{N}+1)^{k/2}\mathcal{U}_N(t,0)\xi\|^2 \end{aligned} \tag{3.55}$$

for a suitable constant $C > 0$ (depending on k). Consider now the second term on the r. h. s. of (3.51),

$$\begin{aligned} \mathrm{II} := \Big|\frac{1}{N}\int \mathrm{d}x\mathrm{d}y\, V(x-y)\Big\langle &\mathcal{U}_N(t,0)\xi, (\mathcal{N}+1)^{j-1} \\ &\times a(\overline{v}_{t,x})a(\overline{v}_{t,y})a(u_{t,y})a(u_{t,x})(\mathcal{N}+1)^{k-j}\mathcal{U}_N(t,0)\xi\Big\rangle\Big|. \end{aligned}$$

Inserting a $1 = (\mathcal{N}+5)^{k/2+1-j}(\mathcal{N}+5)^{-k/2-1+j}$ and pulling $(\mathcal{N}+5)^{-k/2-1+j}$ through the annihilation operators to the right, we get:

$$\begin{aligned} \mathrm{II} &\leq \frac{1}{N}\int \mathrm{d}p\mathrm{d}x\mathrm{d}y\,|\widehat{V}(p)|\left\|(\mathcal{N}+1)^{j-1}(\mathcal{N}+5)^{k/2+1-j}\mathcal{U}_N(t,0)\xi\right\| \\ &\qquad \times \left\|\int \mathrm{d}x\mathrm{d}y\, a(\overline{v}_{t,x})e^{ip\cdot x}a(u_{t,x})a(\overline{v}_{t,y})e^{-ip\cdot y}a(u_{t,y})(\mathcal{N}+1)^{k/2-1}\mathcal{U}_N(t,0)\xi\right\| \end{aligned} \tag{3.56}$$

Using that $v_t u_t = 0$ and that $u_t = 1 - \omega_{N,t}$, we obtain, for any $\phi \in \mathcal{F}$:

$$\begin{aligned}\left\| \int \mathrm{d}x\, a(\overline{v}_{t,x}) e^{ipx} a(u_{t,x})\phi \right\| &= \left\| \int \mathrm{d}r_1 \mathrm{d}r_2 \mathrm{d}x\, v_t(r_1,x) e^{ipx} u_t(x,r_2) a_{r_1} a_{r_2} \phi \right\| \\ &\leq \|v_t [e^{ip\cdot x}, \omega_{N,t}]\|_{\mathrm{HS}} \|\mathcal{N}^{1/2}\phi\| \\ &\leq \left(2\,\mathrm{tr}\left|[e^{ip\cdot x}, \omega_{N,t}]\right|\right)^{1/2} \|\mathcal{N}^{1/2}\phi\| \\ &\leq (2K\varepsilon(1+|p|)N)^{1/2} e^{c|t|}\, \|\mathcal{N}^{1/2}\phi\| \end{aligned} \tag{3.57}$$

where the second line follows from Lemma 3.4.1, the third from $\|v_t\| \leq 1$, $\|e^{ip\cdot x}\| \leq 1$, $\|\omega_{N,t}\| \leq 1$ and the last follows from Proposition 3.4.4 (the constants K, $c > 0$ depend on V but not on k). Applying this bound twice, we can estimate the last norm in the r. h. s. of (3.56) as:

$$\begin{aligned}&\left\| \int \mathrm{d}x\mathrm{d}y\, a(\overline{v}_{t,x}) e^{ip\cdot x} a(u_{t,x}) a(\overline{v}_{t,y}) e^{-ip\cdot y} a(u_{t,y}) (\mathcal{N}+1)^{k/2-1} \mathcal{U}_N(t,0)\xi \right\| \\ &\leq (2K\varepsilon(1+|p|)N)^{1/2} e^{c|t|} \left\| \int \mathrm{d}y\, a(\overline{v}_{t,y}) e^{-ip\cdot y} a(u_{t,y}) \mathcal{N}^{1/2} (\mathcal{N}+1)^{k/2-1} \mathcal{U}_N(t,0)\xi \right\| \\ &\leq 2K\varepsilon(1+|p|)N e^{2c|t|} \left\| \mathcal{N}(\mathcal{N}+1)^{k/2-1} \mathcal{U}_N(t,0)\xi \right\| \\ &\leq 2K\varepsilon(1+|p|)N e^{2c|t|} \left\| (\mathcal{N}+1)^{k/2} \mathcal{U}_N(t,0)\xi \right\|. \end{aligned} \tag{3.58}$$

Plugging this bound into (3.56), we conclude that

$$\begin{aligned}\mathrm{II} &\leq 2K\varepsilon \left(\int \mathrm{d}p\, |\widehat{V}(p)|(1+|p|) \right) e^{2c|t|} \left\| (\mathcal{N}+5)^{k/2} \mathcal{U}_N(t,0)\xi \right\|^2 \\ &\leq C\varepsilon e^{2c|t|} \left\| (\mathcal{N}+1)^{k/2} \mathcal{U}_N(t,0)\xi \right\|^2 \end{aligned}$$

where the constant $c > 0$ depends on V while the constant $C > 0$ depends on V and on k. The last term in (3.51) is bounded analogously to term I. This completes the proof of (3.51). □

Proof of Theorem 3.4.2. Combining Proposition 3.4.3 and Lemma 3.4.5, we find

$$\left| i\varepsilon \frac{\mathrm{d}}{\mathrm{d}t} \left\langle \mathcal{U}_N(t,0)\xi, (\mathcal{N}+1)^k \mathcal{U}_N(t,0)\xi \right\rangle \right| \leq C\varepsilon e^{c_1|t|} \left\langle \mathcal{U}_N(t,0)\xi, (\mathcal{N}+1)^k \mathcal{U}_N(t,0)\xi \right\rangle.$$

Grönwall's Lemma implies that

$$\left\langle \mathcal{U}_N(t,0)\xi, (\mathcal{N}+1)^k \mathcal{U}_N(t,0)\xi \right\rangle \leq \exp(c_2 \exp(c_1|t|)) \left\langle \xi, (\mathcal{N}+1)^k \xi \right\rangle$$

where the constant c_1 depends only on the potential V, while c_2 depends on V and on $k \in \mathbb{N}$. □

3.5. Proof of main results

In this section we prove our main results, Theorem 3.3.1 and Theorem 3.3.2. As in Section 3.4, we will use the notation $R_t \equiv R_{\nu_{N,t}}$, $u_t \equiv u_{N,t}$, $v_t \equiv v_{N,t}$, $\overline{v}_t \equiv \overline{v}_{N,t}$. Moreover, we define the functions $u_{t,x}(y) = u_{N,t}(y,x)$, $v_{t,x}(y) = v_{N,t}(y,x)$ and $\overline{v}_{t,x}(y) = \overline{v}_{N,t}(y,x)$.

Proof of Theorem 3.3.1. We start from the expression

$$\begin{aligned}\gamma^{(1)}_{N,t}(x,y) &= \langle \psi_{N,t}, a^*_y a_x \psi_{N,t}\rangle \\ &= \langle e^{-i\mathcal{H}_N t/\varepsilon} R_0 \xi_N, a^*_y a_x e^{-i\mathcal{H}_N t/\varepsilon} R_0 \xi_N\rangle \\ &= \langle \xi_N, R^*_0 e^{i\mathcal{H}_N t/\varepsilon} a^*_y a_x e^{-i\mathcal{H}_N t/\varepsilon} R_0 \xi_N\rangle.\end{aligned} \tag{3.59}$$

Introducing the fluctuation dynamics $\mathcal{U}_N$ defined in (3.36), we obtain

$$\begin{aligned}\gamma^{(1)}_{N,t}(x,y) &= \big\langle \xi_N, \mathcal{U}^*_N(t,0) R^*_t a^*_y a_x R_t \mathcal{U}_N(t,0)\xi_N\big\rangle \\ &= \big\langle \xi_N, \mathcal{U}^*_N(t,0)\,(a^*(u_{t,y}) + a(\overline{v}_{t,y}))\,(a(u_{t,x}) + a^*(\overline{v}_{t,x}))\,\mathcal{U}_N(t,0)\xi_N\big\rangle \\ &= \big\langle \xi_N, \mathcal{U}^*_N(t,0)\big\{a^*(u_{t,y})a(u_{t,x}) - a^*(\overline{v}_{t,x})a(\overline{v}_{t,y}) + \langle \overline{v}_{t,y}, \overline{v}_{t,x}\rangle \\ &\qquad + a^*(u_{t,y})a^*(\overline{v}_{t,x}) + a(\overline{v}_{t,y})a(u_{t,x})\big\}\,\mathcal{U}_N(t,0)\xi_N\big\rangle.\end{aligned}$$

Here we used the defining property (3.42) of the Bogoliubov transformation R_t and, in the third line, the canonical anticommutation relations (1.33). We observe that

$$\langle \overline{v}_{t,y}, \overline{v}_{t,x}\rangle = \int dz v_t(z,y)\overline{v}_t(z,x) = (v_t\overline{v}_t)(y,x) = \omega_{N,t}(x,y).$$

This implies that

$$\begin{aligned}\gamma^{(1)}_{N,t}(x,y) - \omega_{N,t}(x,y) &= \big\langle \xi_N, \mathcal{U}^*_N(t,0)\big\{a^*(u_{t,y})a(u_{t,x}) - a^*(\overline{v}_{t,x})a(\overline{v}_{t,y}) \\ &\qquad + a^*(u_{t,y})a^*(\overline{v}_{t,x}) + a(\overline{v}_{t,y})a(u_{t,x})\big\}\,\mathcal{U}_N(t,0)\xi_N\big\rangle.\end{aligned}$$

Step 1: Proof of (3.27). We integrate this difference against the integral kernel of a Hilbert-Schmidt operator O on $L^2(\mathbb{R}^3)$ and find

$$\begin{aligned}&\mathrm{tr}\; O\left(\gamma^{(1)}_{N,t} - \omega_{N,t}\right) \\ &\quad = \big\langle \xi_N, \mathcal{U}^*_N(t,0)\left(d\Gamma(u_t O u_t) - d\Gamma(\overline{v}_t \overline{O^*} v_t)\right)\mathcal{U}_N(t,0)\xi_N\big\rangle \\ &\qquad + 2\mathrm{Re}\;\big\langle \xi_N, \mathcal{U}^*_N(t,0)\left(\int \mathrm{d}r_1 \mathrm{d}r_2 (v_t O u_t)(r_1,r_2) a_{r_1} a_{r_2}\right)\mathcal{U}_N(t,0)\xi_N\big\rangle.\end{aligned} \tag{3.60}$$

From Lemma 3.4.1, and using $\|u_t\| = \|v_t\| = 1$, we conclude that

$$\begin{aligned}\left|\mathrm{tr}\, O\left(\gamma^{(1)}_{N,t} - \omega_{N,t}\right)\right| &\leq \left(\|u_t O u_t\| + \|\overline{v}_t \overline{O^*} v_t\|\right)\big\langle \xi_N, \mathcal{U}^*_N(t,0)\mathcal{N}\mathcal{U}_N(t,0)\xi_N\big\rangle \\ &\quad + 2\|v_t O u_t\|_{\mathrm{HS}}\left\|(\mathcal{N}+1)^{1/2}\mathcal{U}_N(t,0)\xi_N\right\|\|\xi_N\| \\ &\leq C\|O\|_{\mathrm{HS}}\big\langle \xi_N, \mathcal{U}^*_N(t,0)(\mathcal{N}+1)\mathcal{U}_N(t,0)\xi_N\big\rangle.\end{aligned} \tag{3.61}$$

From Theorem 3.4.2 and from the assumption $\langle \xi_N, \mathcal{N}\xi_N\rangle \leq C$, we obtain

$$\left\|\gamma^{(1)}_{N,t} - \omega_{N,t}\right\|_{\mathrm{HS}} \leq C\exp(c_1\exp(c_2|t|))$$

which completes the proof of (3.27).

Step 2: Proof of (3.28)*.* We start anew from (3.60), assuming now O to be a compact operator on $L^2(\mathbb{R}^3)$, not necessarily Hilbert-Schmidt. Proceeding as in (3.61), we find

$$\begin{aligned}&\left|\operatorname{tr} O\left(\gamma^{(1)}_{N,t} - \omega_{N,t}\right)\right| \\ &\leq 2\|O\|\,\|(\mathcal{N}+1)^{1/2}\mathcal{U}_N(t,0)\xi_N\|^2 + 2\|v_t O u_t\|_{\mathrm{HS}}\left\|(\mathcal{N}+1)^{1/2}\mathcal{U}_N(t,0)\xi_N\right\|\,\|\xi_N\| \\ &\leq 2\|O\|\,\|(\mathcal{N}+1)^{1/2}\mathcal{U}_N(t,0)\xi_N\|^2 + \|O\|\,\|v_t\|_{\mathrm{HS}}\|(\mathcal{N}+1)^{1/2}\mathcal{U}_N(t,0)\xi_N\|\|\xi_N\|.\end{aligned}$$

Applying Theorem 3.4.2, the assumption $\langle \xi_N, \mathcal{N}\xi_N\rangle \leq C$, and $\|v_t\|_{\mathrm{HS}} = N^{1/2}$, we obtain

$$\left|\operatorname{tr} O\left(\gamma^{(1)}_{N,t} - \omega_{N,t}\right)\right| \leq C N^{1/2}\exp(c_1\exp(c_2|t|))\,.$$

This completes the proof of (3.28).

Step 3: Proof of (3.29)*.* Let us now assume additionally $d\Gamma(\omega_N)\xi_N = 0$. Let $\xi_N^{(n)}$ the n-particle component of the Fock space vector ξ_N. With a slight abuse of notation, we denote again by $\xi_N^{(n)}$ the Fock space vector $(0,\dots,0,\xi_N^{(n)},0,\dots)\in\mathcal{F}$. The assumption implies that $d\Gamma(\omega_N)\xi_N^{(n)} = 0$ for all $n\in\mathbb{N}$. Hence

$$\mathcal{N}R_{\nu_N}\xi_N^{(n)} = R_{\nu_N}(\mathcal{N}+N-2d\Gamma(\omega_N))\xi_N^{(n)} = R_{\nu_N}(n+N)\xi_N^{(n)} = (n+N)R_{\nu_N}\xi_N^{(n)}\,. \tag{3.62}$$

In other words, $R_{\nu_N}\xi_N^{(n)}$ is an eigenstate of the number of particles operator with eigenvalue $n+N$. Hence

$$\begin{aligned}&\gamma^{(1)}_{N,t}(x,y) \\ &\quad= \sum_{n\geq 0}\langle e^{-i\mathcal{H}_N t/\varepsilon}R_{\nu_N}\xi_N^{(n)}, a_y^* a_x e^{-i\mathcal{H}_N t/\varepsilon}R_{\nu_N}\xi_N^{(n)}\rangle \\ &\quad= \sum_{n\geq 0}\langle \mathcal{U}_N(t,0)\xi_N^{(n)}, (a^*(u_{t,y}) + a(\bar{v}_{t,y}))(a(u_{t,x}) + a^*(\bar{v}_{t,x}))\mathcal{U}_N(t,0)\xi_N^{(n)}\rangle.\end{aligned}$$

Proceeding as in the proof of the first part of Theorem 3.3.1, for a compact operator O on $L^2(\mathbb{R}^3)$, we end up with:

$$\begin{aligned}&\operatorname{tr} O(\gamma^{(1)}_{N,t} - \omega_{N,t}) \\ &\quad= \sum_{n\geq 0}\langle \xi_N^{(n)}, \mathcal{U}_N^*(t,0)\left(d\Gamma(u_t O u_t) - d\Gamma(\bar{v}_t\overline{O^*}v_t)\right)\mathcal{U}_N(t,0)\xi_N^{(n)}\rangle \\ &\qquad + 2\,\mathrm{Re}\sum_{n\geq 0}\langle \xi_N^{(n)}, \mathcal{U}_N^*(t,0)\left(\int \mathrm{d}r_1\mathrm{d}r_2 (v_t O u_t)(r_1,r_2)a_{r_1}a_{r_2}\right)\mathcal{U}_N(t,0)\xi_N^{(n)}\rangle \\ &\quad=: \mathrm{I} + \mathrm{II}\,.\end{aligned} \tag{3.63}$$

We estimate separately the two lines in the r. h. s. of Eq. (3.63). Let us start with

$$\mathrm{I} = \sum_{n\geq 0}\langle \xi_N^{(n)}, \mathcal{U}_N^*(t,0)\left(d\Gamma(u_t O u_t) - d\Gamma(\bar{v}_t\overline{O^*}v_t)\right)\mathcal{U}_N(t,0)\xi_N^{(n)}\rangle.$$

From Lemma 3.4.1, we get

$$\begin{aligned} \mathrm{I} &\leq (\|u_t O u_t\| + \|\overline{v}_t \overline{O^*} v_t\|) \sum_{n\geq 0} \langle \xi_N^{(n)}, \mathcal{U}_N^*(t,0) \mathcal{N} \mathcal{U}_N(t,0) \xi_N^{(n)} \rangle \\ &\leq C\|O\| \exp(c_1 \exp(c_2|t|)) \sum_{n\geq 0} \langle \xi_N^{(n)}, \mathcal{N} \xi_N^{(n)} \rangle \\ &= C\|O\| \exp(c_1 \exp(c_2|t|)) \langle \xi_N, \mathcal{N} \xi_N \rangle \leq C\|O\| \exp(c_1 \exp(c_2|t|)) \end{aligned} \tag{3.64}$$

where we used the fact that $\|u_t\| = \|v_t\| = 1$, Theorem 3.4.2 to control the growth of the expectation of $\mathcal{N}$ w. r. t. the fluctuation dynamics $\mathcal{U}_N$, and that by assumption $\langle \xi_N, \mathcal{N} \xi_N \rangle \leq C$. Therefore, we are left with

$$\mathrm{II} = 2\,\mathrm{Re} \sum_{n\geq 0} \langle \xi_N^{(n)}, \mathcal{U}_N^*(t,0) \left(\int \mathrm{d}r_1 \mathrm{d}r_2 (v_t O u_t)(r_1, r_2) a_{r_1} a_{r_2} \right) \mathcal{U}_N(t,0) \xi_N^{(n)} \rangle \,. \tag{3.65}$$

We now introduce the generator $\mathcal{L}_N(t)$ through $i\varepsilon \partial_t \mathcal{U}_N(t,s) = \mathcal{L}_N(t) \mathcal{U}(t,s)$. The generator has a part which commutes with the number operator $\mathcal{N}$; this operator we call $\mathcal{E}(t)$. From Proposition 3.4.3 we know the part of the generator which does not commute with the number operator; writing this part explicitly we get

$$\begin{aligned} \mathcal{L}_N(t) = \frac{1}{N} \int \mathrm{d}x \mathrm{d}y\, V(x-y) \Big\{ & a^*(u_{t,x}) a(\overline{v}_{t,y}) a(u_{t,y}) a(u_{t,x}) \\ & + \frac{1}{2} a(\overline{v}_{t,x}) a(\overline{v}_{t,y}) a(u_{t,y}) a(u_{t,x}) - a^*(u_{t,y}) a^*(\overline{v}_{t,y}) a^*(\overline{v}_{t,x}) a(\overline{v}_{t,x}) + \text{h.c.} \Big\} \\ & + \mathcal{E}(t). \end{aligned} \tag{3.66}$$

We are going to compare the dynamics $\mathcal{U}_N(t,s)$ with a modified dynamics $\mathcal{U}_N^{(1)}(t,s)$, whose generator $\mathcal{L}_N^{(1)}(t)$ only contains one of the three explicitly written terms on the r. h. s. of (3.66), and the term $\mathcal{E}(t)$, which commutes with $\mathcal{N}$. We define

$$\mathcal{L}_N^{(1)}(t) := \frac{1}{N} \int \mathrm{d}x \mathrm{d}y V(x-y) \Big\{ \frac{1}{2} a(\overline{v}_{t,x}) a(\overline{v}_{t,y}) a(u_{t,y}) a(u_{t,x}) + \text{h.c.} \Big\} + \mathcal{E}(t).$$

Notice that $\mathcal{L}_N^{(1)}(t)$ can only create or annihilate four particles at a time. This implies that, although $\mathcal{L}_N^{(1)}(t)$ does not commute with $\mathcal{N}$, it satisfies

$$\mathbf{1}(\mathcal{N} \in n + 4\mathbb{Z})\, \mathcal{U}_N^{(1)}(t,0) = \mathcal{U}_N^{(1)}(t,0)\, \mathbf{1}(\mathcal{N} \in n + 4\mathbb{Z}) \qquad \text{for all } n \in \mathbb{N}. \tag{3.67}$$

Here $\mathbf{1}(\mathcal{N} \in n+4\mathbb{Z})$ is the projection defined by applying the functional calculus of $\mathcal{N}$ to the characteristic function of the set $n+4\mathbb{Z}$. We will use the shorthand $\mathbf{1}_{n+4\mathbb{Z}} = \mathbf{1}(\mathcal{N} \in n+4\mathbb{Z})$ from now on.

We now rewrite (3.65) as

$$\begin{aligned} \mathrm{II} = 2\,\mathrm{Re} \sum_{n\geq 0} \Big\{ & \langle \xi_N^{(n)}, \mathcal{U}_N^{(1)*}(t,0) \left(\int \mathrm{d}r_1 \mathrm{d}r_2 (v_t O u_t)(r_1,r_2) a_{r_1} a_{r_2} \right) \mathcal{U}_N^{(1)}(t,0) \xi_N^{(n)} \rangle \\ & + \langle \xi_N^{(n)}, \left(\mathcal{U}_N^*(t,0) - \mathcal{U}_N^{(1)*}(t,0) \right) \left(\int \mathrm{d}r_1 \mathrm{d}r_2 (v_t O u_t)(r_1,r_2) a_{r_1} a_{r_2} \right) \mathcal{U}_N^{(1)}(t,0) \xi_N^{(n)} \rangle \\ & + \langle \xi_N^{(n)}, \mathcal{U}_N^*(t,0) \left(\int \mathrm{d}r_1 \mathrm{d}r_2 (v_t O u_t)(r_1,r_2) a_{r_1} a_{r_2} \right) \left(\mathcal{U}_N(t,0) - \mathcal{U}_N^{(1)}(t,0) \right) \xi_N^{(n)} \rangle \Big\} \\ =: {} & \mathrm{II}_1 + \mathrm{II}_2 + \mathrm{II}_3 \,. \end{aligned} \tag{3.68}$$

The key observation which allows us to improve the rate of convergence with respect to Eq. (3.28) is that $\mathrm{II}_1 = 0$. This follows from the remark that $\mathcal{U}_N^{(1)}$ can only create or annihilate particles in groups of four. Thus, the expectation of a product of two annihilation operators (or two creation operators) in the vector $\mathcal{U}_N^{(1)}(t,0)\xi_N^{(n)}$ must vanish. To prove this fact rigorously, we use (3.67), which implies that for each $n \in \mathbb{N}$

$$\begin{aligned}
&\langle \xi_N^{(n)}, \mathcal{U}_N^{(1)*}(t,0)\left(\int \mathrm{d}r_1\mathrm{d}r_2(v_tOu_t)(r_1,r_2)a_{r_1}a_{r_2}\right)\mathcal{U}_N^{(1)}(t,0)\xi_N^{(n)}\rangle \\
&= \langle \mathbf{1}_{n+4\mathbb{Z}}\xi_N^{(n)}, \mathcal{U}_N^{(1)*}(t,0)\left(\int \mathrm{d}r_1\mathrm{d}r_2(v_tOu_t)(r_1,r_2)a_{r_1}a_{r_2}\right)\mathcal{U}_N^{(1)}(t,0)\mathbf{1}_{n+4\mathbb{Z}}\xi_N^{(n)}\rangle \\
&= \langle \xi_N^{(n)}, \mathcal{U}_N^{(1)*}(t,0)\mathbf{1}_{n+4\mathbb{Z}}\left(\int \mathrm{d}r_1\mathrm{d}r_2(v_tOu_t)(r_1,r_2)a_{r_1}a_{r_2}\right)\mathbf{1}_{n+4\mathbb{Z}}\mathcal{U}_N^{(1)}(t,0)\xi_N^{(n)}\rangle \\
&= \langle \xi_N^{(n)}, \mathcal{U}_N^{(1)*}(t,0)\mathbf{1}_{n+4\mathbb{Z}}\mathbf{1}_{n+4\mathbb{Z}+2}\left(\int \mathrm{d}r_1\mathrm{d}r_2(v_tOu_t)(r_1,r_2)a_{r_1}a_{r_2}\right)\mathcal{U}_N^{(1)}(t,0)\xi_N^{(n)}\rangle \\
&= 0,
\end{aligned} \tag{3.69}$$

where in the last step we used that the range of the projections is disjoint, $\mathbf{1}_{n+4\mathbb{Z}}\mathbf{1}_{n+4\mathbb{Z}+2} = 0$. We are left with bounding the last two terms in (3.68); let us start with

$$\begin{aligned}
\mathrm{II}_2 = 2\,\mathrm{Re}\sum_{n\geq 0}\Big\langle \xi_N^{(n)}, \Big(\mathcal{U}_N^*(t,0) - \mathcal{U}_N^{(1)*}(t,0)\Big) \\
\times\left(\int \mathrm{d}r_1\mathrm{d}r_2(v_tOu_t)(r_1,r_2)a_{r_1}a_{r_2}\right)\mathcal{U}_N^{(1)}(t,0)\xi_N^{(n)}\Big\rangle.
\end{aligned} \tag{3.70}$$

We expand $\mathcal{U}_N$ in terms of $\mathcal{U}_N^{(1)}$ using the Duhamel formula

$$\mathcal{U}_N(t,0) - \mathcal{U}_N^{(1)}(t,0) = -\frac{i}{\varepsilon}\int_0^t \mathrm{d}s\,\mathcal{U}(t,s)\widetilde{\mathcal{L}}_N(s)\mathcal{U}_N^{(1)}(s,0), \tag{3.71}$$

wherein

$$\begin{aligned}
\widetilde{\mathcal{L}}_N(t) &= \mathcal{L}_N(t) - \mathcal{L}_N^{(1)}(t) \\
&= \frac{1}{N}\int \mathrm{d}x\mathrm{d}y\,V(x-y)\Big\{a^*(u_{t,x})a(\overline{v}_{t,y})a(u_{t,y})a(u_{t,x}) \\
&\qquad - a^*(u_{t,y})a^*(\overline{v}_{t,y})a^*(\overline{v}_{t,x})a(\overline{v}_{t,x}) + \mathrm{h.c.}\Big\}
\end{aligned} \tag{3.72}$$

Plugging (3.71) into (3.70) and using (3.72) we end up with

$$\begin{aligned}
\mathrm{II}_2 \leq \frac{4}{\varepsilon N}\sum_{n\geq 0}\Big\{\Big|\Big\langle \xi_N^{(n)}, \int_0^t \mathrm{d}s\,\mathcal{U}_N^{(1)*}(s,0) \\
\times\left(\int \mathrm{d}x\mathrm{d}y\,V(x-y)a^*(u_{s,x})a(\overline{v}_{s,y})a(u_{s,y})a(u_{s,x}) + \mathrm{h.c.}\right) \\
\times\ \mathcal{U}_N^*(t,s)\left(\int \mathrm{d}r_1\mathrm{d}r_2(v_tOu_t)(r_1,r_2)a_{r_1}a_{r_2}\right)\mathcal{U}_N^{(1)}(t,0)\xi_N^{(n)}\Big\rangle\Big| \\
+\Big|\Big\langle \xi_N^{(n)}, \int_0^t \mathrm{d}s\,\mathcal{U}_N^{(1)*}(s,0)\left(\int \mathrm{d}x\mathrm{d}y\,V(x-y)a^*(u_{s,y})a^*(\overline{v}_{s,y})a^*(\overline{v}_{s,x})a(\overline{v}_{s,x}) + \mathrm{h.c.}\right)\times
\end{aligned}$$

$$
\begin{aligned}
&\qquad \times\ \mathcal{U}_N^*(t,s)\left(\int \mathrm{d}r_1\mathrm{d}r_2(v_tOu_t)(r_1,r_2)a_{r_1}a_{r_2}\right)\mathcal{U}^{(1)}(t,0)\xi_N^{(n)}\Big\rangle\Big|\Big\}\\
&=: \mathrm{II}_{2.1}+\mathrm{II}_{2.2}\,. \qquad (3.73)
\end{aligned}
$$

We start by estimating $\mathrm{II}_{2.1}$. We find

$$
\begin{aligned}
\mathrm{II}_{2.1} \leq\ & \frac{2}{\varepsilon N}\sum_{n\geq 0}\int_0^t \mathrm{d}s\int \mathrm{d}p\,|\hat{V}(p)|\\
&\times\Big\{\Big|\Big\langle \xi_N^{(n)},\mathcal{U}_N^{(1)*}(s,0)d\Gamma(u_se^{ipx}\bar{u}_s)\\
&\qquad\times\left(\int \mathrm{d}\omega_1\mathrm{d}\omega_2\,(v_se^{-ipx}\bar{u}_s)(\omega_1,\omega_2)a_{\omega_1}a_{\omega_2}\right)\mathcal{U}_N^*(t,s)\\
&\qquad\times\left(\int \mathrm{d}r_1\mathrm{d}r_2(v_tOu_t)(r_1,r_2)a_{r_1}a_{r_2}\right)\mathcal{U}_N^{(1)}(t,0)\xi_N^{(n)}\Big\rangle\Big|\\
&\quad+\Big|\Big\langle \xi_N^{(n)},\mathcal{U}_N^{(1)*}(s,0)\left(\int \mathrm{d}\omega_1\mathrm{d}\omega_2\,(\bar{v}_se^{-ipx}u_s)(\omega_1,\omega_2)a^*_{\omega_1}a^*_{\omega_2}\right)\\
&\qquad\times d\Gamma(u_se^{ipx}\bar{u}_s)\mathcal{U}_N^*(t,s)\left(\int \mathrm{d}r_1\mathrm{d}r_2(v_tOu_t)(r_1,r_2)a_{r_1}a_{r_2}\right)\mathcal{U}_N^{(1)}(t,0)\xi_N^{(n)}\Big\rangle\Big|\Big\}\,.
\end{aligned}
$$

Using the Cauchy-Schwarz inequality, we obtain

$$
\begin{aligned}
\mathrm{II}_{2.1} \leq\ & \frac{2}{\varepsilon N}\sum_{n\geq 0}\int_0^t \mathrm{d}s\int \mathrm{d}p|\hat{V}(p)|\left\|d\Gamma(u_se^{ipx}\bar{u}_s)\mathcal{U}_N^{(1)}(s,0)\xi_N^{(n)}\right\|\\
&\times\left\|\left(\int \mathrm{d}\omega_1\mathrm{d}\omega_2\,(v_se^{-ipx}\bar{u}_s)(\omega_1,\omega_2)a_{\omega_1}a_{\omega_2}\right)\mathcal{U}_N^*(t,s)\right.\\
&\qquad\left.\times\left(\int \mathrm{d}r_1\mathrm{d}r_2(v_tOu_t)(r_1,r_2)a_{r_1}a_{r_2}\right)\mathcal{U}_N^{(1)}(t,0)\xi_N^{(n)}\right\|\\
&+\frac{2}{\varepsilon N}\sum_{n\geq 0}\int_0^t \mathrm{d}s\int \mathrm{d}p\,|\hat{V}(p)|\\
&\quad\times\left\|(\mathcal{N}+2)^{-1/2}d\Gamma(u_se^{ipx}\bar{u}_s)\right.\\
&\qquad\left.\times\left(\int \mathrm{d}\omega_1\mathrm{d}\omega_2\,(v_se^{-ipx}\bar{u}_s)(\omega_1,\omega_2)a_{\omega_1}a_{\omega_2}\right)\mathcal{U}_N^{(1)}(s,0)\xi_N^{(n)}\right\|\\
&\quad\times\left\|(\mathcal{N}+2)^{1/2}\mathcal{U}_N^*(t,s)\left(\int \mathrm{d}r_1\mathrm{d}r_2(v_tOu_t)(r_1,r_2)a_{r_1}a_{r_2}\right)\mathcal{U}_N^{(1)}(t,0)\xi_N^{(n)}\right\|\,.
\end{aligned}
$$

From Lemma 3.4.1, it follows that

$$
\begin{aligned}
\mathrm{II}_{2.1} \leq\ & \frac{2}{\varepsilon N}\sum_{n\geq 0}\int_0^t \mathrm{d}s\int \mathrm{d}p\,|\hat{V}(p)|\left\|\mathcal{N}\mathcal{U}_N^{(1)}(s,0)\xi_N^{(n)}\right\|\left\|v_se^{-ipx}\bar{u}_s\right\|_{\mathrm{HS}}\\
&\times\left\|\mathcal{N}^{1/2}\mathcal{U}_N^*(t,s)\left(\int \mathrm{d}r_1\mathrm{d}r_2(v_tOu_t)(r_1,r_2)a_{r_1}a_{r_2}\right)\mathcal{U}_N^{(1)}(t,0)\xi_N^{(n)}\right\|\\
&+\frac{2}{\varepsilon N}\sum_{n\geq 0}\int_0^t \mathrm{d}s\int \mathrm{d}p\,|\hat{V}(p)|\|v_se^{-ipx}\bar{u}_s\|_{\mathrm{HS}}\left\|\mathcal{N}\mathcal{U}_N^{(1)}(s,0)\xi_N^{(n)}\right\|\\
&\quad\times\left\|(\mathcal{N}+2)^{1/2}\mathcal{U}_N^*(t,s)\left(\int \mathrm{d}r_1\mathrm{d}r_2(v_tOu_t)(r_1,r_2)a_{r_1}a_{r_2}\right)\mathcal{U}_N^{(1)}(t,0)\xi_N^{(n)}\right\|\,.
\end{aligned}
$$

Using Theorem 3.4.2 to control the growth of $\mathcal{N}$ w. r. t. the unitary evolutions, and again Lemma 3.4.1, we conclude that

$$\begin{aligned}\mathrm{II}_{2.1} \leq \; & \frac{C\exp(c_1\exp(c_2|t|))}{\varepsilon N} \\ & \times \sum_{n\geq 0}\int_0^t \mathrm{d}s \int \mathrm{d}p\, |\hat{V}(p)|\, \left\| v_s e^{-ipx}\bar{u}_s \right\|_{\mathrm{HS}} \|v_t O u_t\|_{\mathrm{HS}} \left\| (\mathcal{N}+2)\xi_N^{(n)} \right\|^2 .\end{aligned} \tag{3.74}$$

Here we also used a bound of the form $\|\mathcal{N}\mathcal{U}_N^{(1)}(t,0)\xi\| \leq C\exp(c_1\exp(c_2|t|))\|\mathcal{N}\xi\|$ for the growth of the expectation of the number of particles w. r. t. the modified dynamics $\mathcal{U}_N^{(1)}(t,0)$. This bound can be proven exactly as the estimate in Theorem 3.4.2 for the dynamics $\mathcal{U}_N(t,0)$, with the only difference that when we compute the derivative of $\langle \xi, \mathcal{U}_N^{(1)}(t,0)(\mathcal{N}+1)^k \mathcal{U}_N^{(1)}\xi\rangle$ only one of the three terms on the r. h. s. of (3.43) appears.

Since $\|u_t O v_t\|_{\mathrm{HS}} \leq \|O\| N^{1/2}$ and, using Proposition 3.4.4,

$$\left\| v_s e^{ipx}\bar{u}_s \right\|_{\mathrm{HS}}^2 \leq \operatorname{tr}\left|[\gamma_s, e^{ipx}]\right| \leq C(1+|p|)N\varepsilon\exp(c|s|),$$

we find that

$$\begin{aligned}\mathrm{II}_{2.1} &\leq C\|O\|\varepsilon^{-1/2}\exp(c_1\exp(c_2|t|))\sum_{n\geq 0}\|(\mathcal{N}+2)\xi_N^{(n)}\|^2 \\ &\leq C\|O\|\varepsilon^{-1/2}\exp(c_1\exp(c_2|t|))\|(\mathcal{N}+2)\xi_N\|^2.\end{aligned}$$

The same strategy is followed to bound $\mathrm{II}_{2.2}$ in (3.73), and II_3 in (3.68). Hence, we have shown that, for every compact operator O,

$$\begin{aligned}\left|\operatorname{tr} O\,(\gamma_{N,t}^{(1)} - \omega_{N,t})\right| &\leq C\|O\|N^{1/6}\exp\left(c_2\exp(c_1|t|)\right)\langle \xi_N, (\mathcal{N}+2)^2\xi_N\rangle \\ &\leq C\|O\|N^{1/6}\exp\left(c_2\exp(c_1|t|)\right)\end{aligned}$$

where we used the assumption $\langle \xi_N, \mathcal{N}^2\xi_N\rangle \leq C$. This completes the proof of (3.29).

Step 4: Proof of (3.30). We consider an observable $O = e^{ix\cdot q+\varepsilon p\cdot\nabla}$ with $p,\, q \in \mathbb{R}^3$. As in (3.63) we decompose

$$\operatorname{tr} O(\gamma_{N,t}^{(1)} - \omega_{N,t}) = \mathrm{I} + \mathrm{II}.$$

The bound for I obtained in (3.64) for an arbitrary bounded operator O is already consistent with (3.30). However, we have to improve the bound for II, using the special structure of the observable O. Writing $\mathrm{II} = \mathrm{II}_1 + \mathrm{II}_2 + \mathrm{II}_3$ as in (3.68), and noticing again that $\mathrm{II}_1 = 0$, we are left with the problem of improving the bound for II_2 and II_3. To bound II_2, we use (3.74) and the remark that, for $O = e^{ix\cdot q+\varepsilon\nabla\cdot p}$,

$$\begin{aligned}\|v_t O u_t\|_{\mathrm{HS}}^2 &= \left\|v_t e^{ix\cdot q+\varepsilon p\cdot\nabla}u_t\right\|_{\mathrm{HS}}^2 \\ &\leq \operatorname{tr}\left|\left[\omega_{N,t}, e^{ix\cdot q+\varepsilon p\cdot\nabla}\right]\right| \leq \operatorname{tr}\left|\left[\omega_{N,t}, e^{ix\cdot q}\right]\right| + \operatorname{tr}\left|\left[\omega_{N,t}, e^{\varepsilon p\cdot\nabla}\right]\right|.\end{aligned} \tag{3.75}$$

Using that

$$\begin{aligned}[\omega_{N,t}, e^{\varepsilon p\cdot\nabla}] = \omega_{N,t}e^{\varepsilon p\cdot\nabla} - e^{\varepsilon p\cdot\nabla}\omega_{N,t} &= -\int_0^1 \mathrm{d}s\, \frac{\mathrm{d}}{\mathrm{d}s} e^{s\varepsilon p\cdot\nabla}\omega_{N,t}e^{(1-s)\varepsilon p\cdot\nabla} \\ &= -\int_0^1 \mathrm{d}s\, e^{s\varepsilon p\cdot\nabla}[\varepsilon p\cdot\nabla, \omega_{N,t}]e^{(1-s)\varepsilon p\cdot\nabla}\end{aligned}$$

we conclude from Proposition 3.4.4 that

$$\operatorname{tr}|[\omega_{N,t}, e^{\varepsilon p\cdot\nabla}]| \leq |p| \operatorname{tr}|[\varepsilon\nabla, \omega_{N,t}]| \leq C|p|N\varepsilon \exp(c|t|).$$

Therefore, using Proposition 3.4.4 also to bound $\operatorname{tr}|[\omega_{N,t}, e^{ix\cdot q}]|$, (3.75) implies that

$$\|v_t O u_t\|_{\mathrm{HS}}^2 \leq C(1+|q|+|p|)N\varepsilon \exp(c|t|).$$

Inserting this bound in (3.74), we obtain that, for $O = e^{ix\cdot q+\varepsilon\nabla\cdot p}$,

$$\mathrm{II}_2 \leq C\exp(c_1\exp(c_2|t|))(1+|p|+|q|)^{1/2}\|(\mathcal{N}+1)\xi_N\|^2.$$

A similar bound can be found for the contribution II_3. Hence

$$\begin{aligned}\left|\operatorname{tr}\, e^{ix\cdot q+\varepsilon\nabla\cdot p}\left(\gamma_{N,t}^{(1)} - \omega_{N,t}\right)\right| &\leq C(1+|p|+|q|)^{1/2}\exp(c_1\exp(c_2|t|))\|(\mathcal{N}+1)\xi_N\|^2 \\ &\leq C(1+|p|+|q|)^{1/2}\exp(c_1\exp(c_2|t|)),\end{aligned}$$

where we used the assumption $\|(\mathcal{N}+1)\xi_N\|^2 < C$. This concludes the proof of Theorem 3.3.1. □

Next, we proceed with the proof of Theorem 3.3.2.

Proof of Theorem 3.3.2. We start from the expression

$$\begin{aligned}&\gamma_{N,t}^{(k)}(x_1,\ldots,x_k,x_1',\ldots x_k') \\ &\quad= \langle e^{-i\mathcal{H}_N t/\varepsilon}R_0\xi, a_{x_k'}^*\ldots a_{x_1'}^* a_{x_1}\ldots a_{x_k} e^{-i\mathcal{H}_N t/\varepsilon}R_0\xi\rangle \\ &\quad= \langle \mathcal{U}_N(t,0)\xi, R_t^* a_{x_k'}^*\ldots a_{x_1'}^* a_{x_1}\ldots a_{x_k} R_t\mathcal{U}_N(t,0)\xi\rangle \\ &\quad= \langle \mathcal{U}_N(t,0)\xi, \left(a^*(u_{t,x_k'}) + a(\overline{v}_{t,x_k'})\right)\cdots\left(a^*(u_{t,x_1'}) + a(\overline{v}_{t,x_1'})\right) \\ &\qquad\qquad \times (a(u_{t,x_1}) + a^*(\overline{v}_{t,x_1}))\cdots(a(u_{t,x_k}) + a^*(\overline{v}_{t,x_k}))\,\mathcal{U}_N(t,0)\xi\rangle.\end{aligned} \tag{3.76}$$

This product will be expanded as a sum of 2^{2k} summands. Each summand will be put in normal order using Wick's theorem, which gives rise to contractions. The completely contracted contribution will be identified with the Hartree-Fock density matrix $\omega_{N,t}^{(k)}$, all other contributions will be of smaller order.

Step 1: Expanding the product and applying Wick's theorem. We recall Wick's theorem. For $j = 1,\ldots,2k$, we denote by $a_j^\sharp$ either an annihilation or a creation operator acting on the fermionic Fock space $\mathcal{F}$. We denote by $: a_{j_1}^\sharp \ldots a_{j_\ell}^\sharp :$ the product $a_{j_1}^\sharp \ldots a_{j_\ell}^\sharp$ in normal order (obtained by moving all creation operators on the left and all annihilation operators on the right, proceeding as if they were all anticommuting operators). Wick's theorem states that

$$\begin{aligned}a_1^\sharp a_2^\sharp\cdots a_{2k}^\sharp = \,: a_1^\sharp a_2^\sharp\cdots a_{2k}^\sharp : + \sum_{j=1}^{k}\sum_{n_1<\cdots<n_{2j}} &: a_1^\sharp\cdots\widehat{a_{n_1}^\sharp}\cdots\widehat{a_{n_{2j}}^\sharp}\cdots a_{2k}^\sharp : \\ &\times \sum_{\sigma\in P_{2j}}(-1)^{|\sigma|}\langle\Omega, a_{n_{\sigma(1)}}^\sharp a_{n_{\sigma(2)}}^\sharp\Omega\rangle\cdots\langle\Omega, a_{n_{\sigma(2j-1)}}^\sharp a_{n_{\sigma(2j)}}^\sharp\Omega\rangle\end{aligned}$$

where P_{2j} is the set of pairings

$$P_{2j} = \big\{\sigma \in S_{2j} : \sigma(2\ell-1) < \sigma(2\ell) \; \forall \ell = 1,\dots,j \text{ and} \\ \sigma(2\ell-1) < \sigma(2\ell+1) \; \forall \ell = 1,\dots,j-1\big\}, \tag{3.77}$$

and $|\sigma|$ denotes the number of pair interchanges needed to bring the contracted operators in the order $a^\sharp_{n_{\sigma(1)}} a^\sharp_{n_{\sigma(2)}} \dots a^\sharp_{n_{\sigma(2j)}}$. We call $\langle \Omega, a^\sharp_i a^\sharp_j \Omega\rangle$ the contraction of $a^\sharp_i$ and $a^\sharp_j$. The notation with the hats indicates operators that do not appear in the product.

Next, we apply Wick's theorem to the products arising from (3.76). To this end, we observe that the contraction of a $a^\sharp(u_{t,z_1})$-operator with a $a^\sharp(\overline{v}_{t,z_2})$-operator is always zero because $u_t \overline{v}_t = v_t u_t = 0$. Furthermore, the $a^\sharp(u_{t,z})$-operators among themselves are already in normal order, so their contractions always vanish. Hence, the only non-vanishing contractions arising from the terms on the r. h. s. of (3.76) have the form

$$\big\langle \Omega, a(\overline{v}_{t,x'_i}) a^*(\overline{v}_{t,x_j})\Omega\big\rangle = \omega_{N,t}(x_j, x'_i)\,. \tag{3.78}$$

Since each contraction of the form (3.78) involves one x- and one x'-variable, the normal-ordered products in the non-vanishing contributions arising from Wick's theorem always have the same number of x- and x'-variables. So, all terms emerging from (3.76) after applying Wick's theorem have the form

$$\pm \Big\langle \mathcal{U}_N(t,0)\xi, : a^\sharp(w_1(\cdot, x'_{\sigma(1)})) \cdots a^\sharp(w_{k-j}(\cdot, x'_{\sigma(k-j)})) \\ \times a^\sharp(\eta_1(\cdot, x_{\pi(1)})) \cdots a^\sharp(\eta_{k-j}(\cdot, x_{\pi(k-j)})) : \mathcal{U}_N(t,0)\xi\Big\rangle \\ \times \omega_{N,t}(x_{\pi(k-j+1)}, x'_{\sigma(k-j+1)}) \cdots \omega_{N,t}(x_{\pi(k)}, x'_{\sigma(k)}) \tag{3.79}$$

where $j \le k$ denotes the number of contractions, $\pi, \sigma \in S_k$ are two appropriate permutations, and, for every $j = 1,\dots,k-j$, $w_j, \eta_j : L^2(\mathbb{R}^3) \to L^2(\mathbb{R}^3)$ are either the operator u_t or the operator $\overline{v}_t$ (the operators are identified with their integral kernels).

Step 2: Estimating (3.79) *in the case* $0 \le j < k$. We will use the shorthand notation $\mathbf{x}_k = (x_1,\dots,x_k) \in \mathbb{R}^{3k}$ and similarly $\mathbf{x}'_k = (x'_1,\dots,x'_k) \in \mathbb{R}^{3k}$. Let O be a Hilbert-Schmidt operator on $L^2(\mathbb{R}^{3k})$, with integral kernel $O(\mathbf{x}_k, \mathbf{x}'_k)$. Integrating (3.79) against $O(\mathbf{x}_k, \mathbf{x}'_k)$, we set

$$\mathrm{I} := \Big| \int \mathrm{d}\mathbf{x}_k \mathrm{d}\mathbf{x}'_k \, O(\mathbf{x}_k, \mathbf{x}'_k) \, \langle \mathcal{U}_N(t,0)\xi, : a^\sharp(w_1(\cdot, x'_{\sigma(1)})) \cdots a^\sharp(w_{k-j}(\cdot, x'_{\sigma(k-j)})) \\ \times a^\sharp(\eta_1(\cdot, x_{\pi(1)})) \cdots a^\sharp(\eta_{k-j}(\cdot, x_{\pi(k-j)})) : \mathcal{U}_N(t,0)\xi\rangle \\ \times \omega_{N,t}(x_{\pi(k-j+1)}, x'_{\sigma(k-j+1)}) \cdots \omega_{N,t}(x_{\pi(k)}, x'_{\sigma(k)}) \Big|. \tag{3.80}$$

We remark that

$$\mathrm{I} = \Big| \int \mathrm{d}\mathbf{x}_k \mathrm{d}\mathbf{x}'_k \left[\eta_1^{(\pi(1))} \cdots \eta_{k-j}^{(\pi(k-j))} \, O \, w_1^{(\sigma(1))} \cdots w_{k-j}^{(\sigma(k-j))}\right](\mathbf{x}_k, \mathbf{x}'_k) \\ \times \langle \mathcal{U}_N(t,0)\xi, : a^\sharp_{x'_{\sigma(1)}} \cdots a^\sharp_{x'_{\sigma(k-j)}} a^\sharp_{x_{\pi(1)}} \cdots a^\sharp_{x_{\pi(k-j)}} : \mathcal{U}_N(t,0)\xi\rangle \\ \times \omega_{N,t}(x_{\pi(k-j+1)}, x'_{\sigma(k-j+1)}) \cdots \omega_{N,t}(x_{\pi(k)}, x'_{\sigma(k)}) \Big|$$

where $\eta_\ell^{(\pi(\ell))}$ and $w_\ell^{(\sigma(\ell))}$ denote the one-particle operators η_ℓ and w_ℓ acting only on particle $\pi(\ell)$ and, respectively, on particle $\sigma(\ell)$. Notice that to be precise some of the operators

$\eta_\ell^{(\pi(\ell))}$ and $w_\ell^{(\sigma(\ell))}$ may need to be replaced by their transpose, their complex conjugate, or their hermitian conjugate. In the end, this change does not affect our analysis, since we will only need the bounds $\|\eta_j\|, \|w_j\| \leq 1$ for the operator norms. From Hölder's inequality, we get

$$\begin{aligned}
\mathrm{I} \leq & \, \|\eta_1^{(\pi(1))} \cdots \eta_{k-j}^{(\pi(k-j))} \, O \, w_1^{(\sigma(1))} \cdots w_{k-j}^{(\sigma(k-j))}\|_{\mathrm{HS}} \\
& \times \bigg(\int \mathrm{d}\mathbf{x}_k \mathrm{d}\mathbf{x}'_k \, \big| \langle \mathcal{U}_N(t,0)\xi, \, : a^\sharp_{x'_{\sigma(1)}} \cdots a^\sharp_{x'_{\sigma(k-j)}} a^\sharp_{x_{\pi(1)}} \cdots a^\sharp_{x_{\pi(k-j)}} : \mathcal{U}_N(t,0)\xi \rangle \big|^2 \\
& \qquad \times \big| \omega_{N,t}(x_{\pi(k-j+1)}, x'_{\sigma(k-j+1)}) \big|^2 \cdots \big| \omega_{N,t}(x_{\pi(k)}, , x'_{\sigma(k)}) \big|^2 \bigg)^{1/2} \\
\leq & \, \|O\|_{\mathrm{HS}} \|\omega_{N,t}\|_{\mathrm{HS}}^j \\
& \times \bigg(\int \mathrm{d}x_{\pi(1)} \cdots \mathrm{d}x_{\pi(k-j)} \mathrm{d}x'_{\sigma(1)} \cdots dx'_{\sigma(k-j)} \\
& \qquad \times \big| \langle \mathcal{U}_N(t,0)\xi, : a^\sharp_{x'_{\sigma(1)}} \cdots a^\sharp_{x'_{\sigma(k-j)}} a^\sharp_{x_{\pi(1)}} \cdots a^\sharp_{x_{\pi(k-j)}} : \mathcal{U}_N(t,0)\xi \rangle \big|^2 \bigg)^{1/2} .
\end{aligned}$$

Since $\|\omega_{N,t}\|_{\mathrm{HS}} = N^{1/2}$ and since the operators in the inner product are normal-ordered, we obtain

$$\mathrm{I} \leq C\|O\|_{\mathrm{HS}} N^{j/2} \langle \mathcal{U}_N(t,0)\xi, (\mathcal{N}+1)^{k-j} \mathcal{U}_N(t,0)\xi \rangle \, .$$

Hence, the contribution of each term with $j < k$ arising from (3.76) after applying Wick's theorem and integrating against a Hilbert-Schmidt operator O can be bounded by

$$C\|O\|_{\mathrm{HS}} \, N^{(k-1)/2} \langle \mathcal{U}_N(t,0)\xi, (\mathcal{N}+1)^k \mathcal{U}_N(t,0)\xi \rangle \, . \tag{3.81}$$

Step 3: Fully contracted terms, $j = k$. To finish the proof of Theorem 3.3.2, we consider the fully contracted terms with $j = k$ arising from (3.76) after expanding and applying Wick's theorem. Since $\langle \Omega, a(\overline{v}_{t,\cdot,y_i}) a^*(\overline{v}_{t,x_j}) \Omega \rangle = \omega_{N,t}(x_j, y_i)$ are the only nonzero contractions, only the term

$$a(\overline{v}_{t,y_k}) \cdots a(\overline{v}_{t,y_1}) a^*(\overline{v}_{t,x_1}) \cdots a^*(\overline{v}_{t,x_k})$$

on the r. h. s. of (3.76) produces a non-vanishing, fully contracted, contribution. From (3.78) and comparing with the definition (3.32), this contribution is given by

$$\sum_{\pi \in S_k} \mathrm{sgn}(\pi) \, \omega_{N,t}(x_1, x'_{\pi(1)}) \ldots \omega_{N,t}(x_k, x'_{\pi(k)}) = \omega_{N,t}^{(k)}(\mathbf{x}_k, \mathbf{x}'_k).$$

Combining the results of Step 2 and Step 3, we conclude that

$$\left| \mathrm{tr} \, O \left(\gamma_{N,t}^{(k)} - \omega_{N,t}^{(k)} \right) \right| \leq C N^{(k-1)/2} \|O\|_{\mathrm{HS}} \langle \mathcal{U}_N(t,0)\xi, (\mathcal{N}+1)^{k-1} \mathcal{U}_N(t,0)\xi \rangle$$

for every Hilbert-Schmidt operator O on $L^2(\mathbb{R}^{3k})$. Eq. (3.33) now follows from Theorem 3.4.2.

Step 4: Bound for the trace norm. Eq. (3.34) follows, similarly to (3.33), if we can show that, for any bounded operator O on $L^2(\mathbb{R}^{3k})$, the contribution (3.80) can be bounded by

$$\mathrm{I} \leq C\|O\| \, N^{\frac{k+j}{2}} \exp(c_1 \exp(c_2|t|)) \tag{3.82}$$

for all $\xi \in \mathcal{F}$ with $\langle \xi, \mathcal{N}^k \xi \rangle < \infty$, and the number of contractions $0 \leq j < k$. In fact, because of the fermionic symmetry of $\gamma^{(k)}_{N,t}$ and $\omega^{(k)}_{N,t}$, it is enough to establish (3.82) for all bounded O with the symmetry

$$O(x_{\pi(1)}, \dots, x_{\pi(k)}, x'_{\sigma(1)}, \dots, x'_{\sigma(k)}) = \mathrm{sgn}(\pi)\mathrm{sgn}(\sigma)\, O(x_1, \dots, x_k, x'_1, \dots x'_k)$$

for any permutations $\pi, \sigma \in S_k$. For such observables, (3.80) can be rewritten as

$$\begin{aligned}
\mathrm{I} = \Big| \int \mathrm{d}\mathbf{x}_k \mathrm{d}\mathbf{x}'_k\, O(\mathbf{x}_k, \mathbf{x}'_k) \, &\langle \mathcal{U}_N(t,0)\xi, : a^\sharp(w_1(\cdot, x'_1)) \cdots a^\sharp(w_{k-j}(\cdot, x'_{k-j})) \\
&\times a^\sharp(\eta_1(\cdot, x_1)) \cdots a^\sharp(\eta_{k-j}(\cdot, x_{k-j})) : \mathcal{U}_N(t,0)\xi \rangle \\
&\qquad \times \omega_{N,t}(x_{k-j+1}, x'_{k-j+1}) \cdots \omega_{N,t}(x_k, x'_k) \Big| \\
= \Big| \int \mathrm{d}\mathbf{x}_{k-j} \mathrm{d}\mathbf{x}'_{k-j} &\left[\eta^{(1)}_1 \cdots \eta^{(k-j)}_{k-j} \left(\mathrm{tr}_{k-j+1,\dots,k}\; O(1 \otimes \omega^{\otimes j}_{N,t}) \right) w^{(1)}_1 \cdots w^{(k-j)}_{k-j} \right] (\mathbf{x}_{k-j}, \mathbf{x}'_{k-j}) \\
&\times \langle \mathcal{U}_N(t,0)\xi, : a^\sharp_{x'_1} \cdots a^\sharp_{x'_{k-j}} a^\sharp_{x_1} \cdots a^\sharp_{x_{k-j}} : \mathcal{U}_N(t,0)\xi \rangle
\end{aligned}$$

where

$$\begin{aligned}
&\left(\mathrm{tr}_{k-j+1,\dots,k}\, O(1 \otimes \omega^{\otimes j}_{N,t}) \right) (\mathbf{x}_{k-j}, \mathbf{x}'_{k-j}) \\
&\qquad = \int \mathrm{d}x_{k-j+1} \mathrm{d}x'_{k-j+1} \dots \mathrm{d}x_k \mathrm{d}x'_k\, O(\mathbf{x}_k, \mathbf{x}'_k) \prod_{\ell = k-j+1}^{k} \omega_{N,t}(x_\ell, x'_\ell)
\end{aligned}$$

denotes the partial trace over the last j particles. Using Cauchy-Schwarz, we obtain

$$\begin{aligned}
\mathrm{I} \;&\leq\; \left\| \eta^{(1)}_1 \dots \eta^{(k-j)}_{k-j} \left(\mathrm{tr}_{k-j+1,\dots,k}\; O\,(1 \otimes \omega^{\otimes j}_{N,t}) \right) w^{(1)}_1 \dots w^{(k-j)}_{k-j} \right\|_{\mathrm{HS}} \left\| \mathcal{N}^{\frac{k-j}{2}} \mathcal{U}_N(t,0)\xi \right\|^2 \\
&\leq\; \left\| \eta^{(1)}_1 \dots \eta^{(k-j)}_{k-j} \right\|_{\mathrm{HS}} \left\| \mathrm{tr}_{k-j+1,\dots,k}\; O(1 \otimes \omega^{\otimes j}_{N,t}) \right\| \left\| \mathcal{N}^{\frac{k-j}{2}} \mathcal{U}_N(t,0)\xi \right\|^2 \\
&\leq\; N^{\frac{k-j}{2}} \left\| \mathrm{tr}_{k-j+1,\dots,k}\; O(1 \otimes \omega^{\otimes j}_{N,t}) \right\| \left\| \mathcal{N}^{\frac{k-j}{2}} \mathcal{U}_N(t,0)\xi \right\|^2
\end{aligned}$$

where in the second line we used that $\|w^{(j)}_j\| = 1$ for all $j = 1, \dots, k-j$. Since

$$\begin{aligned}
\left\| \mathrm{tr}_{k-j+1,\dots,k}\; O(1 \otimes \omega^{\otimes j}_{N,t}) \right\| \;&=\; \sup_{\substack{\phi, \varphi \in L^2(\mathbb{R}^{3(k-j)}) \\ \|\phi\| = \|\psi\| \leq 1}} \left| \left\langle \phi, \left(\mathrm{tr}_{k-j+1,\dots,k}\; O(1 \otimes \omega^{\otimes j}_{N,t}) \right) \varphi \right\rangle \right| \\
&=\; \sup_{\substack{\phi, \varphi \in L^2(\mathbb{R}^{3(k-j)}) \\ \|\phi\| = \|\psi\| \leq 1}} \left| \mathrm{tr}\; O \left(|\varphi\rangle\langle\phi| \otimes \omega^{\otimes j}_{N,t} \right) \right| \\
&\leq\; (\mathrm{tr}|\omega_{N,t}|)^j \, \|O\| \leq N^j \, \|O\| \,,
\end{aligned} \tag{3.83}$$

we get

$$\mathrm{I} \leq N^{\frac{k+j}{2}} \, \|O\| \, \left\| \mathcal{N}^{\frac{k-j}{2}} \mathcal{U}_N(t,0)\xi \right\|^2 ,$$

which, by Theorem 3.4.2, proves (3.82). □

3.6. Propagation of semiclassical structure

In this section we prove Proposition 3.4.4, which propagates the bounds (3.24) along the solution of the Hartree-Fock equation and plays a central role in our analysis.

Proof of Proposition 3.4.4. Let $\omega_{N,t}$ denote the solution of the Hartree-Fock equation (3.26). We define the (time-dependent) Hartree-Fock Hamiltonian

$$h_{\mathrm{HF}}(t) = -\varepsilon^2\Delta + (V * \rho_t) - X_t$$

where $\rho_t(x) = (1/N)\omega_{N,t}(x,x)$, $(V*\rho_t)$ is the operator of multiplication with $(V*\rho_t)(x)$ and X_t is the exchange operator, having the integral kernel $X_t(x,y) = V(x-y)\omega_{N,t}(x,y)$. Then $\omega_{N,t}$ satisfies the equation

$$i\varepsilon\partial_t\omega_{N,t} = [h_{\mathrm{HF}}(t), \omega_{N,t}].$$

Therefore, we obtain

$$\begin{aligned} i\varepsilon\frac{\mathrm{d}}{\mathrm{d}t}[e^{ip\cdot x}, \omega_{N,t}] &= [e^{ip\cdot x}, [h_{\mathrm{HF}}(t), \omega_{N,t}]] \\ &= [h_{\mathrm{HF}}(t), [e^{ip\cdot x}, \omega_{N,t}]] + [\omega_{N,t}, [h_{\mathrm{HF}}(t), e^{ip\cdot x}]] \\ &= [h_{\mathrm{HF}}(t), [e^{ip\cdot x}, \omega_{N,t}]] - [\omega_{N,t}, [\varepsilon^2\Delta, e^{ip\cdot x}]] - [\omega_{N,t}, [X_t, e^{ip\cdot x}]] \end{aligned} \tag{3.84}$$

where we used the Jacobi identity and the fact that $[\rho_t * V, e^{ipx}] = 0$. We compute

$$[\varepsilon^2\Delta, e^{ip\cdot x}] = i\varepsilon\nabla\cdot\varepsilon p e^{ip\cdot x} + e^{ip\cdot x}\varepsilon p\cdot i\varepsilon\nabla$$

and hence

$$\begin{aligned} [\omega_{N,t}, [\varepsilon^2\Delta, e^{ip\cdot x}]] &= [\omega_{N,t}, i\varepsilon\nabla\cdot\varepsilon p e^{ip\cdot x} + e^{ip\cdot x}\varepsilon p\cdot i\varepsilon\nabla] \\ &= [\omega_{N,t}, i\varepsilon\nabla]\cdot\varepsilon p e^{ip\cdot x} + i\varepsilon^2\nabla\cdot p[\omega_{N,t}, e^{ip\cdot x}] \\ &\quad + \varepsilon p e^{ip\cdot x}[\omega_{N,t}, i\varepsilon\nabla] + [\omega_{N,t}, e^{ip\cdot x}]i\varepsilon^2\nabla\cdot p\,. \end{aligned}$$

From (3.84) we find

$$\begin{aligned} i\varepsilon\frac{\mathrm{d}}{\mathrm{d}t}[e^{ip\cdot x}, \omega_{N,t}] &= A(t)[e^{ip\cdot x}, \omega_{N,t}] - [e^{ip\cdot x}, \omega_{N,t}]B(t) \\ &\quad - \varepsilon p e^{ip\cdot x}[\omega_{N,t}, i\varepsilon\nabla] - [\omega_{N,t}, i\varepsilon\nabla]\cdot\varepsilon p e^{ip\cdot x} - [\omega_{N,t}, [X_t, e^{ip\cdot x}]] \end{aligned}$$

where we defined the time dependent operators

$$A(t) = h_{\mathrm{HF}}(t) + i\varepsilon^2\nabla\cdot p \quad \text{and} \quad B(t) = h_{\mathrm{HF}}(t) - i\varepsilon^2\nabla\cdot p\,.$$

Observe that $A(t)$ and $B(t)$ are selfadjoint for every $t\in\mathbb{R}$ (the factor $\pm i\varepsilon^2 p\cdot\nabla$ can be interpreted as originating from a constant vector potential). They generate two unitary evolutions $\mathcal{U}_1(t,s)$ and $\mathcal{U}_2(t,s)$ satisfying

$$i\varepsilon\partial_t\mathcal{U}_1(t,s) = A(t)\mathcal{U}_1(t,s) \quad \text{and} \quad i\varepsilon\partial_t\mathcal{U}_2(t,s) = B(t)\mathcal{U}_2(t,s)$$

with the initial conditions $\mathcal{U}_1(s,s) = \mathcal{U}_2(s,s) = 1$. We observe that, by definition of the unitary maps $\mathcal{U}_1(t,s)$ and $\mathcal{U}_2(t,s)$,

$$\begin{aligned} &i\varepsilon\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{U}_1^*(t,0)[e^{ip\cdot x}, \omega_{N,t}]\mathcal{U}_2(t,0) \\ &\quad = \mathcal{U}_1^*(t,0)\left\{-A(t)[e^{ip\cdot x}, \omega_{N,t}] + [e^{ip\cdot x}, \omega_{N,t}]B(t) + i\varepsilon\frac{\mathrm{d}}{\mathrm{d}t}[e^{ip\cdot x}, \omega_{N,t}]\right\}\mathcal{U}_2(t,0) \\ &\quad = -\mathcal{U}_1^*(t,0)\left\{\varepsilon p e^{ip\cdot x}[\omega_{N,t}, i\varepsilon\nabla] + [\omega_{N,t}, i\varepsilon\nabla]\cdot\varepsilon p e^{ip\cdot x} + [\omega_{N,t}, [X_t, e^{ip\cdot x}]]\right\}\mathcal{U}_2(t,0). \end{aligned}$$

Hence

$$
\begin{aligned}
&\mathcal{U}_1^*(t,0)[e^{ip\cdot x},\omega_{N,t}]\,\mathcal{U}_2(t,0)\\
&= [e^{ip\cdot x},\omega_N]\\
&\quad + \frac{i}{\varepsilon}\int_0^t \mathrm{d}s\,\mathcal{U}_1^*(s,0)\big\{\varepsilon p e^{ip\cdot x}[\omega_{N,s}, i\varepsilon\nabla] + [\omega_{N,s}, i\varepsilon\nabla]\cdot \varepsilon p e^{ip\cdot x} + [\omega_{N,s},[X_s, e^{ip\cdot x}]]\big\}\mathcal{U}_2(s,0)
\end{aligned}
$$

and therefore

$$
\begin{aligned}
&[e^{ip\cdot x},\omega_{N,t}]\\
&\quad = \mathcal{U}_1(t,0)[e^{ip\cdot x},\omega_N]\,\mathcal{U}_2^*(t,0)\\
&\qquad + \frac{i}{\varepsilon}\int_0^t \mathrm{d}s\,\mathcal{U}_1(t,s)\big\{\varepsilon p e^{ip\cdot x}[\omega_{N,s}, i\varepsilon\nabla] + [\omega_{N,s}, i\varepsilon\nabla]\cdot \varepsilon p e^{ip\cdot x} + [\omega_{N,s},[X_s, e^{ip\cdot x}]]\big\}\mathcal{U}_2(s,t).
\end{aligned}
$$

Taking the trace norm, we find

$$
\operatorname{tr}|[e^{ip\cdot x},\omega_{N,t}]| \leq \operatorname{tr}|[e^{ip\cdot x},\omega_N]| + 2|p|\int_0^t \mathrm{d}s\ \operatorname{tr}|[\varepsilon\nabla,\omega_{N,s}]| + \frac{1}{\varepsilon}\int_0^t \mathrm{d}s\,\operatorname{tr}|[\omega_{N,s},[X_s,e^{ip\cdot x}]]|. \tag{3.85}
$$

To control the contribution of the last term, we observe that

$$
X_s(x,y) = \frac{1}{N}V(x-y)\omega_{N,s}(x,y) = \frac{1}{N}\int \mathrm{d}q\,\widehat{V}(q)e^{iq\cdot(x-y)}\omega_{N,s}(x,y) = \frac{1}{N}\int \mathrm{d}q\,\widehat{V}(q)\omega_{q,t}(x,y)
$$

where we defined the operator $\omega_{q,t} = e^{iq\cdot x}\omega_{N,t}e^{-iq\cdot x}$ (here x indicates the multiplication operator). Hence, we get

$$
[\omega_{N,t},[X_t,e^{ip\cdot x}]] = \frac{1}{N}\int \mathrm{d}q\,\widehat{V}(q)[\omega_{N,t},[\omega_{q,t},e^{ip\cdot x}]]
$$

and therefore, using $\|\omega_{N,t}\| \leq 1$,

$$
\begin{aligned}
\operatorname{tr}|[\omega_{N,t},[X_t,e^{ip\cdot x}]]| &\leq \frac{1}{N}\int \mathrm{d}q|\widehat{V}(q)|\ \operatorname{tr}|[\omega_{N,t},[\omega_{q,t},e^{ip\cdot x}]]|\\
&\leq \frac{2}{N}\int \mathrm{d}q|\widehat{V}(q)|\ \operatorname{tr}|[\omega_{q,t},e^{ip\cdot x}]|\\
&\leq \frac{2}{N}\left(\int \mathrm{d}q|\widehat{V}(q)|\right)\ \operatorname{tr}|[\omega_{N,t},e^{ip\cdot x}]|
\end{aligned}
$$

where in the last line we used that $[\omega_{q,t},e^{ipx}] = e^{iqx}[\omega_{N,t},e^{ipx}]e^{-iqx}$. From (3.85), we conclude that

$$
\operatorname{tr}|[e^{ip\cdot x},\omega_{N,t}]| \leq \operatorname{tr}|[e^{ip\cdot x},\omega_N]| + 2|p|\int_0^t \mathrm{d}s\ \operatorname{tr}|[\varepsilon\nabla,\omega_{N,s}]| + \frac{C}{N\varepsilon}\int_0^t \mathrm{d}s\,\operatorname{tr}|[e^{ip\cdot x},\omega_{N,s}]| \tag{3.86}
$$

and therefore, from (3.49), we find

$$
\begin{aligned}
\sup_p \frac{1}{1+|p|}\operatorname{tr}|[e^{ip\cdot x},\omega_{N,t}]| &\leq C\varepsilon N + 2\int_0^t \mathrm{d}s\ \operatorname{tr}|[\varepsilon\nabla,\omega_{N,s}]|\\
&\quad + C\int_0^t \mathrm{d}s\ \sup_p \frac{1}{1+|p|}\operatorname{tr}|[e^{ip\cdot x},\omega_{N,s}]|.
\end{aligned} \tag{3.87}
$$

Next, we need to control the growth of $\operatorname{tr}|[\varepsilon\nabla, \omega_{N,t}]|$. Consider

$$\begin{aligned} i\varepsilon\frac{\mathrm{d}}{\mathrm{d}t}[\varepsilon\nabla, \omega_{N,t}] =& [\varepsilon\nabla, [h_{\mathrm{HF}}(t), \omega_{N,t}]] \\ =& [h_{\mathrm{HF}}(t), [\varepsilon\nabla, \omega_{N,t}]] + [\omega_{N,t}, [h_{\mathrm{HF}}(t), \varepsilon\nabla]] \\ =& [h_{\mathrm{HF}}(t), [\varepsilon\nabla, \omega_{N,t}]] + [\omega_{N,t}, [V * \rho_t, \varepsilon\nabla]] - [\omega_{N,t}, [X_t, \varepsilon\nabla]] \,. \end{aligned}$$

As before, the first term on the r. h. s. can be eliminated by an appropriate unitary conjugation. Denote namely by $\mathcal{U}_3(t,s)$ the two-parameter unitary group satisfying

$$i\varepsilon\partial_t \mathcal{U}_3(t,s) = h_{\mathrm{HF}}(t)\mathcal{U}_3(t,s)$$

and $\mathcal{U}_3(s,s) = 1$. Then we compute

$$\begin{aligned} i\varepsilon\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{U}_3^*(t,0)[\varepsilon\nabla, \omega_{N,t}]\mathcal{U}_3(t,0) &= \mathcal{U}_3^*(t,0)\left\{-[h_{\mathrm{HF}}(t), [\varepsilon\nabla, \omega_{N,t}]] + i\varepsilon\frac{\mathrm{d}}{\mathrm{d}t}[\varepsilon\nabla, \omega_{N,t}]\right\}\mathcal{U}_3(t,0) \\ &= \mathcal{U}_3^*(t,0)\left\{[\omega_{N,t}, [V * \rho_t, \varepsilon\nabla]] - [\omega_{N,t}, [X_t, \varepsilon\nabla]]\right\}\mathcal{U}_3(t,0). \end{aligned}$$

This gives

$$\begin{aligned} [\varepsilon\nabla, \omega_{N,t}] =& \mathcal{U}_3(t,0)[\varepsilon\nabla, \omega_N]\mathcal{U}_3^*(t,0) \\ &+ \frac{1}{i\varepsilon}\int_0^t \mathrm{d}s\, \mathcal{U}_3(t,s)\left\{[\omega_{N,s}, [V * \rho_s, \varepsilon\nabla]] - [\omega_{N,s}, [X_s, \varepsilon\nabla]]\right\}\mathcal{U}_3(s,t) \end{aligned}$$

and therefore

$$\begin{aligned} \operatorname{tr}|[\varepsilon\nabla, \omega_{N,t}]| \leq& \operatorname{tr}|[\varepsilon\nabla, \omega_N]| \\ &+ \frac{1}{\varepsilon}\int_0^t \mathrm{d}s\, \operatorname{tr}|[\omega_{N,s}, [V * \rho_s, \varepsilon\nabla]]| + \frac{1}{\varepsilon}\int_0^t \mathrm{d}s\, \operatorname{tr}|[\omega_{N,s}, [X_s, \varepsilon\nabla]]|. \end{aligned} \tag{3.88}$$

The second term on the r. h. s. can be controlled by

$$\begin{aligned} \operatorname{tr}|[\omega_{N,s}, [V * \rho_s, \varepsilon\nabla]]| &= \varepsilon\, \operatorname{tr}|[\omega_{N,s}, \nabla(V * \rho_s)]| \\ &\leq \varepsilon \int \mathrm{d}q\, |\widehat{V}(q)||q||\widehat{\rho}_s(q)|\, \operatorname{tr}|[\omega_{N,s}, e^{iq\cdot x}]| \\ &\leq \varepsilon\left(\int \mathrm{d}q\, |\widehat{V}(q)|(1+|q|)^2\right)\sup_q \frac{1}{1+|q|}\operatorname{tr}|[\omega_{N,s}, e^{iq\cdot x}]| \end{aligned}$$

where we used the bound $\|\widehat{\rho}_s\|_\infty \leq \|\rho_s\|_1 = 1$. As for the last term on the r. h. s. of (3.88), we note that

$$[\omega_{N,s}, [X_s, \varepsilon\nabla]] = \frac{1}{N}\int \mathrm{d}q\, \widehat{V}(q)[\omega_{N,s}, [\omega_{q,s}, \varepsilon\nabla]]$$

where, as above, we set $\omega_{q,s} = e^{iq\cdot x}\omega_{N,s}e^{-iq\cdot x}$. Hence, we obtain

$$\begin{aligned} \operatorname{tr}|[\omega_{N,s}, [X_s, \varepsilon\nabla]]| &\leq \frac{2}{N}\int \mathrm{d}q\, |\widehat{V}(q)|\, \operatorname{tr}|[\omega_{q,s}, \varepsilon\nabla]| \\ &\leq \frac{2}{N}\left(\int \mathrm{d}q\, |\widehat{V}(q)|\right)\operatorname{tr}|[\omega_{N,s}, \varepsilon\nabla]| \end{aligned}$$

where in the last inequality we used that

$$[\omega_{q,s}, \varepsilon\nabla] = e^{iqx}[\omega_{N,s}, \varepsilon(\nabla + iq)]e^{-iqx} = e^{iqx}[\omega_{N,s}, \varepsilon\nabla]e^{-iqx} \,.$$

From (3.88), we conclude that

$$\operatorname{tr}|[\varepsilon\nabla, \omega_{N,t}]| \leq C\varepsilon N + C\int_0^t \mathrm{d}s \sup_q \frac{1}{1+|q|} \operatorname{tr}|[\omega_{N,s}, e^{iq\cdot x}]| + C\int_0^t \mathrm{d}s \operatorname{tr}|[\omega_{N,s}, \varepsilon\nabla]|.$$

Summing up the last equation with (3.87) and applying Grönwall's lemma, we find constants $C, c > 0$ such that

$$\begin{aligned} \sup_p \frac{1}{1+|p|} \operatorname{tr}|[e^{ip\cdot x}, \omega_{N,t}]| &\leq C\varepsilon N \exp(c|t|), \\ \operatorname{tr}|[\varepsilon\nabla, \omega_{N,t}] &\leq C\varepsilon N \exp(c|t|). \end{aligned}$$

□

3.A. Comparison between Hartree and Hartree-Fock dynamics

In the next proposition we show that, under the assumptions of Theorem 3.3.1, the solution $\omega_{N,t}$ of the Hartree-Fock equation (3.26) is well-approximated by the solution $\widetilde{\omega}_{N,t}$ of the Hartree equation (3.31). Since we can show that the difference $\omega_{N,t} - \widetilde{\omega}_{N,t}$ remains of order one in N for all fixed times $t \in \mathbb{R}$, this result implies that all bounds in Theorem 3.3.1 remain true if we replace $\omega_{N,t}$ by $\widetilde{\omega}_{N,t}$.

Proposition 3.A.1. *Assume that the interaction potential $V \in L^1(\mathbb{R}^3)$ satisfies (3.23) and that the sequence ω_N of orthogonal projections on $L^2(\mathbb{R}^3)$ with $\operatorname{tr}\omega_N = N$ satisfies (3.24). Let $\omega_{N,t}$ denote the solution of the Hartree-Fock equation*

$$i\varepsilon\partial_t\omega_{N,t} = \left[-\varepsilon^2\Delta + (V * \rho_t) - X_t, \omega_{N,t}\right]$$

and $\widetilde{\omega}_{N,t}$ the solution of the Hartree equation

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

with initial data $\omega_{N,t=0} = \widetilde{\omega}_{N,t=0} = \omega_N$ (recall here that $\rho_t(x) = N^{-1}\omega_{N,t}(x,x)$, $\widetilde{\rho}_t(x) = N^{-1}\widetilde{\omega}_{N,t}(x,x)$ and $X_t(x,y) = N^{-1}V(x-y)\omega_{N,t}(x,y)$). Then there exist constants $C, c_1, c_2 > 0$ such that

$$\operatorname{tr}|\omega_{N,t} - \widetilde{\omega}_{N,t}| \leq C\exp(c_1\exp(c_2|t|))$$

for all $t \in \mathbb{R}$.

Proof. Let $\mathcal{W}(t,s)$ be the unitary dynamics generated by the Hartree Hamiltonian $h_H(t) = -\varepsilon^2\Delta + (V * \widetilde{\rho}_t)$. In other words, $\mathcal{W}(s,s) = 1$ for all $s \in \mathbb{R}$ and

$$i\varepsilon\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{W}(t,s) = h_H(t)\mathcal{W}(t,s)\,.$$

Then, we have

$$\begin{aligned} &i\varepsilon\partial_t\mathcal{W}^*(t,0)\widetilde{\omega}_{N,t}\mathcal{W}(t,0) = 0\,, \\ &i\varepsilon\partial_t\mathcal{W}^*(t,0)\omega_{N,t}\mathcal{W}(t,0) = \mathcal{W}^*(t,0)\left(\left[V * \left(\rho_t - \widetilde{\rho}_t\right), \omega_{N,t}\right] - \left[X_t, \omega_t\right]\right)\mathcal{W}(t,0). \end{aligned}$$

Integrating over time, we end up with

$$\begin{aligned} \widetilde{\omega}_{N,t} &= \mathcal{W}(t,0)\omega_N\mathcal{W}^*(t,0)\,, \\ \omega_{N,t} &= \mathcal{W}(t,0)\omega_N\mathcal{W}^*(t,0) \\ &\quad - \frac{i}{\varepsilon}\int_0^t \mathrm{d}s\,\mathcal{W}(t,s)\left(\left[V * \left(\widetilde{\rho}_s - \rho_s\right), \omega_{N,s}\right] - \left[X_s, \omega_{N,s}\right]\right)\mathcal{W}^*(t,s) \end{aligned}$$

and thus

$$\operatorname{tr}|\omega_{N,t}-\widetilde{\omega}_{N,t}| \leq \frac{1}{\varepsilon}\int_0^t \mathrm{d}s \left\{\operatorname{tr}|[V*(\widetilde{\rho}_s-\rho_s),\omega_{N,s}]| + \operatorname{tr}|[X_s,\omega_{N,s}]|\right\} =: \mathrm{I}+\mathrm{II}. \tag{3.89}$$

Let us first estimate II. We get

$$\begin{aligned}
\mathrm{II} &= \frac{1}{\varepsilon}\int_0^t \mathrm{d}s \operatorname{tr}|[X_s,\omega_{N,s}]| \\
&\leq \frac{1}{\varepsilon N}\int_0^t \mathrm{d}s \int \mathrm{d}p\, |\widehat{V}(p)| \operatorname{tr}\left|\left[e^{ip\cdot x}\omega_{N,s}e^{-ip\cdot x},\omega_{N,s}\right]\right| \\
&\leq \frac{2}{\varepsilon N}\int_0^t \mathrm{d}s \int \mathrm{d}p\, |\widehat{V}(p)| \operatorname{tr}\left|\left[e^{ip\cdot x},\omega_{N,s}\right]\right| \\
&\leq C\exp(c|t|),
\end{aligned} \tag{3.90}$$

where in the last step we used Proposition 3.4.4 ($e^{ip\cdot x}$ denotes here the multiplication operator). We are left with I. Writing

$$V*(\widetilde{\rho}_s-\rho_s)(x) = \int \mathrm{d}p\, \widehat{V}(p)\left(\widehat{\widetilde{\rho}}_s(p)-\widehat{\rho}_s(p)\right)e^{ip\cdot x}$$

we find

$$\begin{aligned}
\mathrm{I} &\leq \frac{1}{\varepsilon}\int_0^t \mathrm{d}s \int \mathrm{d}p\, |\hat{V}(p)| \left|\widehat{\widetilde{\rho}}_s(p)-\widehat{\rho}_s(p)\right| \operatorname{tr}\left|\left[e^{ip\cdot x},\omega_{N,s}\right]\right| \\
&\leq CN\exp(c|t|)\int_0^t \mathrm{d}s \sup_{p\in\mathbb{R}^3}\left|\widehat{\rho}_s(p)-\widehat{\widetilde{\rho}}_s(p)\right| \\
&\leq C\exp(c|t|)\int_0^t \mathrm{d}s \operatorname{tr}|\omega_{N,s}-\widetilde{\omega}_{N,s}|
\end{aligned} \tag{3.91}$$

where in the second inequality we used again Proposition 3.4.4, while in the last inequality we used the bound

$$\left|\widehat{\rho}_s(p)-\widehat{\widetilde{\rho}}_s(p)\right| = \frac{1}{N}\left|\operatorname{tr} e^{ip\cdot x}(\omega_{N,s}-\widetilde{\omega}_{N,s})\right| \leq \frac{1}{N}\operatorname{tr}|\omega_{N,s}-\widetilde{\omega}_{N,s}|.$$

Inserting (3.90), (3.91) into (3.89), and applying the Grönwall lemma, we get

$$\operatorname{tr}|\omega_{N,t}-\widetilde{\omega}_{N,t}| \leq C\exp(c_1\exp(c_2|t|)) \tag{3.92}$$

for some C, c_1, c_2 only depending on the potential V. □

4. Mean-field Evolution of Fermions with Relativistic Dispersion

In this chapter we provide an extension of the derivation of the Hartree-Fock equation in Chapter 3 to the analogous model with relativistic dispersion law. This chapter is based on the article [BPS13b].

We use the fermionic convention $\operatorname{tr} \gamma_N^{(k)} = \frac{N!}{(N-k)!}$ for the normalization of density matrices, see Section 1.A.

4.1. Introduction

As in the previous chapter, we are interested in the dynamics of a system of N fermions moving in three spatial dimensions, but now with a relativistic dispersion law. In units where the Planck constant and the speed of light are $\hbar = c = 1$, the evolution is governed by the Schrödinger equation

$$i\partial_t \psi_{N,t} = \left[\sum_{j=1}^{N} \sqrt{-\Delta_{x_j} + m^2} + \lambda \sum_{i<j}^{N} V(x_i - x_j) \right] \psi_{N,t} \tag{4.1}$$

for the wave function $\psi_{N,t} \in L^2_a(\mathbb{R}^{3N})$, in accordance with Pauli's principle. The constant $m > 0$ is the mass and $\lambda \in \mathbb{R}$ a coupling constant.

We are interested in the mean-field limit, characterized by $N \gg 1$ and weak interaction $|\lambda| \ll 1$. Notice that in contrast to the non-relativistic case, the kinetic energy of N fermions in a volume of order one is only of order $N^{4/3}$, so that we take $\lambda N^{2/3} = 1$ fixed. For technical reasons, we also consider large masses m, keeping $mN^{-1/3} = m_0$ fixed in the limit. Introducing the semiclassical parameter $\varepsilon = N^{-1/3}$, we can then rewrite (4.1) as

$$i\varepsilon\partial_t \psi_{N,t} = \left[\sum_{j=1}^{N} \sqrt{-\varepsilon^2\Delta_{x_j} + m_0^2} + \frac{1}{N} \sum_{i<j}^{N} V(x_i - x_j) \right] \psi_{N,t}. \tag{4.2}$$

Unlike in the non-relativistic case, the velocity of particles (think of the group velocity for the free evolution) with relativistic dispersion is always bounded by one, so it is physically plausible that we have not rescaled time.

From the physical point of view, it is important to understand the dynamics of initial data which can be easily prepared in labs. Hence, it makes sense to study the evolution of initial data close to the ground state of a Hamiltonian of the form

$$H_N^{\text{trap}} = \sum_{j=1}^{N} \left[\sqrt{-\varepsilon^2\Delta_{x_j} + m_0^2} + V_{\text{ext}}(x_j) \right] + \frac{1}{N} \sum_{i<j}^{N} V(x_i - x_j), \tag{4.3}$$

where $V_{\text{ext}} : \mathbb{R}^3 \to \mathbb{R}$ is an external potential, trapping the particles in a volume of order one. It is expected that the ground state of (4.3) can be approximated by the Slater determinant with one-particle reduced density ω_N minimizing the (relativistic) Hartree-Fock energy functional

$$\begin{aligned}\mathcal{E}_{\text{HF}}(\omega_N) = \; &\operatorname{tr}\left[\sqrt{-\varepsilon^2\Delta + m_0^2} + V_{\text{ext}}\right]\omega_N \\ &+ \frac{1}{2N}\int \mathrm{d}x\mathrm{d}y\, V(x-y)\left(\omega_N(x,x)\omega_N(y,y) - |\omega_N(x,y)|^2\right)\end{aligned} \tag{4.4}$$

among all orthogonal projections ω_N on $L^2(\mathbb{R}^3)$ with $\operatorname{tr}\omega_N = N$ (recall that the reduced density of an N-particle Slater determinant is such an orthogonal projection).

In Chapter 3, we considered the evolution of N non-relativistic fermions, governed by the Schrödinger equation

$$i\varepsilon\partial_t\psi_{N,t} = \left[\sum_{j=1}^{N} -\frac{\varepsilon^2\Delta_{x_j}}{2m_0} + \frac{1}{N}\sum_{i<j}^{N} V(x_i - x_j)\right]\psi_{N,t}. \tag{4.5}$$

In particular, we were interested in the evolution of initial data close to Slater determinants minimizing a non-relativistic Hartree-Fock energy (similar to (4.4), but with a non-relativistic dispersion law). To this end, we argued that minimizers of the Hartree-Fock energy satisfy semiclassical commutator estimates of the form

$$\operatorname{tr}|[x,\omega_N]| \le CN\varepsilon, \qquad \text{and} \qquad \operatorname{tr}|[\varepsilon\nabla,\omega_N]| \le CN\varepsilon, \tag{4.6}$$

where x denotes the position operator (i. e. multiplication with x). Motivated by this observation, we assumed initial data to be close to Slater determinants with reduced one-particle density satisfying (4.6). For such initial data[1], we proved that for sufficiently regular interaction potential V the many-body evolution can be approximated by the time-dependent non-relativistic Hartree-Fock equation

$$i\varepsilon\partial_t\omega_{N,t} = \left[-\frac{\varepsilon^2\Delta}{2m_0} + (V*\rho_t) - X_t, \omega_{N,t}\right]. \tag{4.7}$$

Here $\rho_t(x) = N^{-1}\omega_{N,t}(x,x)$ is the density of particles close to $x \in \mathbb{R}^3$ and X_t is the exchange operator, having the integral kernel $X_t(x,y) = N^{-1}V(x-y)\omega_{N,t}(x,y)$.

In this chapter we proceed analogously but for fermions with relativistic dispersion. Similar to the non-relativistic case, the arguments presented in Chapter 3 and semiclassical analysis suggest that (approximate) minimizers of the Hartree-Fock energy (4.4) satisfy the commutator bounds (4.6). For this reason, we will consider the evolution (4.2) for initial data close to Slater determinants, with reduced density ω_N satisfying (4.6). For such initial data, we will show in Theorem 4.2.1 below that the solution of the Schrödinger equation (4.2) stays close to a Slater determinant with one-particle reduced density evolving according to the relativistic Hartree-Fock equation

$$i\varepsilon\partial_t\omega_{N,t} = \left[\sqrt{-\varepsilon^2\Delta + m_0^2} + (V*\rho_t) - X_t, \omega_{N,t}\right], \tag{4.8}$$

[1] In fact, instead of assuming $\operatorname{tr}|[x,\omega_N]| \le CN\varepsilon$, we only imposed the weaker condition $\operatorname{tr}|[e^{ip\cdot x},\omega_N]| \le CN(1+|p|)\varepsilon$, for all $p \in \mathbb{R}$. However, here we find it more convenient to work with $[x,\omega_N]$.

where, like in (4.7), $\rho_t(x) = N^{-1}\omega_{N,t}(x,x)$ and $X_t(x,y) = N^{-1}V(x-y)\omega_{N,t}(x,y)$.

For initial data minimizing the Hartree-Fock energy (4.4), the typical momentum of the particles is of order ε^{-1}, meaning that the expectation of $\varepsilon|\nabla|$ is typically of order one. Hence, for $m_0 \gg 1$, we can expand the relativistic dispersion as

$$\sqrt{-\varepsilon^2\Delta + m_0^2} = m_0\sqrt{1 - \frac{\varepsilon^2\Delta}{m_0^2}} \simeq m_0\left(1 - \frac{\varepsilon^2\Delta}{2m_0^2}\right) = m_0 + \frac{-\varepsilon^2\Delta}{2m_0}.$$

Since the constant m_0 only produces a harmless phase, this implies that in the limit of large m_0, one can approximate the solutions of the relativistic Schrödinger equation (4.2) and of the relativistic Hartree-Fock equation (4.8) by the solutions of the corresponding non-relativistic equations (4.5) and, respectively, (4.7). On the other hand, for fixed m_0 of order one as we consider it here, the relativistic dynamics cannot be compared to the non-relativistic dynamics.

If we start from (4.1) and consider the limit of large $N \gg 1$ and weak interaction $\lambda N^{2/3} = 1$ without scaling the mass m, we obtain a Schrödinger equation like (4.2), but with m_0 replaced by εm (recall that $\varepsilon = N^{-1/3}$). In the limit $N \gg 1$, this evolution can be compared with the massless relativistic Schrödinger equation

$$i\varepsilon\partial_t\psi_{N,t} = \left[\sum_{j=1}^{N}\varepsilon|\nabla_{x_j}| + \frac{1}{N}\sum_{i<j}^{N}V(x_i - x_j)\right]\psi_{N,t}. \tag{4.9}$$

In this case, we expect the dynamics of initial data close to Slater determinants satisfying the commutator estimates (4.6) to be approximated by the Hartree-Fock equation

$$i\varepsilon\partial_t\omega_{N,t} = \Big[\varepsilon|\nabla| + (V*\rho_t) - X_t, \omega_{N,t}\Big]. \tag{4.10}$$

For technical reasons, we do not consider this case in the present work. Proving the convergence of (4.9) towards (4.10) remains an interesting open problem.

4.2. Main result and sketch of its proof

To state our main theorem, we switch to the Fock space representation. In terms of the operator-valued distributions a_x^*, a_x we define the Hamilton operator

$$\mathcal{H}_N = \int dx\, a_x^*\sqrt{-\varepsilon^2\Delta_x + m_0^2}\, a_x + \frac{1}{2N}\int \mathrm{d}x\mathrm{d}y\, V(x-y)a_x^*a_y^*a_ya_x \tag{4.11}$$

on fermionic Fock space $\mathcal{F}$. As in the other models discussed, $\mathcal{H}_N$ commutes with the number of particles operator $\mathcal{N}$. When restricted to the N-particle sector, $\mathcal{H}_N$ agrees with the Hamiltonian generating the evolution (4.2).

Let ω_N be an orthogonal projection on $L^2(\mathbb{R}^3)$, with tr $\omega_N = N$. Then there are orthonormal functions $f_1, \dots, f_N \in L^2(\mathbb{R}^3)$ with $\omega_N = \sum_{j=1}^N |f_j\rangle\langle f_j|$. We complete $f_1, \dots, f_N$ to an orthonormal basis $(f_j)_{j\in\mathbb{N}}$ of $L^2(\mathbb{R}^3)$. We introduce a (unitary) particle-hole transformation $R_{\omega_N} : \mathcal{F} \to \mathcal{F}$ by setting as before

$$R_{\omega_N}\Omega = a^*(f_1)\cdots a^*(f_N)\Omega, \tag{4.12}$$

a Slater determinant with reduced density ω_N. Moreover we require that

$$R^*_{\omega_N} a(f_i) R_{\omega_N} = \begin{cases} a(f_i) & \text{if } i > N \\ a^*(f_i) & \text{if } i \leq N. \end{cases} \tag{4.13}$$

The operator $R^*_{\omega_N}$ implements a fermionic Bogoliubov transformation on $\mathcal{F}$. We consider the time evolution of initial data of the form $R_{\omega_N}\xi_N$, for a $\xi_N \in \mathcal{F}$ with $\langle \xi_N, \mathcal{N}\xi_N\rangle \leq C$ uniformly in N (i. e. $R_{\omega_N}\xi_N$ is close to the N-particle Slater determinant $R_{\omega_N}\Omega$).

We are now ready to state our main theorem.

Theorem 4.2.1. *Let $V \in L^1(\mathbb{R}^3)$ with*

$$\int |\widehat{V}(p)|(1+|p|)^2 \, dp < \infty. \tag{4.14}$$

Let ω_N be a sequence of orthogonal projections on $L^2(\mathbb{R}^3)$ with $\operatorname{tr} \omega_N = N$, satisfying the semiclassical commutator bounds (4.6). Let ξ_N be a sequence in $\mathcal{F}$ with $\langle \xi_N, \mathcal{N}\xi_N\rangle \leq C$ uniformly in N. We consider the time evolution

$$\psi_{N,t} = e^{-i\mathcal{H}_N t/\varepsilon} R_{\omega_N}\xi_N \tag{4.15}$$

generated by the Hamiltonian (4.11), with $\varepsilon = N^{-1/3}$ and with a fixed $m_0 > 0$. Here R_{ω_N} denotes the unitary implementor of a Bogoliubov transformation defined in (4.13) and (4.12). Let $\gamma^{(1)}_{N,t}$ be the one-particle reduced density associated with $\psi_{N,t}$. Then there exist constants $c, C > 0$ such that

$$\operatorname{tr} \left| \gamma^{(1)}_{N,t} - \omega_{N,t} \right|^2 \leq C \exp(c \exp(c|t|)) \tag{4.16}$$

where $\omega_{N,t}$ is the solution of the time-dependent Hartree-Fock equation (4.8) with initial data $\omega_{N,t=0} = \omega_N$.

Remarks:

(i) The bound (4.16) should be compared with $\operatorname{tr}(\gamma^{(1)}_{N,t})^2$ and $\operatorname{tr}(\omega_{N,t})^2$, which are both of order N. The N-dependence in (4.16) is optimal, since one can easily find a sequence $\xi_N \in \mathcal{F}$ with $\langle \xi_N, \mathcal{N}\xi_N \rangle \leq C$ such that $\gamma^{(1)}_{N,0} - \omega_{N,0} = \mathcal{O}(1)$ (for example, just take $\xi_N = a^*(f_{N+1})\Omega$).

(ii) As in Chapter 3, under the additional assumptions that we have $\mathrm{d}\Gamma(\omega_N)\xi_N = 0$ and $\langle \xi_N, \mathcal{N}^2 \xi_N \rangle \leq C$ for all $N \in \mathbb{N}$, we find the trace norm estimate

$$\operatorname{tr}|\gamma^{(1)}_{N,t} - \omega_{N,t}| \leq C N^{1/6} \exp(c \exp(c|t|)). \tag{4.17}$$

(iii) We can also control the convergence of higher order reduced densities. If $\gamma^{(k)}_{N,t}$ denotes the k-particles reduced density associated with (4.15), and if $\omega^{(k)}_{N,t}$ is the antisymmetric tensor product of k copies of the solution $\omega_{N,t}$ of the Hartree-Fock equation (4.8), we find, similarly to 3.3.2,

$$\operatorname{tr} \left| \gamma^{(k)}_{N,t} - \omega^{(k)}_{N,t} \right|^2 \leq C N^{k-1} \exp(c \exp(c|t|)). \tag{4.18}$$

This should be compared with $\operatorname{tr}(\gamma^{(k)}_{N,t})^2$ and $\operatorname{tr}(\omega^{(k)}_{N,t})^2$, which are of order N^k.

(iv) Just like in the non-relativistic model (see Appendix 3.A) the exchange term $[X_t, \omega_{N,t}]$ in the Hartree-Fock equation (4.8) is of smaller order and can be neglected. The bounds (4.16), (4.17), (4.18) remain true if we replace $\omega_{N,t}$ with the solution of the Hartree equation

$$i\varepsilon\partial_t\widetilde{\omega}_{N,t} = \left[\sqrt{-\varepsilon^2\Delta + m_0^2} + (V * \widetilde{\rho}_t), \widetilde{\omega}_{N,t}\right] \tag{4.19}$$

with the density $\widetilde{\rho}_t(x) = N^{-1}\widetilde{\omega}_{N,t}(x,x)$.

(v) The relativistic Hartree-Fock equation (4.8) and the relativistic Hartree equation (4.19) still depend on N through the semiclassical parameter $\varepsilon = N^{-1/3}$. As $N \to \infty$, the Hartree-Fock and the Hartree dynamics can be approximated by the relativistic Vlasov evolution. If $W_{N,t}(x,v)$ denotes the Wigner transform of the solution $\omega_{N,t}$ of (4.8) (or, analogously, of the solution $\widetilde{\omega}_{N,t}$ of (4.19)), we expect that in an appropriate sense $W_{N,t} \to W_{\infty,t}$ as $N \to \infty$, where $W_{\infty,t}$ satisfies the relativistic Vlasov equation

$$\partial_t W_{\infty,t} + \frac{v}{\sqrt{v^2 + m_0^2}} \cdot \nabla_x W_{\infty,t} - \nabla_v W_{\infty,t} \cdot \nabla\left(V * \rho_{\infty,t}\right) = 0\,,$$

where $\rho_{\infty,t}(x) = \int \mathrm{d}v\, W_{\infty,t}(x,v)$. In fact, the convergence of the relativistic Hartree evolution towards the relativistic Vlasov dynamics has been shown in [AMS08] for particles interacting through a Coulomb potential. In this case, however, a rigorous mathematical understanding of the relation with many-body quantum dynamics is still missing (because of the regularity assumption (4.14), Theorem 4.2.1 does not cover the Coulomb interaction). In view of applications to the dynamics of gravitating fermionic stars (such as white dwarfs and neutron stars) and the related phenomenon of gravitational collapse studied in [HS09, HLLS10], this is an interesting and important open problem (at the level of the ground state energy, this problem has been solved in [LY87]). Notice that the corresponding questions for bosonic stars have been addressed in [ES07, MS12].

Next, we explain the strategy of the proof of Theorem 4.2.1, which is based on the proof of Theorem 3.3.1. In fact, the main body of the proof can be taken over without significant changes. There is, however, one important ingredient of the analysis which requires non-trivial modifications, namely the propagation of the commutator bounds (4.6) along the solution of the Hartree-Fock equation (4.8). We will discuss this part of the proof of Theorem 4.2.1 separately in Section 4.3.

Sketch of the proof of Theorem 4.2.1. We introduce the vector $\xi_{N,t} \in \mathcal{F}$ describing the fluctuations around the Slater determinant with reduced density $\omega_{N,t}$ given by the solution of the Hartree-Fock equation (4.8) by requiring that

$$\psi_{N,t} = e^{-i\mathcal{H}_N t/\varepsilon} R_{\omega_N}\xi_N = R_{\omega_{N,t}}\xi_{N,t}.$$

This gives $\xi_{N,t} = \mathcal{U}_N(t,0)\xi_N$, with the fluctuation dynamics

$$\mathcal{U}_N(t,s) = R^*_{\omega_{N,t}} e^{-i\mathcal{H}_N t/\varepsilon} R_{\omega_{N,s}}.$$

Notice that $\mathcal{U}_N(t,s)$ is a two-parameter group of unitary transformations. The problem of proving that $\psi_{N,t}$ is close to the Slater determinant $R_{\omega_{N,t}}\Omega$ reduces to showing that the expectation of the number of particles in $\xi_{N,t}$ stays of order one, i. e. small compared to the N particles in the Slater determinant. In fact, it is easy to check (see Section 3.5) the bound for the Hilbert-Schmidt norm

$$\|\gamma^{(1)}_{N,t} - \omega_{N,t}\|_{\text{HS}} \leq C\langle \xi_{N,t}, \mathcal{N}\xi_{N,t}\rangle = C\langle \xi_N, U_N^*(t,0)\mathcal{N}U_N(t,0)\xi_N\rangle \,. \tag{4.20}$$

To bound the growth of the expectation of the number of particles with respect to the fluctuation dynamics $U_N(t,s)$ we use Grönwall's Lemma. Differentiating the expectation on the r. h. s. of (4.20) with respect to time gives (see Proof of Proposition 3.4.3)

$$\begin{aligned} i\varepsilon\frac{\mathrm{d}}{\mathrm{d}t}&\langle \xi_N, U_N^*(t,0)\mathcal{N}U_N(t,0)\xi_N\rangle \\ &= \langle \xi_N, U_N^*(t,0)R^*_{\omega_{N,t}}\Big(d\Gamma(i\varepsilon\partial_t\omega_{N,t}) - [\mathcal{H}_N, d\Gamma(\omega_{N,t})]\Big)R_{\omega_{N,t}}U_N(t,0)\xi_N\rangle. \end{aligned}$$

There are important cancellations between the two terms in the parenthesis. In particular, since

$$\begin{aligned} \left[\int \mathrm{d}x\, a_x^*\sqrt{-\varepsilon^2\Delta + m_0^2}\,a_x\,,\, d\Gamma(\omega_{N,t})\right] &= \left[d\Gamma\left(\sqrt{-\varepsilon^2\Delta+m_0^2}\right), d\Gamma(\omega_{N,t})\right] \\ &= d\Gamma\left(\left[\sqrt{-\varepsilon^2\Delta+m_0^2}\,,\,\omega_{N,t}\right]\right) \end{aligned}$$

the contributions of the kinetic energy cancel exactly. The remaining terms are then identical to those found in the non-relativistic case. Hence, analogously to Proposition 3.4.3, we conclude that

$$\begin{aligned} i\varepsilon\frac{\mathrm{d}}{\mathrm{d}t}&\langle \xi_N, U_N^*(t,0)\mathcal{N}U_N(t,0)\xi_N\rangle \\ = -\frac{4i}{N}\mathrm{Im}\int \mathrm{d}x\mathrm{d}y\, V(x-y)\big\{&\langle U_N(t,0)\xi_N, a^*(u_{t,x})a(u_{t,x})a(\overline{v}_{t,y})a(u_{t,y})U_N(t,0)\xi_N\rangle \\ &+ \langle U_N(t,0)\xi_N, a^*(\overline{v}_{t,x})a(\overline{v}_{t,x})a(\overline{v}_{t,y})a(u_{t,y})U_N(t,0)\xi_N\rangle \\ &+ \langle U_N(t,0)\xi_N, a(\overline{v}_{t,x})a(u_{t,x})a(\overline{v}_{t,y})a(u_{t,y})U_N(t,0)\xi_N\rangle\big\} \end{aligned} \tag{4.21}$$

where the functions $u_{t,x}$ and $v_{t,x}$ are defined by[2]

$$R^*_{\omega_{N,t}}a_xR_{\omega_{N,t}} = a(u_{t,x}) + a^*(\overline{v}_{t,x}).$$

It is easy to express $u_{t,x}$ (which is actually a distribution) and $v_{t,x}$ (a L^2-function) in terms of $\omega_{N,t}$; see, for example, (1.66). Notice that in Proposition 3.4.3, we also considered the expectation of higher moments of $\mathcal{N}$. This can be done in the relativistic setting as well, and is needed to prove the trace norm bound (4.17).

Proceeding as in the proof of Lemma 3.4.5, we can bound the terms on the r. h. s. of (4.21) to show that

$$\begin{aligned} &\left|i\varepsilon\frac{\mathrm{d}}{\mathrm{d}t}\,\langle \xi_N, U_N^*(t,0)(\mathcal{N}+1)U_N(t,0)\xi_N\rangle\right| \\ &\qquad\leq CN^{-1}\sup_{p\in\mathbb{R}^3}\frac{\mathrm{tr}|[e^{ip\cdot x}, \omega_{N,t}]|}{1+|p|}\,\langle \xi_N, U_N^*(t,0)(\mathcal{N}+1)U_N(t,0)\xi_N\rangle. \end{aligned} \tag{4.22}$$

[2] We changed $\overline{v}$ to v compared to [BPS13b], to make the notation in this thesis consistent.

Using the integral representation

$$[e^{ip\cdot x}, \omega_{N,t}] = \int_0^1 \mathrm{d}s \, e^{isp\cdot x} \, [ip \cdot x, \omega_{N,t}] \, e^{i(1-s)p\cdot x}$$

we conclude that

$$\sup_{p\in\mathbb{R}^3} \frac{\operatorname{tr}|[e^{ip\cdot x}, \omega_{N,t}]|}{1+|p|} \leq \operatorname{tr}|[x, \omega_{N,t}]|. \tag{4.23}$$

Hence, (4.22) implies the bound (4.16) in Theorem 4.2.1, if we can show that there exist constants $C, c > 0$ with

$$\operatorname{tr} \, |[x, \omega_{N,t}]| \leq CN\varepsilon \exp(c|t|) \tag{4.24}$$

for all $t \in \mathbb{R}$. We show (4.24) in Proposition 4.3.1 below. □

4.3. Propagation of the semiclassical commutator bounds

The goal of this section is to show the estimate (4.24), which is needed in the proof of Theorem 4.2.1. To this end, we use the assumption (4.6) on the initial data, and we propagate the commutator estimates along the Hartree-Fock evolution. This is the genuinely new part of the present paper, where the ideas of Chapter 3 need to be adapted to the relativistic dispersion of the particles.

Proposition 4.3.1. *Let $V \in L^1(\mathbb{R}^3)$ with*

$$\int |\widehat{V}(p)|(1+|p|)^2 dp < \infty. \tag{4.25}$$

Let ω_N be a trace class operator on $L^2(\mathbb{R}^3)$ with $0 \leq \omega_N \leq 1$ and $\operatorname{tr}\omega_N = N$, satisfying the commutator estimates (4.6). Denote by $\omega_{N,t}$ the solution of the Hartree-Fock equation (4.8) (with $\varepsilon = N^{-1/3}$) with initial data $\omega_{N,0} = \omega_N$. Then there exist constants $C, c > 0$ such that

$$\begin{aligned} \operatorname{tr}|[x, \omega_{N,t}]| &\leq CN\varepsilon \exp(c|t|) \quad \textit{and} \\ \operatorname{tr}|[\varepsilon\nabla, \omega_{N,t}]| &\leq CN\varepsilon \exp(c|t|) \end{aligned}$$

for all $t \in \mathbb{R}$.

Proof. We define the Hartree-Fock Hamiltonian

$$h(t) := \sqrt{-\varepsilon^2\Delta + m_0^2} + (V * \rho_t) - X_t$$

where $\rho_t(x) = N^{-1}\omega_{N,t}(x,x)$ and X_t is the exchange operator defined by the integral kernel $X_t(x,y) = N^{-1}V(x-y)\omega_{N,t}(x,y)$ (note that ρ_t and X_t depend on the solution $\omega_{N,t}$ of the Hartree-Fock equation (4.8)). Then $\omega_{N,t}$ satisfies the equation

$$i\varepsilon\partial_t\omega_{N,t} = [h(t), \omega_{N,t}]. \tag{4.26}$$

Using the Jacobi identity we obtain

$$\begin{aligned} i\varepsilon\partial_t[x, \omega_{N,t}] &= [x, [h(t), \omega_{N,t}]] \\ &= [h(t), [x, \omega_{N,t}]] + \left[\omega_{N,t}, \left[\sqrt{-\varepsilon^2\Delta + m_0^2}\,, \, x\right]\right] - [\omega_{N,t}, [X_t, x]]. \end{aligned} \tag{4.27}$$

We can eliminate the first term on the r. h. s. of the last equation by conjugating $[x, \omega_{N,t}]$ with the two-parameter group $W(t,s)$ generated by the selfadjoint operators $h(t)$, satisfying

$$i\varepsilon\partial_t W(t,s) = h(t)W(t,s) \quad \text{with} \quad W(s,s) = 1 \quad \text{for all } s \in \mathbb{R}. \tag{4.28}$$

In fact, we have

$$\begin{aligned} &i\varepsilon\partial_t \, W^*(t,0)[x, \omega_{N,t}]W(t,0) \\ &\qquad = W^*(t,0)\Big(\Big[\omega_{N,t}, \Big[\sqrt{-\varepsilon^2\Delta + m_0^2}\,,\, x\Big]\Big] - [\omega_{N,t}, [X_t, x]]\Big)W(t,0) \end{aligned}$$

and therefore

$$\begin{aligned} &W^*(t,0)[x, \omega_{N,t}]W(t,0) \\ &\quad = [x, \omega_{N,0}] + \frac{1}{i\varepsilon}\int_0^t \mathrm{d}s \, \frac{\mathrm{d}}{\mathrm{d}s}\big(W^*(s,0)[x, \omega_{N,s}]W(s,0)\big) \\ &\quad = [x, \omega_{N,0}] + \frac{1}{i\varepsilon}\int_0^t \mathrm{d}s \, W^*(s,0)\Big(\Big[\omega_{N,t}, \Big[\sqrt{-\varepsilon^2\Delta + m_0^2}, x\Big]\Big] - [\omega_{N,t}, [X_t, x]]\Big)W(s,0). \end{aligned}$$

This implies that

$$\operatorname{tr}|[x, \omega_{N,t}]| \le \operatorname{tr}|[x, \omega_{N,0}]| + \frac{1}{\varepsilon}\int_0^t \mathrm{d}s \; \operatorname{tr}\Big|\Big[\omega_{N,s}, \Big[\sqrt{-\varepsilon^2\Delta + m_0^2}, x\Big]\Big]\Big| \tag{4.29}$$

$$+ \frac{1}{\varepsilon}\int_0^t \mathrm{d}s \; \operatorname{tr}|[\omega_{N,s}, [X_s, x]]|. \tag{4.30}$$

To control the term (4.30) we observe that

$$X_s = \frac{1}{N}\int \mathrm{d}q \, \widehat{V}(q) \, e^{iq\cdot x}\omega_{N,s}e^{-iq\cdot x}. \tag{4.31}$$

Since $\|\omega_{N,s}\| \le 1$ (because of the assumption $0 \le \omega_{N,s} \le 1$, as required for fermionic one-particle density matrices), we find

$$\begin{aligned} \operatorname{tr}|[\omega_{N,s}, [X_s, x]]| &\le \frac{1}{N}\int \mathrm{d}q \, |\widehat{V}(q)| \; \operatorname{tr}|[\omega_{N,s}, [e^{iq\cdot x}\omega_{N,s}e^{-iq\cdot x}, x]]| \\ &\le \frac{2}{N}\int \mathrm{d}q \, |\widehat{V}(q)| \; \operatorname{tr}|[e^{iq\cdot x}\omega_{N,s}e^{-iq\cdot x}, x]| \\ &= \frac{2}{N}\int \mathrm{d}q \, |\widehat{V}(q)| \; \operatorname{tr}|e^{iq\cdot x}[\omega_{N,s}, x]e^{-iq\cdot x}| \le \frac{2\|\widehat{V}\|_1}{N} \operatorname{tr}|[\omega_{N,s}, x]|. \end{aligned} \tag{4.32}$$

To control (4.29) we notice that

$$\Big[\sqrt{-\varepsilon^2\Delta + m_0^2}\,,\, x\Big] = -\varepsilon\frac{\varepsilon\nabla}{\sqrt{-\varepsilon^2\Delta + m_0^2}}.$$

Hence

$$\Big[\omega_{N,s}, \Big[\sqrt{-\varepsilon^2\Delta + m_0^2}, x\Big]\Big] = -\varepsilon[\omega_{N,s}, \varepsilon\nabla]\frac{1}{\sqrt{-\varepsilon^2\Delta + m_0^2}} - \varepsilon^2\nabla\left[\omega_{N,s}, \frac{1}{\sqrt{-\varepsilon^2\Delta + m_0^2}}\right]$$

and thus

$$\operatorname{tr}\left|\left[\omega_{N,s},\left[\sqrt{-\varepsilon^2\Delta+m_0^2},x\right]\right]\right| \leq \varepsilon m_0^{-1}\operatorname{tr}|[\varepsilon\nabla,\omega_{N,s}]| + \varepsilon\operatorname{tr}\left|\varepsilon\nabla\left[\omega_{N,s},\frac{1}{\sqrt{-\varepsilon^2\Delta+m_0^2}}\right]\right|. \tag{4.33}$$

Here we used the estimate $\|(-\varepsilon^2\Delta+m_0^2)^{-1/2}\| \leq m_0^{-1}$. To bound the second term on the r. h. s. we will use the integral representation[3]

$$\frac{1}{\sqrt{A}} = \frac{1}{\pi}\int_0^\infty \frac{\mathrm{d}\lambda}{\sqrt{\lambda}}(A+\lambda)^{-1} \tag{4.34}$$

and the identity

$$[(A+\lambda)^{-1},B] = (A+\lambda)^{-1}[B,A](A+\lambda)^{-1}$$

for $A>0, B$ selfadjoint operators. Now consider the j-th component ($j\in\{1,2,3\}$) of the operator whose trace norm we have to estimate:

$$\begin{aligned}
&\operatorname{tr}\left|\varepsilon\partial_j\left[\omega_{N,s},\frac{1}{\sqrt{-\varepsilon^2\Delta+m_0^2}}\right]\right| \\
&\leq \frac{1}{\pi}\int_0^\infty\frac{\mathrm{d}\lambda}{\sqrt{\lambda}}\operatorname{tr}\left|\varepsilon\partial_j\frac{1}{-\varepsilon^2\Delta+m_0^2+\lambda}[\omega_{N,s},\varepsilon^2\Delta]\frac{1}{-\varepsilon^2\Delta+m_0^2+\lambda}\right| \\
&\leq \frac{1}{\pi}\sum_{k=1}^3\int_0^\infty\frac{\mathrm{d}\lambda}{\sqrt{\lambda}}\left\|\frac{-\varepsilon^2\partial_j\partial_k}{-\varepsilon^2\Delta+m_0^2+\lambda}\right\|\operatorname{tr}|[\omega_{N,s},\varepsilon\partial_k]|\left\|\frac{1}{-\varepsilon^2\Delta+m_0^2+\lambda}\right\| \\
&\quad+\frac{1}{\pi}\sum_{k=1}^3\int_0^\infty\frac{\mathrm{d}\lambda}{\sqrt{\lambda}}\left\|\frac{-i\varepsilon\partial_j}{(-i\varepsilon\nabla)^2+m_0^2+\lambda}\right\|\operatorname{tr}|[\omega_{N,s},\varepsilon\partial_k]|\left\|\frac{-i\varepsilon\partial_k}{(-i\varepsilon\nabla)^2+m_0^2+\lambda}\right\|.
\end{aligned}$$

Using the bounds $\|(-\varepsilon^2\Delta+m_0^2+\lambda)^{-1}\| \leq (m_0^2+\lambda)^{-1}$,

$$\left\|\frac{-i\varepsilon\partial_k}{-\varepsilon^2\Delta+m_0^2+\lambda}\right\| \leq \frac{1}{\sqrt{m_0^2+\lambda}} \quad\text{and}\quad \left\|\frac{-\varepsilon^2\partial_k\partial_j}{-\varepsilon^2\Delta+m_0^2+\lambda}\right\| \leq 1,$$

all of which can be easily proved in Fourier space, we conclude that

$$\begin{aligned}
\operatorname{tr}\left|\varepsilon\partial_j\left[\omega_{N,s},\frac{1}{\sqrt{-\varepsilon^2\Delta+m_0^2}}\right]\right| &\leq C\operatorname{tr}|[\varepsilon\nabla,\omega_{N,s}]|\int_0^\infty\frac{\mathrm{d}\lambda}{\sqrt{\lambda}}\frac{1}{\lambda+m_0^2} \\
&\leq Cm_0^{-1}\operatorname{tr}|[\varepsilon\nabla,\omega_{N,s}]|.
\end{aligned}$$

Inserting this estimate in (4.33), we obtain

$$\operatorname{tr}\left|\left[\omega_{N,s},\left[\sqrt{-\varepsilon^2\Delta+m_0^2},x\right]\right]\right| \leq C\varepsilon m_0^{-1}\operatorname{tr}|[\varepsilon\nabla,\omega_{N,s}]|.$$

Plugging this bound and (4.32) into (4.29) and (4.30), we arrive at

$$\operatorname{tr}|[x,\omega_{N,t}]| \leq \operatorname{tr}|[x,\omega_{N,0}]| + Cm_0^{-1}\int_0^t\mathrm{d}s\operatorname{tr}|[\varepsilon\nabla,\omega_{N,s}]| + CN^{-2/3}\int_0^t\mathrm{d}s\operatorname{tr}|[x,\omega_{N,s}]|. \tag{4.35}$$

[3]To check this operator identity, first use the functional calculus and Fubini's theorem to reduce it to the analogous identity for $A\in\mathbb{R}$. Then substitute $\lambda=t^2$ and use the residue theorem to calculate the integral.

Next, we bound the growth of the commutator $[\varepsilon\nabla, \omega_{N,t}]$. Since the kinetic energy commutes with the observable $\varepsilon\nabla$, we can proceed here exactly as in the non-relativistic case. For completeness, we reproduce the short argument. Differentiating w. r. t. time and applying Jacobi identity, we find

$$\begin{aligned} i\varepsilon\frac{\mathrm{d}}{\mathrm{d}t}\,[\varepsilon\nabla, \omega_{N,t}] =& [\varepsilon\nabla, [h(t), \omega_{N,t}]] \\ =& [h(t), [\varepsilon\nabla, \omega_{N,t}]] + [\omega_{N,t}, [h(t), \varepsilon\nabla]] \\ =& [h(t), [\varepsilon\nabla, \omega_{N,t}]] + [\omega_{N,t}, [V * \rho_t, \varepsilon\nabla]] - [\omega_{N,t}, [X_t, \varepsilon\nabla]]\,. \end{aligned}$$

As before, the first term on the r. h. s. can be eliminated by conjugation with the unitary maps $W(t,0)$ defined in (4.28). Thus we find

$$\begin{aligned} \operatorname{tr}|[\varepsilon\nabla, \omega_{N,t}]| \leq& \operatorname{tr}\,|[\varepsilon\nabla, \omega_{N,0}]| \\ &+ \frac{1}{\varepsilon}\int_0^t ds\ \operatorname{tr}|[\omega_{N,s}, [V * \rho_s, \varepsilon\nabla]]| + \frac{1}{\varepsilon}\int_0^t ds\ \operatorname{tr}\,|[\omega_{N,s}, [X_s, \varepsilon\nabla]]|. \end{aligned} \tag{4.36}$$

The second term on the r. h. s. of the last equation can be controlled by

$$\begin{aligned} \operatorname{tr}|[\omega_{N,s}, [V * \rho_s, \varepsilon\nabla]]| &= \varepsilon\ \operatorname{tr}|[\omega_{N,s}, \nabla(V * \rho_s)]| \\ &\leq \varepsilon \int \mathrm{d}q\, |\widehat{V}(q)||q||\widehat{\rho}_s(q)|\ \operatorname{tr}|[\omega_{N,s}, e^{iq\cdot x}]| \\ &\leq \varepsilon \left(\int \mathrm{d}q\, |\widehat{V}(q)|(1+|q|)^2\right) \sup_q \frac{1}{1+|q|}\ \operatorname{tr}|[\omega_{N,s}, e^{iq\cdot x}]| \\ &\leq C\varepsilon\ \operatorname{tr}|[x, \omega_{N,s}]| \end{aligned}$$

where we used the bound $\|\widehat{\rho}_s\|_\infty \leq \|\rho_s\|_1 = 1$, the estimate (4.23) and the assumption (4.25) on the interaction potential. As for the last term on the r. h. s. of (4.36), we note that, writing the exchange operator as in (4.31),

$$\begin{aligned} \operatorname{tr}|[\omega_{N,s}, [X_s, \varepsilon\nabla]]| &\leq \frac{1}{N}\int \mathrm{d}q\, |\widehat{V}(q)|\ \operatorname{tr}\left|[\omega_{N,s}, [e^{iq\cdot x}\omega_{N,s}e^{-iq\cdot x}, \varepsilon\nabla]]\right| \\ &\leq \frac{2}{N}\int \mathrm{d}q\, |\widehat{V}(q)|\operatorname{tr}|[e^{iq\cdot x}\omega_{N,s}e^{-iq\cdot x}, \varepsilon\nabla]| \\ &\leq \frac{2\|\widehat{V}\|_1}{N}\ \operatorname{tr}|[\omega_{N,s}, \varepsilon\nabla]|. \end{aligned}$$

In the last inequality we used that

$$[e^{iq\cdot x}\omega_{N,s}e^{-iq\cdot x}, \varepsilon\nabla] = e^{iq\cdot x}[\omega_{N,s}, \varepsilon(\nabla + iq)]e^{-iq\cdot x} = e^{iq\cdot x}[\omega_{N,s}, \varepsilon\nabla]e^{-iq\cdot x}\,.$$

From (4.36), we conclude that

$$\operatorname{tr}|[\varepsilon\nabla, \omega_{N,t}]| \leq \operatorname{tr}|[\varepsilon\nabla, \omega_{N,0}]| + C\int_0^t ds\ \operatorname{tr}|[x, \omega_{N,s}]| + CN^{-2/3}\int_0^t ds\ \operatorname{tr}|[\varepsilon\nabla, \omega_{N,s}]|.$$

Summing up the last equation with (4.35), using the conditions (4.6) on the initial data and applying Grönwall's lemma, we find constants $C, c > 0$ such that

$$\begin{aligned} \operatorname{tr}|[x, \omega_{N,t}]| &\leq CN\varepsilon\ \exp(c|t|) \quad \text{and} \\ \operatorname{tr}|[\varepsilon\nabla, \omega_{N,t}] &\leq CN\varepsilon\ \exp(c|t|). \end{aligned}$$

□

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